RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2015

Section New Results

Edition: 2016-03-21

ACUMES Team

6. New Results

6.1. Mathematical analysis and control of macroscopic traffic flow models

6.1.1. Vehicular traffic

Participants: Guillaume Costeseque, Paola Goatin, Christophe Chalons [UVST], Simone Göttlich [U Mannheim, Germany], Jerôme Härri [EURECOM], Oliver Kolb [U Mannheim, Germany], Sosina Mengistu-Gashaw [EURECOM], Francesco Rossi [U Aix-Marseille], Stefano Villa [U Milano-Bicocca].

In collaboration with the University of Mannheim and in the framework of the PHC Procope project "Transport Networks Modeling and Analysis", we studied how to manage variable speed limits combined with coordinated ramp metering within the framework of the LWR network model. Following a "first discretize then optimize" approach, we derived the first order optimality system and explained the switch of speeds at certain fixed points in time and the boundary control for the ramp metering as well. Sequential quadratic programming methods are used to solve the control problem numerically. For application purposes, we present experimental setups where variable speed limits are used as a traffic guidance system to avoid traffic jams on highway interchanges and on-ramps, see [35].

The thesis of S. Mengistu-Gashaw, funded by the Labex UCN@Sophia (http://ucnlab.eu/) and co-supervised by P. Goatin and J. Härri, is devoted to understanding and modeling mobility characteristics of scooters and motorcycles for user-centric ITS application. We are currently developing a macroscopic model for heterogeneous traffic including car and motorcycles.

A new traffic flow model has been designed in [44] for taking into account the multiclass and multilane features of real traffic. This model is based on a system of coupled Hamilton-Jacobi PDEs for an appropriate choice of framework that mixes spatial and Lagrangian coordinates. The coupling conditions emerge from the moving bottleneck theory that has been developed in the traffic flow literature several years ago but for which a real mathematical sound basis lacked. Very recently, there were some new results dealing with the existence of a solution under suitable assumptions. However, these results were set for the hyperbolic conservation law in Eulerian coordinates and they are not straightforward to extend to Hamilton-Jacobi equations in different coordinates. Despite that the well-posedness of the problem is still an open problem, a numerical method is developed and it takes advantage of the classical representation formula available for HJ PDEs. This numerical scheme has been proved to provide good qualitative results.

In collaboration with F. Rossi, we proved existence and uniqueness of solutions to a transport equation modelling vehicular traffic in which the velocity field depends non-locally on the downstream traffic density via a discontinuous anisotropic kernel. The result is obtained recasting the problem in the space of probability measures equipped with the ∞-Wasserstein distance. We also show convergence of solutions of a finite dimensional system, which provide a particle method to approximate the solutions to the original problem. See, [45].

Finally, the internship of S. Villa, co-supervised by M. Garavello (U Milano-Bicocca), was devoted to the analytical and numerical study of the Aw-Rascle-Zhang model with moving bottleneck. Two Riemann Solver have been proposed, and two numerical strategies have been developed. A journal article is in preparation in collaboration with C. Chalons.

6.1.2. Crowd motion

Participants: Paola Goatin, Matthias Mimault.

M. Mimault defended hid PhD on December 14th, 2015. The last part of his thesis was devoted to the numerical study of scalar conservation laws with non-local flow in two space dimensions. These equations are meant to model crowd motion, where the movement direction of each pedestrian depends on a weighted mean of the crowd density around him. In particular, he implemented a finite volume numerical scheme which has been used for flow optimization purposes: he applied the adjoint method to compute the gradient for the evacuation time minimization depending on the initial crowd distribution.

6.2. Characterization of model uncertainty for turbulent flows

Participants: Régis Duvigneau, Jérémie Labroquère, Emmanuel Guilmineau [CNRS ECN, Nantes], Marianna Brazza [CNRS IMFT, Toulouse], Mathieu Szubert [CNRS IMFT, Toulouse].

The uncertainty related to turbulence modeling is still a bottleneck in realistic flows simulation. Therefore, some studies have been conducted to quantify this uncertainty for two problems in which turbulence plays a critical role. Firstly, the impact of the model choice has been estimated in the case of a massively detached flow over a 2D backward facing step including an oscillatory active control device, whose parameters are optimized [41], [34]. Secondly, the influence of the transition point location has been investigated, in the case of the 3D flow around a bluff-body, using models ranging from RANS to DES models [40].

6.3. Sensitivity analysis for unsteady flows

Participants: Régis Duvigneau, Dominique Pelletier [Ecole Polytechnique Montreal], Alexander Hay [Ecole Polytechnique Montreal].

Although sensitivity analysis is now commonly used for steady systems, usually on the basis of the adjoint equation method, the application to unsteady problems is still tedious, due to the backward time integration required. Therefore, an alternative approach, namely the sensitivity equation method, has been studied in the framework of the compressible Navier-Stokes equations. A continuous version has preferred to the discrete one for its flexibility and easier implementation. The proposed approach has been verified on several problems of increasing difficulty and the computational efficiency quantified [42].

6.4. Optimization accounting for experimental and numerical uncertainties

Participants: Régis Duvigneau, Olivier Le Maitre [CNRS LIMSI, Orsay], Matthieu Sacher [Ecole Navale, Brest], Alban Leroyer [ECN, Nantes], Patrick Queutey [CNRS ECN, Nantes].

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

The first case corresponds to the optimization of the shape of a racing kayak. The performance is estimated by coupling Newton's law with Navier-Stokes equations to compute the kayak velocity from the effort of the athlete, considered as input. The proposed method has been used here to filter the noise arising from the numerical simulation.

The second case corresponds to the optimization of a sail trimming, whose performance can be estimated either experimentally in a wind tunnel, or numerically by solving a fluid-structure interaction problem. In the former case, uncertainty has been estimated according to measurements accuracy, while in the latter case the numerical noise has be inferred from a set of observations collected during the optimization.

6.5. High-order numerical schemes for convection-dominated problems

Participants: Régis Duvigneau, Asma Gdhami [ENIT, Tunisia].

The use of high-order numerical schemes is necessary to reduce numerical diffusion in simulations, maintain a reasonable computational time for 3D problems, estimate accurately uncertainties or sensitivities, etc. Consequently, we work to develop high-order numerical schemes for the applications targeted by the team, in particular for convection-dominated problems. More precisely, we intend to include in a unified framework, based on Discontinuous Galerkin approximations, numerical methods accounting for complex geometries (isogeometric methods), uncertainty propagation (high-dimensional cubature) and sensitivity analysis.

6.6. Validation of time dependent diffusion approaches for activated and inhibited cell sheet closure

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

We have studied in [21] five MDCK cell monolayer assays in a reference, activated and inhibited migration conditions. Modulo the inherent variability of biological assays, we have shown that in the assay where migration was not exogeneously activated or inhibited, the wound velocity was constant and the Fisher-KPP equation was able to accurately predict, until the final closure of the wound, the evolution of the wound area, the mean velocity of the cell front, and the time at which the closure occurred. When activated or inhibited, the F-KPP equation with constant parameters was unable to reproduce the observed biological cell sheet behavior. We modify the original equation, making the diffusion and proliferation parameters time dependent, following a sigmoid profile. We then set up an optimization loop to identify the sigmoids parameters, by computing a classical error indicator (difference between a computed density and the observed one, obtained through image processing) as done in the cited reference. We then obtain results which convincingly show that our approach is efficient : in both cases, inhibited and activated, the time varying identified parameters allow us to accurately predict until the final closure the evolution of the wound area.

6.7. Game strategies for joint data completion and parameter identification

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

We have demonstrated in previous works [22], [23] that Nash game approaches are efficient to tackle ill-posedness for linear second order elliptic Cauchy problems. We next developed a mathematical formulation for the linear elasticity model. The reconstruction is based on data completion and material identification, making it a harsh ill posed inverse problem. Up to now, we have obtained successful results for the Lamé parameter recovery in linear elasticity, using the so-called Kohn and Vogelius functional. Simultaneous data completion and parameter identification is under investigation.

6.8. Revised definition of the Multiple Gradient Descent Algorithm (MGDA)

Participant: Jean-Antoine Désidéri.

The Multiple Gradient Descent Algorithm (MGDA) had been defined originally to identify a descent direction common to a set of gradient vectors. According to a completely general principle, the direction is opposite to the vector of minimum Euclidean norm in the convex hull of the gradients. The Euclidean norm is defined via a general scalar product in $\mathbf{R}^n$. From a theoretical viewpoint, the notion of Pareto-stationarity had been introduced and it was established that if a point is Pareto-optimal and if the objective functions are locally differentiable and convex, then the point is Pareto-stationary. From a computational viewpoint, the descent direction can be determined as the solution of a Quadratic-Programming (QP) formulation. However, when the gradients are linearly independent a direct construction via a Gram-Schmidt orthogonalization process was preferred. We have now generalized the orthogonalization process by the introduction of a hierarchical strategy in the ordering of the subfamily of gradients utilized to construct the orthogonal basis. This strategy aims at making the (multi-dimensional) cone associated with the convex hull of the subfamily as large as possible. As

a result, in the case of linearly-dependent gradients, the orthogonalization process not only provides a basis of the spanned subspace, but the subfamily is selected such that its the convex hull is also very representative of a large cone, encompassing in the most favorable cases all the given gradients. By this change in the definition of the algorithm, we were able to reformulate the QP formulation, now stated in a suitable basis, in a way that is well-suited for the treatment of cases where the number of gradients exceeds, possibly vastly, the dimension of the vector space. This revision makes the algorithm much more general and robust [43].

6.9. Multi-point optimization of a time-periodic system of pulsating jets

Participants: Jean-Antoine Désidéri, Régis Duvigneau.

A multi-point optimization exercise governed by the time-dependent compressible Navier-Stokes equations has been solved based on the sensitivity analysis (see above). A system was considered consisting of three pulsating jets acting on a flat-plate boundary layer. As it is well-known, the flow mixing by the jets has the effect of reducing the drag, as this was confirmed by the simulation of the flow in the somewhat arbitrary initial setting of the jets. Then, positions and pulsation frequencies of the jets have been maintained fixed, while their amplitudes and phases, six parameters in total, have been optimized to minimize the drag force. The finite-volume simulation of the time-periodic flow provides the drag force as a function of time over a large number of timesteps (800 for an accurate description of a period). The sensitivity analysis simultaneously provides the derivatives of drag with respect to the six design parameters. These derivatives were averaged over 20 distinct time-intervals, thus yielding 20 averaged gradient vectors of dimension 6. The MGDA was then used to define a descent direction common to the 20 vectors, a descent step was applied to the design parameters, and the process was continued iteratively.

The experiment confirmed the possibility to reduce the drag force at all times of the period, and not only in the average. In contrast, using the average gradient to define the direction of search resulted in a more important reduction of the average drag but at the cost of an increase of drag in a critical portion of the time period. Hence our optimization algorithm is more versatile and powerful than one aiming at minimizing purely statistical functions obtained by time averaging. We also demonstrated the possibility to optimize over a subinterval of the time interval.

6.10. Quasi-Riemannian approach to constrained optimization

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

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

However the BFGS method does extend to constrained problems very simply. Following Gabay [95] and other authors, Chunhong Qi *et al* [128] have proposed a "Riemannian" variant, RBFGS that indeed incorporates equality constraints in the formulation and actually demonstrates superior convergence rates for problems with a large number of variables. However these Riemannian formulations are non trivial to implement since they require procedures implementing non-trivial differential-geometry operators ('retraction' and 'metric transport') to be developed. In their paper, they assume a formal expression of the constraint to be known. But, in PDE-constrained optimization, many constraints are functional, and it is not clear how can the metric transport operator in particular can be defined.

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

6.11. Unstructured mesh adaptation using an adjoint-based sensor

Participants: Sébastien Bourasseau [Doctoral student, ONERA Department of Computational Fluid Dynamics, Châtillon], Jacques Peter [Research Engineer, ONERA Department of Computational Fluid Dynamics, Châtillon], Jean-Antoine Désidéri.

Mesh adaptation is a powerful tool to obtain accurate aerodynamic simulations at limited cost. When the simulation is aimed at the accurate calculation of aerodynamic outputs (forces, moments) goal-oriented methods based on the adjoint vector of the output of interest are often advocated. The calculation of the total derivative dJ/dX of the aerodynamic function of interest, J, with respect to the volume mesh coordinates, X, has been extended to the case of an unstructured grid. The software developments have been validated for inviscid and laminar viscous flows, and implemented in the ONERA code (elsA). Then a local sensor θ based on dJ/dX was devised to identify areas where the location of the volume mesh nodes has a strong impact on the evaluation of the output J. The sensor has been shown to be adequate in different flow regimes (subsonic, transonic, supersonic), for internal (blade and nozzle) and external (airfoils, wings) aerodynamic configurations. The proposed method has been compared to a well-known goal-oriented method (Darmofal and Venditti, 2001) and to a feature-based method; it yields comparable results at lower cost in simple configurations. A publication is currently subject to minor revisions.

6.12. Multi-fidelity surrogate modeling with application to the optimization of nanophotonic devices

Participants: Cédric Durantin [Doctoral student, CEA LETI Grenoble], Alain Glière [Research Engineer, CEA LETI Grenoble], Jean-Antoine Désidéri.

Multiple models of a physical phenomenon are sometimes available with different levels of approximation, the high fidelity model being more demanding in terms of computational time than the coarse approximation. In this context, including information from the lower fidelity model to build a surrogate model is desirable. A new multi-fidelity metamodeling method, based on Radial Basis Function, the co-RBF, is proposed. The new method is compared with the classical co-kriging on two analytical benchmarks and a realistic validation test, namely the design of a miniaturized photoacoustic gas sensor. The co-RBF method brings better results on high dimensional problem and could be considered as an alternative to co-kriging for multi-fidelity metamodeling.

CAGIRE Team

7. New Results

7.1. DNS of a jet in crossflow

One main achievement of this year is to have done our first DNS computations at third order with the Aerosol software. Two configurations of jet in cross flow have been computed: one with a hole direction aligned with the main flow direction (Fig. 3 -left), and another one with a 90-degree jet skidding (Fig. 3 -right). The first case has been validated by using analytical models of jet trajectory, and has also been compared with experiments made with our experimental bench MAVERIC. The comparison of experiments and DNS showed a good agreement.

The DNS database includes:

- The instantaneous flow at the vertices of the mesh.
- the instantaneous flow at some probes.
- The mean flow.
- The value of the Reynolds stress tensor in all the degrees of freedom.

7.2. Extension of the momentum interpolation method to low Mach Rieman problems

In a previous study [9], the momentum interpolation (MI) method was considered as a guideline to develop a Godunov-like flux scheme called AUSM-IT and able to preserve the acoustic energy at the discrete level for a low-order finite volume approach. This year, the MI method has been successfully extended to the case of low Mach flows featuring discontinuities [8]. The undesirable dispersive effect directly connected to the upwinding of the MI formulation of the face velocity has been corrected (up to second-order errors) by using a central interpolation of momentum in the face velocity definition.

7.3. Main features of highly underexpanded jets

Despite the numerous studies dealing with underexpanded jets, many aspects of their structure were not clearly described, particularly when one seeks for quantitative predictions. Since such flow configuration may be of interest in case of the accidental boring of an aeronautical combustion chamber, an exhaustive review of the main experimental papers dealing with underexpanded jets has been carried out [5]. This study aimed at clarifying the characteristics which were well known, from those where there is clearly a lack of confidence. Curiously enough, such a work has never been done and no exhaustive review was available on such a topic.

7.4. Formulation of a reference EB-RSM model

The Elliptic Blending Reynolds Stress Model (EB-RSM), originally proposed by Manceau & Hanjalic in 2002, has been subject to various modifications by several authors during the last decade, mainly for numerical robustness reasons. We have revisited all these modifications from the theoretical standpoint and investigated in detail their influence on the reproduction of the physical mechanisms at the origin of the influence of the wall on turbulence. Theoretical arguments and comparison with DNS results led to the selection of a recommended formulation for the EB-RSM model [7].

7.5. Development of a new enrichment method

A complex issue in multi-scale simulations is the necessity to *enrich* the solution at the interface between a region described at coarse grain (e.g., using RANS) and a region described at fine grain (e.g., using LES). In order to rapidly generate realistic fluctuations at the beginning of the LES region, we have proposed [4] a method of volumic forcing, the so-called ALF (Anisotropic Linear Forcing). In an overlap region, a time-dependent volume force is introducted into the filtered equations of motion in order to amplify the turbulent fluctuations in order that the LES field satisfy the statistics of the RANS solution, a method that proved simple, efficient and computationnaly cheap.

7.6. A new criterion to analyse hybrid RANS/LES approaches

Most of the available hybrid RANS/LES methods are completely empirical or based on a formalism which is not applicable in practical application, due to a mismatch between the statistical average and the spatial filetring in inhomogeneous flows. The lack of clear formalism leads to limitations in terms of modeling of the unresolved turbulent motion. We have established a criterion [6] to assess the equivalence between hybrid RANS/LES methods, called *H-equivalence*, that makes it possible to view different hybrid methods as models for the same system of equations: as a consequence, empirical hybrid methods, such as the detached-eddy simulation (DES), can be interpreted as a model for the subfilter stress involved in the *temporally filtered* Navier-Stokes equations, which is an answer to the issue raised above about the formalism underlying such methods.

CARDAMOM Team

7. New Results

7.1. High order discretizations on unstructured meshes

Participants: Héloise Beaugendre [Corresponding member], Cécile Dobrzynski, Léo Nouveau, Mario Ricchiuto, Quentin Viville.

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

- We have extended the team's previous work on the consistent residual based approximation of viscous flow equations to the framework of Immersed Boundary Methods (IBM). This is an increasingly popular approach in Computational Fluid Dynamics as it simplifies the mesh generation problem. In our work, we consider a echnique based on the addition of a penalty term to the Navier-Stokes equations to account for the wall boundary conditions. To adapt the residual distribution method method to the IBM, we developed a new formulation based on a Strang splitting appproach in time. This approach, couples in a fully consistent manner an implicit asymptoticly exact integration procedure of the penalization ODE, with the explicit residual distribution discretization for the Navier-Stokes equations, based on the method proposed in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010). The ODE integrator provides an operator which is exact up to orders η^2, with η the penalty parameter assuming values of the order of 10^{-10}. To preserve the accuracy of the spatial discretization in the Navier-Stokes step, we have introduced, in vicinity of the penalised region, a modification of the solution gradient reconstruction required for the evaluation of the viscous fluxes. We have shown formally and numerically that the approach proposed is second order accurate for smooth solutions, and shown its potential when combined with unstructured mesh adaptation strategies w.r.t. the (implicitly described) solid walls. This work has been accepted on *Comp.Meth.Appl.Mech.Eng.* ;
- Another research axis consists in proposing a novel approach that allows to use p-adaptation with continuous finite elements. Under certain conditions, primarily the use of a residual distribution scheme, it is possible to avoid the continuity constraint imposed to the approximate solution, while still retaining the advantages of a method using continuous finite elements. The theoretical material, the complete numerical method and practical results show as a proof of concept that p-adaptation is possible with continuous finite elements. Its extension to penalized Navier-Stokes equations are under progress ;
- We have continued the study of the properties of residual based methods in the time dependent case. We have been able to further characterize one of the variants of the approach proposed in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010) in terms of preservation of the positivity of the density showing this property in practical applications involving the shallow water equations [130]. The impact of the simplified construction leading to these schemes has also been investigated. In particular, we have shown that despite the additional complexity associated to the inversion of the mass matrix, non-linear methods providing monotone solution and yet featuring linear mass matrices can be constructed [142]. These methods, have been shown to have some potential w.r.t. fully diagonal approaches as those used in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010), in terms of error as fucntion of CPU time : the non-diagonal schemes showing error reductions up to one order of magnitude. Current work is devoted to the use of other multistage (defect correction type) and multistep (extrapolated methods) techniques, comparing them to space time approaches.

7.2. Modelling of free surface flows

Participants: Luca Arpaia, Stevan Bellec, Mathieu Colin, Sebastien de Brye, Andrea Filippini, Maria Kazolea, Mario Ricchiuto [Corresponding member].

We have introduced a new systematic method to obtain discrete numerical models for incompressible free-surface flows. The method consists in first discretizing the Euler equations with respect to the horizontal variables, keeping the vertial z variable and time continuous. We have focused so far on (continuous) Galerkin n finite element discretizations in the horizontal. We then perform an asymptotic analysis on the resulting semi-discrete system. Our initial result, has led to a new dicrete approximation, which we have shown to be consistent with the Boussinesq system known as Peregrine model. We have proven that the method obtained by means of this discrete asymptotic method, has phase and linear shoaling errors far lower that those obtained by discretizing the continuous model directly by means of the Galerkin method. Extensions to other weakly non-linear models have been obtained, and the study of fully nonlinear variants is under way.
We have also investigated the relations between some of the most common weakly nonlinear Boussinesq models. It is known since many years that, for given phase linear shoaling relations, two families of models exist depending on whether the dispersive terms are evaluated using derivatives of the speed, of of the flux (depth times speed). We have shown both analytically and numerically, that, independently on the phase and linear shoaling relations, these two families provide (quanlitatively *and* quantitatively) only two distinct behaviours when approaching the nonlinear regime. Models based on velocity derivatives, provide taller more asymmetric waves, all models of the same family produce stunningly similar results, even when the linear relations differ considerably.
To extend our initial work on unstructured solvers for dispersive wave models to the fully nonlinear case we have proposed a new framework to approximate the so-called Green-Naghdi equations [99]. The method proposed, while remaining unsplit in time, is based on a separation of the elliptic and hyperbolic components of the equations. This separation is designed to recover the standard shallow water equations in the hyperbolic step, so that the method can be written as an *algebraic* correction to an existing shallow water code. In particular, in our approach we fix the method used for the elliptic component (a continuous Galerkin method), and couple it to different hyperbolic shallow water solvers. As long as the hyperbolic step is more than second order accurate, the approach proposed allows accuracies comparable to those of a fourth order finite difference method, with a natural potential for h and $p-$ adaptation on unstructured grids. The two-dimensional extension in in the testing phase.
The tools developed have been also used intensively in funded research programs. Within the TANDEM project, several benchmarks relevant to tsunami modelling have been performed and several common publications with the project partners are in preparation. Independently on this activity, this year we used our codes to investigate two case studies. The first is the study of the wave conditions for the old Venetian harbour of Chania in Crete [109]. The study compares fully nonlinear-weakly dispersive COULWAVE code, developed at the University of South California, and TUCWave. The models are used to explore the appearance of resonance, eventually determining the resonant frequencies for the entire basin. The second study concerns the conditions for tidal bore formation in convergent alluvial estuaries [69]. A new set of dimensionless parameters has been introduced to describe the problem, and the code SLOWS has been used to explore the space of these parameters allowing to determine a critical curve allowing to characterize an estuary as "bore forming" or not. Surprising physical behaviours, in terms of dissipation and nonlinearity of the tides, have been highlighted. Part of this work has been accepted on *Estuarine, Coastal and Shelf Science*, with a manuscript on the numerical aspects in review on *Ocean Modelling*.

7.3. Wave energy conversion hydrodynamics

Participants: Umberto Bosi, Mario Ricchiuto [Corresponding member].

We have developed a prototype spectral element solver four a coupled set of differential equations modelling wave propagation (so-called outer domain), and the submerged flow under a floating body (inner domain). Both systems of equations are depth-averaged (Boussinesq type) systems involving some dispersive terms. They are further coupled to a force balance providing a (system of) ODE(s) for the floater. This model constitutes an intermediate fidelity approximation for the hydrodynamics of a wave energy converter. Differently from all industrial state of the art, it is a (fully) nonlinear model. However, its cost is extremely low when compared to full three-dimensional CFD analyses, due to the dimensional reduction brought from the depth averaged modelling. This year we have shown the potential of this Boussinesq-type model to predict the hydrodynamics

of a floater in a siplified case [97], [98] (journal version to appear on *J. Ocean Eng. and Marine Energy*). This result paves the way to the construction of new medium fidelity models to be used in the optimization of converters. This will be achieved in the framework of the MIDWEST project funded this year under the EU OCEANEranet call.

7.4. Two-phase flow numerical simulation with real-gas effects and occurrence of rarefaction shock waves

Participants: Maria Giovanna Rodio, Pietro Marco Congedo [Corresponding member].

We have studied the prediction in numerical simulation of turbulent cavitating flows, which could be strongly influenced by the presence of several empirical coefficients. The aim of this work is to explore the interaction between the cavitation model and turbulence in terms of uncertainty propagation through an unsteady numerical solver, for assessing the robustness and the accuracy of the physical models at different times. Furthermore, the influence of experimental data in the setting of some turbulence and cavitation model coefficients is investigated by means of a Bayesian approach. Finally, the interest is to provide some innovative insights for improving the understanding of these models for cavitating flows.

7.5. Formulation of stochastic methods for CFD

Participants: Maria Giovanna Rodio, Pietro Marco Congedo [Corresponding member].

We have worked on the extension of the Truncate and Encode (TE) approach, previously proposed by some of the authors (Abgrall et al. in J Comput Phys 257:19?56, 2014. doi:10.1016/j.jcp.2013.08.006), for taking into account uncertainty in partial differential equations (PDEs). Innovative ingredients are given by an algorithm permitting to recover the multiresolution representation without requiring the fully resolved solution, the possibility to treat a whatever form of pdf and the use of high-order (even non-linear, i.e. data-dependent) reconstruction in the stochastic space. Moreover, the spatial-TE method is introduced, which is a weakly intrusive scheme for uncertainty quantification (UQ), that couples the physical and stochastic spaces by minimizing the computational cost for PDEs. The proposed scheme is particularly attractive when treating moving discontinuities (such as shock waves in compressible flows), even if they appear during the simulations as it is common in unsteady aerodynamics applications. The proposed method is very flexible since it can easily coupled with different deterministic schemes, even with high-resolution features. Flexibility and performances of the present method are demonstrated on various numerical test cases (algebraic functions and ordinary differential equations), including partial differential equations, both linear and non-linear, in presence of randomness. The efficiency of the proposed strategy for solving stochastic linear advection and Burgers equation is shown by comparison with some classical techniques for UQ, namely Monte Carlo or the non-intrusive polynomial chaos methods.

A new scheme for the numerical approximation of a five-equation model taking into account Uncertainty Quantification (UQ) is also presented. In particular, the Discrete Equation Method (DEM) for the discretization of the five-equation model is modified for including a formulation based on the adaptive Semi-Intrusive (aSI) scheme, thus yielding a new intrusive scheme (sDEM) for simulating stochastic two-phase flows. Some reference test-cases are performed in order to demonstrate the convergence properties and the efficiency of the overall scheme. The propagation of initial conditions uncertainties is evaluated in terms of mean and variance of several thermodynamic properties of the two phases.

7.6. Sensitivity analysis, metamodelling, and and robust optimization

Participants: Kunkun Tang, Francesca Fusi, Pietro Marco Congedo [Corresponding member].

We have worked on two different formulations for sensitivity analysis. Moreover, we have proposed a new metamodelling technique and an innovative method for performing robust optimization.

Concerning sensitivity analysis, an anchored analysis of variance (ANOVA) method is proposed to decompose the statistical moments. Compared to the standard ANOVA with mutually orthogonal component functions, the anchored ANOVA, with an arbitrary choice of the anchor point, loses the orthogonality if employing the same measure. However, an advantage of the anchored ANOVA consists in the considerably reduced number of deterministic solver?s computations, which renders the uncertainty quantification of real engineering problems much easier. Different from existing methods, the covariance decomposition of the output variance is used to take account of the interactions between non-orthogonal components, yielding an exact variance expansion and thus, with a suitable numerical integration method, provides a strategy that converges. This convergence is verified by studying academic tests. In particular, the sensitivity problem of existing methods to the choice of anchor point is analyzed via the Ishigami case, and we point out that covariance decomposition survives from this issue. Also, with a truncated anchored ANOVA expansion, numerical results prove that the proposed approach is less sensitive to the anchor point. The covariance- based sensitivity indices (SI) are also used, compared to the variance-based SI. Furthermore, we emphasize that the covariance decomposition can be generalized in a straightforward way to decompose higher-order moments. For academic problems, results show the method converges to exact solution regarding both the skewness and kurtosis. Finally, the proposed method is applied on a realistic case, that is, estimating the chemical reactions uncertainties in a hypersonic flow around a space vehicle during an atmospheric reentry.

A sensitivity analysis method is extended in order to compute third and fourth-order statistic moments, i.e. skewness and kurtosis, respectively. It is shown that this decomposition is correlated to a Polynomial Chaos (PC) expansion, permitting to easily compute each term. Then, new sensitivity indexes are proposed basing on the computation of skewness and kurtosis. PC-based numerical technique is used in order to compute the convergence of the sensitivity indexes according to the polynomial order by using the exact solution as the reference one. The interest of the proposed analysis is first depicted by considering several test-functions. In particular, a functional decomposition based on variance, skewness and kurtosis is computed, displaying how sensitivity indexes vary according to the order of the statistical moment. Then, the problem of how reducing the complexity of a stochastic problem is treated by proposing two strategies: i) the reduction of the number of dimensions, the reduction of the order of interaction. In both cases, the impact on the statistics of the reduced function is then assessed. Feasibility of the proposed analysis in a real-case is then demonstrated by presenting a stochastic study about the uncertainty propagation in a challenging engineering simulation: the numerical prediction of a turbine cascade in an Organic Rankine Cycles (ORCs), with the use of complex thermodynamic models and the presence of multiple sources of uncertainty. Basing on high-order statistics decomposition and physical remarks, it is shown how the analysis proposed in this work can help to drive the design process in a real-engineering problem.

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

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

7.7. High order mesh generation and mesh adaptation

Participants: Luca Arpaia, Cécile Dobrzynski [Corresponding member], Ghina El Jannoun, Mario Ricchiuto.

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

- We have enhanced our work on r-adaptation techniques for time dependent equations. These techniques are based on mesh deformations obtained by solving continuous differential equations for the local displacements. These equations are controlled by an error monitor. Several improvements have been made. We have studied in depth the formulation of the coupling of the mesh movement with the flow solver. We have found that for both finite volume and residual distribution methods, a coupling of mesh and solution evolution (by means of an ALE method) provides accuracy enhancements, and is to be preferred to a simpler adapt-project-evolve approach. The method has been fully tested in two space dimensions. The adaptation library has been extended to three dimensions, and benchmarking is under way. We have improved the definition of the error monitor, and we are now able to prescribe directly the local mesh size. For problems with source terms, and in particular problems admitting some important physical invariants as the shallow water equations, we have solved the conflict between the conservation of either mass or the invariant, allowing for the conservation of both quantities up to machine accuracy;
- We upgrade our technique for generating high order curved meshes: starting from a straight mesh with a curved boundary, a new smoothing and untangling approach is proposed to ensure a final valid mesh. The untangling algorithm is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. On the one hand, the local topological optimization consists in simultaneously relocating the vertices and control points of a local patch around the invalid element in order to optimize the quality and validity of the elements inside the patch. The elements' validity problem is formulated as an unconstrained optimization problem using a log-barriers that is solved progressively using the conjugate gradient method. On the other hand, the linear elasticity analogy permits the propagation of the curvature to the volume of the domain hence untangling volume mesh elements.

7.8. Virtual self-healing composite for aeronautic propulsion

Participants: Mathieu Colin [Corresponding member], Xi Lin, Gregory Perrot, Mario Ricchiuto.

As a composite material having excellent properties, Ceramic-matrix composites (CMCs) comprise a ceramic matrix reinforced by a refractory fiber such as silicon carbide fiber. Due to the self-healing process (which consists in filling cracks produced by oxydation by an oxide formed in-situ), CMCs have extremely long lifetimes even under severe mechanical and chemical solicitations. These time spans make most full-scale experimental investigations impractical : laboratory tests have necessarily to be replaced by predictions based on numerical models. Initial results have already been obtained by in the past with simplified crack averaged models based on simple potential approximations of the flow field of the oxide. In this direction, Xi Lin has developed new asymptotic models by creating a hierarchy inside two different families : the Saint-Venant equations and the thin film equations. The hierarchy is based on the use of several different boundary conditions. The main goal is to obtain more accurate hydrodynamic models accounting for surface tension and viscous effects which may be very important for the oxide evolution.

In parallel, we have made great progress in the coupling of the chemistry module with the structural mechanics solver of the LCTS laboratory in Bordeaux. The first fully coupled simulations of a fatigue test for a so-called mini-composite (on single fibre tow). The simulations have allowed to reproduce the gradual breaking mechanism typical of these materials, allowing to reproduce numerically the delayed rupture observed in practice.

7.9. Numerical simulation of the liquid ablation

Participants: Gérard Gallice, Luc Mieussens [Corresponding member], Simon Peluchon.

During the atmospheric re-entry phase, a space vehicle undergoes a heating due to the friction of the atmospheric gases. Conversion of kinetic energy to thermal energy leads to a sudden increase of the temperature of the solid boundary. This leads to a physical-chemical degradation of the thermal protective system, and to a boundary recession. For some materials, this recession occurs with a melting of the materials into a fluid phase. The numerical simulation of this phenomenon requires to take into account a two-phase flow with a compressible gaz (the air flow) and a weakly compressible liquid (the melted material). Numerically, this problem is strongly stiff.

We have proposed a splitting strategy to simulate compressible two-phase flows using the five equation model. The main idea of the splitting is to separate the acoustic and transport phenomena. The acoustic step is solved in Lagrangian coordinates by using a scheme based on an approximate Riemann solver. On the one hand, since the acoustic time step driven by the fast sound velocity is very restrictive, an implicit treatment of the Lagrangian step is performed. On the other hand, we use an explicit scheme for the transport step driven by the slow material waves. The global scheme resulting from this splitting operator strategy is conservative, positive, and preserves contact discontinuities. Numerical simulations of compressible diphasic flows are presented on 2d-structured grids. The implicit-explicit strategy allows large time steps, which do not depend on the fast acoustic waves.

7.10. Boundary conditions for the Navier-Stokes equations in the transitional regime

Participants: Céline Baranger, Pietro Marco Congedo, Giorgio Martalo, Julien Mathiaud, Luc Mieussens [Corresponding member].

In reentry flows at high altitude, the parietal fluxes along the boundary of a space vehicle are computed by solving the Boltzmann equation of the gas kinetic theory. It depends on the way particles are reflected by the solid wall. In this kind of applications, the reflection is usually supposed to be 80% diffuse (the particle are re-emitted in a random direction in thermal equilibrium with the wall), and 20% specular.

In lower altitude, it is possible to use the compressible Navier-Stokes equations, but the standard boundary conditions do not take into account the specular part. These equations are hence not very accurate in the transition regime (in which the Knudsen number is around 0.01).

By using an asymptotic boundary layer analysis, we have derived boundary conditions for the compressible Navier-Stokes equations that formaly make the fluid model a second order approximation of on the Boltzmann equation of the kinetic gas theory (with respect to the Knudsen number), and that can take into account the effect of the specular reflections. These boundary conditions include a slip velocity at the wall and a temperature jump, with some coefficients that depend on some auxiliary half-space problems. An existing numerical method has been extended to solve these problems and give numerical values for these coefficients. This make our boundary conditions practically usable into any Navier-Stokes code.

DEFI Project-Team

6. New Results

6.1. Methods for inverse problems

6.1.1. Identifying defects in an unknown background using differential measurements

L. Audibert and H. Haddar

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

6.1.2. Invisibility in scattering theory for small obstacles

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

We are interested in a time harmonic acoustic problem in a waveguide containing flies. The flies are modelled by small sound soft obstacles. We explain how they should arrange to become invisible to an observer sending waves from $-\infty$ and measuring the resulting scattered field at the same position. We assume that the flies can control their position and/or their size. On the other hand, we show that any sound soft obstacle (non necessarily small) embedded in the waveguide always produces some non exponentially decaying scattered field at $+\infty$. As a consequence, the flies cannot be made completely invisible to an observer equipped with a measurement device located at $+\infty$.

6.1.3. New notion of regularization for Poisson data with an application to nanoparticle volume determination

F. Benvenuto, H. Haddar and B. Lantz

The aim of this work is to develop a fully automatic method for the reconstruction of the volume distribution of diluted polydisperse non-interacting nanoparticles with identical shapes from Small Angle X-ray Scattering measurements. The described method solves a maximum likelihood problem with a positivity constraint on the solution by means of an Expectation Maximization iterative scheme coupled with a robust stopping criterion. We prove that this is a regularization method according to an innovative notion of regularization specifically defined for inverse problems with Poisson data. Such a regularization, together with the positivity constraint results in high fidelity quantitative reconstructions of particle volume distributions making the method particularly effective in real applications. We test the performance of the method on synthetic data in the case of uni- and bi-modal particle volume distributions. Moreover, we show the reliability of the method on real data provided by a Xenocs device prototype.

6.1.4. A conformal mapping algorithm for the Bernoulli free boundary value problem

H. Haddar and R. Kress

We propose a new numerical method for the solution of Bernoulli's free boundary value problem for harmonic functions in a doubly connected domain D in R^2 where an unknown free boundary Γ_0 is determined by prescribed Cauchy data on Γ_0 in addition to a Dirichlet condition on the known boundary Γ_1. Our main idea is to involve the conformal mapping method as proposed and analyzed by Akduman, Haddar and Kress for the solution of a related inverse boundary value problem. For this we interpret the free boundary Γ_0 as the unknown boundary in the inverse problem to construct Γ_0 from the Dirichlet condition on Γ_0 and Cauchy data on the known boundary Γ_1. Our method for the Bernoulli problem iterates on the missing normal derivative on Γ_1 by alternating between the application of the conformal mapping method for the inverse problem and solving a mixed Dirichlet–Neumann boundary value problem in D. We present the mathematical foundations of our algorithm and prove a convergence result. Some numerical examples will serve as proof of concept of our approach.

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

H. Haddar and M. Lakhal

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

6.2. Direct scattering problems

6.2.1. A numerical method to approximate black hole singularities in presence of metamaterials

L. Chesnel, A.-S. Bonnet-Ben Dhia, C. Carvalho and P. Ciarlet.
We investigate in a 2D setting the scattering of time-harmonic electromagnetic waves by a plasmonic device, represented as a non dissipative bounded and penetrable obstacle with a negative permittivity. Using the T-coercivity approach, we proved that the problem is well-posed in the classical frameworks if the negative permittivity does not lie in some critical interval whose definition depends on the shape of the device. When the latter has corners, for values inside the critical interval, unusual strong singularities for the electromagnetic field can appear. In that case, well-posedness is obtained by imposing a radiation condition at the corners to select the outgoing black-hole plasmonic wave, that is the one which carries energy towards the corners. We give a simple and systematic criterion to define what is the outgoing solution. We also propose an original numerical method based on the use of Perfectly Matched Layers at the corners. We emphasize that it is necessary to design an *ad hoc* technique because the field is too singular to be captured with standard finite element methods.

6.2.2. Boundary Integral Equations for the Transmission Eigenvalue Problem for Maxwell's Equations

Houssem Haddar, Shixu Meng and Fioralba Cakoni

We consider the transmission eigenvalue problem for Maxwell's equations corresponding to non-magnetic inhomogeneities with contrast in electric permittivity that changes sign inside its support. We formulate the transmission eigenvalue problem as an equivalent homogeneous system of boundary integral equa- tion, and assuming that the contrast is constant near the boundary of the support of the inhomogeneity, we prove that the operator associated with this system is Fredholm of index zero and depends analytically on the wave number. Then we show the existence of wave numbers that are not transmission eigenvalues which by an application of the analytic Fredholm theory implies that the set of transmission eigenvalues is discrete with positive infinity as the only accumulation point.

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

Houssem Haddar and Thi Phong Nguyen

We investigate the scattering problem for the case of locally perturbed periodic layer in $R^N (N = 2, 3)$. Using Floquet-Bloch transform in x_1-direction we reformulate this scattering problem as an equivalent system of coupled volume integral equations. Using periodization in the x_2-direction we apply a spectral method to discretize the problem and compute a numerical approximation of the solution. The convergence of this method is established and numerical validating results are conducted.

6.3. Shape and topology optimization

6.3.1. Deterministic approximation methods in shape optimization under random uncertainties

G. Allaire and C. Dapogny

This work is concerned with the treatment of uncertainties in shape optimization. We consider uncertainties in the loadings, the material properties, the geometry and the vibration frequency, both in the parametric and geometric optimization setting. We minimize objective functions which are mean values, variances or failure probabilities of standard cost functions under random uncertainties. By assuming that the uncertainties are small and generated by a finite number N of random variables, and using first- or second-order Taylor expansions, we propose a deterministic approach to optimize approximate objective functions. The computational cost is similar to that of a multiple load problems where the number of loads is N. We demonstrate the effectiveness of our approach on various parametric and geometric optimization problems in two space dimensions.

6.3.2. Molding direction constraints in structural optimization via a level-set method

G. Allaire, F. Jouve and G. Michailidis

In the framework of structural optimization via a level-set method, we develop an approach to handle the directional molding constraint for cast parts. A novel molding condition is formulated and a penalization method is used to enforce the constraint. A first advantage of our new approach is that it does not require to start from a feasible initialization, but it guarantees the convergence to a castable shape. A second advantage is that our approach can incorporate thickness constraints too. We do not adress the optimization of the casting system, which is considered a priori defined. We show several 3d examples of compliance minimization in linearized elasticity under molding and minimal or maximal thickness constraints. We also compare our results with formulations already existing in the literature.

6.3.3. Identification of magnetic deposits in 2-D axisymmetric eddy current models via shape optimization

Zixian Jiang, Houssem Haddar, Armin Lechleiter and Mabrouka El-Guedri

The non-destructive control of steam generators is an essential task for the safe and failure-free operation of nuclear power plants. Due to magnetite particles in the cooling water of the plants, a frequent source for failures are magnetic deposits in the cooling loop of steam generators. From eddy current signals measured inside a U-tube in the steam generator, we propose and analyze a regularized shape optimization algorithm to identify magnetic deposits outside the U-tube with either known or unknown physical properties. Motivated by the cylindrical geometry of the U-tubes we assume an axisymmetric problem setting, reducing Maxwell's equations to a 2-D elliptic eddy current problem. The feasibility of the proposed algorithms is illustrated via numerical examples demonstrating in particular the stability of the method with respect to noise.

6.4. Asymptotic Analysis

6.4.1. Ion transport through deformable porous media: derivation of the macroscopic equations using upscaling

G. Allaire, O. Bernard, J.-F. Dufrêche and A. Mikelic

We study the homogenization (or upscaling) of the transport of a multicomponent electrolyte in a dilute Newtonian solvent through a deformable porous medium. The pore scale interaction between the flow and the structure deformation is taken into account. After a careful adimensionalization process, we first consider so-called equilibrium solutions, in the absence of external forces, for which the velocity and diffusive fluxes vanish and the electrostatic potential is the solution of a Poisson-Boltzmann equation. When the motion is governed by a small static electric field and small hydrodynamic and elastic forces, we use O'Brien's argument to deduce a linearized model. Then we perform the homogenization of these linearized equations for a suitable choice of time scale. It turns out that the deformation of the porous medium is weakly coupled to the electrokinetics system in the sense that it does not influence electrokinetics although the latter one yields an osmotic pressure term in the mechanical equations. As a consequence, the effective tensor satisfies Onsager properties, namely is symmetric positive definite.

6.4.2. On the asymptotic behaviour of the kernel of an adjoint convection-diffusion operator in a long cylinder

G. Allaire and A. Piatnitski

This work studies the asymptotic behaviour of the principal eigenfunction of the adjoint Neumann problem for a convection diffusion operator defined in a long cylinder. The operator coefficients are 1-periodic in the longitudinal variable. Depending on the sign of the so-called longitudinal drift (a weighted average of the coefficients), we prove that this principal eigenfunction is equal to the product of a specified periodic function and of an exponential, up to the addition of fast decaying boundary layer terms.

6.4.3. A comparison between two-scale asymptotic expansions and Bloch wave expansions for the homogenization of periodic structures

G. Allaire, M. Briane and M. Vanninathan

In this work we make a comparison between the two-scale asymptotic expansion method for periodic homogenization and the so-called Bloch wave method. It is well-known that the homogenized tensor coincides with the Hessian matrix of the first Bloch eigenvalue when the Bloch parameter vanishes. In the context of the two-scale asymptotic expansion method, there is the notion of high order homogenized equation where the homogenized equation can be improved by adding small additionnal higher order differential terms. The next non-zero high order term is a fourth-order term, accounting for dispersion effects. Surprisingly, this homogenized fourth-order tensor is not equal to the fourth-order tensor arising in the Taylor expansion of the first Bloch eigenvalue, which is often called Burnett tensor. Here, we establish an exact relation between the homogenized fourth-order tensor and the Burnett fourth-order tensor. It was proved by Conca et al. that the Burnett fourth-order tensor has a sign. For the special case of a simple laminate we prove that the homogenized fourth-order tensor may change sign. In the elliptic case we explain the difference between the homogenized and Burnett fourth-order tensors by a difference in the source term which features an additional corrector term.

Finally, for the wave equation, the two fourth-order tensors coincide again, so dispersion is unambiguously defined, and only the source terms differ as in the elliptic case.

6.4.4. Influence of the geometry on plasmonic waves

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

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

6.4.5. Effective boundary conditions for thin periodic coatings Participants

Mathieu Chamaillard, Houssem Haddar and Patrick Joly

We study the derivation of asymptotic model (generalized impedance boundary conditions) for periodic coating in 3-D configurations. The definition of periodicity for $3D$ surfaces cannot be done in an intrinsic way in general. We propose a definition based on the use of local parametrisations of the surface. This parametrization-dependent definition is somehow inspired from practical considerations in the manufacturing of periodic coatings. The asymptoic of the problem is constructed for the scalar problem and also for the electormagnetic problem. Approximate models of order 1 and 2 are derived for the scalar problem and are validated numerically. In the electromagnetic case, only conditions or order 1 are exhibited in the genral case.

6.5. Diffusion MRI

Jing-RebeccaLi, HoussemHaddar, SimonaSchiavi ,Khieu VanNguyen,GabrielleFournet

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.

- We derived using homogenization techniques a model of the time-dependent “apparent diffusion coefficient”(ADC) that is valid at a wide range of diffusion times. The ADC is a very important experimental quantity measured by diffusion MRI in biological tissues. This work resulted in one submitted article to a mathematical journal and we are preparing an article for a physics journal.
- We analyzed a dMRI model called the Karger model that is valid at long diffusion times. This resulted in one submitted article to a mathematical journal.
- We acquired dMRI data of the nerve cells of the Aplysia Californica at the high field brain MRI center Neurospin. This data is useful because the nerve cells are bigger than mammal neurons and so it is easier to obtain segmented geometrical information about these cells for model validation.
- We participated in the data analysis and numerical simulation of a MR imaging method to measure blood flow in micro-vessels in the brain. This resulted in a submitted article to a MRI journal.

ECUADOR Project-Team

6. New Results

6.1. AD-adjoints and C dynamic memory management

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

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

Adjoint AD must reproduce in reversed order the control decisions of the original code. In languages such as C, allocation of dynamic memory and pointer management form a significant part of these control decisions. Reproducing memory (de)allocation in reverse means reallocating memory, possibly receiving a different memory chunk. Reproducing pointer addresses in reverse thus require to convert addresses in the former memory chunks into equivalent addresses in the new reallocated chunks. Together with Krishna Narayanan from Argonne, we experiment on real applications to find the most efficient solution to this address conversion problem. We jointly develop a library (called ADMM, ADjoint Memory Management) whose primitives can be used in AD adjoint code to handle this address conversion. Using this library together with Tapenade, we could obtain a correct AD adjoint code of a medium-size industrial code (“Multibody", structural mechanics) that exhibits a typical usage of C pointer arithmetic. This year, the same effort was conducted with the OpenAD AD tool, leading us to an ADMM library less dependent on the particular target AD tool. A joint publication with our colleagues from Argonne is in preparation.

In parallel, we investigate alternative implementation strategies for ADMM, one of which could be to build our own memory (de)allocation mechanism, This should ultimately rely on the standard C library. As a result, management of adjoint memory addresses could be done deeper in the system and therefore with a smaller overhead, at the cost of some additional portability issues.

We pursue our objective of improving reliability of the AD adjoint model for C codes to a similar level as achieved for Fortran. To this end we apply Tapenade to increasingly larger and complex C codes. In addition to the already mentioned “Multibody" application, we initiated differentiation of two new complex applications:

- “BLN" is a code developed by the Inria team ABS, that computes the potential energy of possible conformations of a macromolecule. Its gradient is used to explore the local minima in the energy landscape of these conformations. The AD adjoint of a Fortran implementation of BLN has been built by Tapenade and successfully validated. The adjoint of the C implementation is a challenge that helps us clarify the adjoint AD model that we use in Tapenade. The C version of BLN that we are considering is actually a (partly mechanical) translation of the actual C++ source. This makes this code an even more appealing and challenging test case. This work was mostly conducted by Raphaël Couronné as a part of his summer internship with us.
- “SEISM" is a code developed by Mathieu Morlighem from UC Irvine, jointly with Eric Larour from JPL. This is a glaciology code closely related to the larger “ISSM" code, in C++. One objective, addressed mostly by Mathieu Morlighem, is to clarify recommendations on the C programming style (again very much inspired here from the C++ style) that allows AD to perform better. The other objective, adressed mostly by our team, it to experiment with quite intricate data structures, where Tapenade’s static pointer destination analysis is used intensively.

6.2. AD-adjoints of MPI-parallel codes

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

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

During her PhD work, Ala Taftaf is considering the question of checkpointing applied to the AD-adjoint of an MPI-parallel code. Checkpointing is a memory/runtime tradeoff which is essential for adjoint AD of large codes, in particular parallel codes. However, for MPI codes this question has always been addressed by ad-hoc hand manipulations of the differentiated code, and with no formal assurance of correctness. Ala Taftaf is investigating the assumptions implicitly made during past experiments, to clarify and generalize them. On one hand we propose an extension of the adjoint of MPI point-to-point communication primitives, so that the semantics of an adjoint program is preserved for any placement of checkpoints. On the other hand, we propose an alternative extension of these adjoint communications, more efficient but that requires a number of restrictions on the placement of checkpoints. We shall try to provide proof of correctness of these strategies, and in particular demonstrate that they cannot introduce deadlocks. Tradeoffs between the two extensions should be investigated. Ala Taftaf presented her research on "'Adjoint-Checkpointing on MPI-parallel codes" at the EuroAD workshop in Paderborn, Germany, december 1-2. A conference article has been submitted to Eccomas 2016 in Crete.

6.3. AD-adjoints of Iterative Processes

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

Adjoint codes naturally propagate partial gradients backwards from the result of the simulation. However, this uses the data flow of the simulation in reverse order, at a cost that increases with the length of the simulation. In the special case of iterative Fixed-Point loops, only the final converged result should be used: the "initial guess" and the intermediate non-converged states should not be considered by the adjoint calculation, and this remark brings enormous gain in memory use. We selected the strategy proposed by Bruce Christianson [22] and this year we continued its application to medium-size testcases provided by Queen Mary University for the AboutFlow project. We also simplified the user interface provided to trigger this special strategy extension in Tapenade. Ala Taftaf presented her results at the ECCOMAS Eurogen conference in Glasgow [15], september 14-16.

In parallel, we collaborated with Krishna Narayanan from ANL and Dan Goldberg from University of Edinburgh (UK) to implement the same strategy into the OpenAD tool, in view of applying it to a glaciology configuration of the MIT GCM code. A joint article describing the results has been submitted for publication.

6.4. AD-adjoints of large real codes

Participants: Laurent Hascoët, Valérie Pascual, Raphaël Couronné, Fabrice Zaoui [EDF R&D, LNHE].

In collaboration with EDF, Valérie Pascual is applying Tapenade to the hydrographic code "Mascaret". Both tangent and adjoint diferentiated codes have been built and validated. Application of the tangent differentiated Mascaret for data assimilation on two real cases is described in a joint publication [14].

During his summer internship, Raphaël Couronné has applied Tapenade to the MIT "GCM", a reference code in the Earth Sciences community. We have obtained a valid adjoint for a recommended configuration of this very large Fortran code. This test showed some maturity of the Tapenade tool for Fortran, as it turned out that no modification nor debug of the tool was needed. We are now discussing with the MIT team to schedule further collaboration.

In cooperation with the partners of the FP7 project UMRIDA, the team has assisted Alenia-Aermacchi (Filomena Cariglino and Nicola Ceresola) in the efficient differentiation of their Euler/Navier Stokes code “UNS3D" in tangent mode, dealing in particular with its use of MPI.

The team has assisted Marcin Wyrozebski from Warsaw University of Technology, to apply Tapenade to a CFD software from WUT.

6.5. Resolution of linearised systems and efficiency

Participants: Olivier Allain [Lemma], Gautier Brèthes, Alain Dervieux, Bruno Koobus [Université Montpellier 2], Emmanuelle Itam [Université Montpellier 2], Vincent Levasseur [Lemma], Stephen Wornom [Lemma].

For Fluid Mechanics as well as for Structural Mechanics, an implicit time-advancing is mandatory. It can be applied efficiently if the large systems involved are solved with a good parallel algorithm. In the 90’s, a generation of solution algorithms was devised on the basis of Domain Decomposition Methods (DDM). For complex models (compressible flows...), Schwarz DDM were combined with quasi-Newton algorithms such as GMRES. These are for example Restrictive Additive Schwarz (RAS), which is used in our platform AIRONUM. RAS was developed by Cai, Farhat and others. RAS is an ancestor of the widely used class of Newton-Krylov-Schwarz (NKS) algorithms. For hundreds of processors many versions of NKS, and in particular RAS, are almost scalable (convergence rate independant of the number of processors). But scalability vanishes for a medium-large number of processors (thousands). In the ANR ECINADS, coordinated by Ecuador, a Coarse-Grid Deflated RAS was developped: iteration-wise scalability holds for all parts, except for the coarse grid direct solver, which concerns a much smaller problem. Effective Convergence Scalability (ECS) was confirmed up to 2048 processors. Beyond this level the asymptotic complexity of the coarse-grid direct solver becomes predominant and ECS is lost. In other words, with a Coarse-Grid Deflated RAS, the size of the coarse grid problem which is solved by a direct algebraic solver must be limited in order to enjoy ECS. For finer meshes, the coarse system cannot be finer, and the efficiency is lower. It is then natural to consider intermediate meshes on which iterative solvers will be applied. In the ANR MAIDESC, Gautier Brèthes has defined a multi-mesh Full MultiGrid (FMG) algorithm adapted to anisotropic mesh adaptation. In 2015, the method has been extended to MPI-based massive parallelism, in cooperation with the Lemma team for the computation of incompressible flows. As a perspective, our parallel MG can be complemented with the previous version of the solver (deflated RAS) for a higher degree of scalability.

A second issue which we addressed is the use of explicit time advancing. Many unsteady flows have to be computed with explicit time advancing. A single explicit time step is of a low cost and can be highly accurate. Explicit time advancing is mandatory for wave propagation: blast shocks of vortices in wakes. However the meshes used may involve small regions in which the explicit time step should be very small and large regions in which such a small time step is a waste. The family of time-advancing methods in which unsteady phenomena are computed using different time steps in different regions is called the multirate methods. In our cooperation with University of Montpellier, a novel multirate method using cell-agglomeration has been designed and developed in our AIRONUM platform. An article is in preparation. This work takes place in the ANR MAIDESC programme.

6.6. Control of approximation errors

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

The study of combination of full multigrid (FMG) with anisotropic mesh adaption (AA), started with the thesis of Gautier Brèthes, has been published [13].

Further studies of mesh adaptation for viscous flows are currently performed and a journal paper, joint with Inria team Gamma3 and University of Paris 6 (Anca Belme) is in preparation.

An important novelty in mesh adaption is the norm-oriented AA method. The method relies on the definition of ad hoc correctors. It has been developed in the academic platform “FMG" for elliptic problems. Gautier Brèthes gave several presentations in conferences, a journal article has been submitted. The introduction of the norm-oriented idea considerably amplifies the impact of adjoint-based AA. The applied mathematician and the engineer now have methods when faced to mesh adaptation for the simulation of a complex PDE system, since they can specify which error norm level they wish, and for which norm [12], [16]. Another version is developed jointly with Inria team Gamma3 for the compressible Euler model [19].

A cooperation has started between Gautier Brèthes et Thierry Coupez (Ecole Centrale de Nantes) concerning discrete metrics. This takes place in the ANR MAIDESC program. An article is in preparation.

Éléonore Gauci started last year a thesis (co-advised by Frédéric Alauzet) on the study of norm-oriented criteria for CFD and coupled CSM-CFD systems. She gave a presentation at the “Coupled Problems" symposium.

Post-doc Guilherme Cunha did a study (in cooperation with Lemma) on the combination of mesh adaptation and coefficient identification for unsteady phenomena.

The theoretical studies are supported by an ANR project MAIDESC coordinated by ECUADOR and Gamma3, which deals with meshes for interfaces, third-order accuracy, meshes for boundary layers, and curved meshes.

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

6.7. Turbulence models

Participants: Alain Dervieux, Bruno Koobus [University of Montpellier 2], Emmanuelle Itam [University of Montpellier 2], Marianna Braza [CNRS-IMFT at Toulouse], Stephen Wornom [Lemma], Bruno Sainte-Rose [Lemma].

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

This year, we have continued the evaluation of a dynamic formulation of Piomelli-Germano type for the Variational-multiscale model. We have also modified the integration of the boundary layer by adding the so-called Menter correction imposing the Bradshaw law. We have studied these improvements on multiple-body flows. An emblematic case is the interaction between two parallel cylinders, one being in the wake of the other. A flow around a space probe at high Reynolds number is also studied [18], [17].

GAMMA3 Project-Team

5. New Results

5.1. Serendipity and reduced elements

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

We give a method to constructing Serendipity elements for quads and hexes with full symmetry properties and indicate the reading of their shape functions. We show that, since the degree 5, the Serendipity elements are no longer symmetric but we propose a method resulting in a Lagrange element of degree 5 with full symmetry properties after adding an adequate number of additional nodes.

On the other hand, we show how to guarantee the geometric validity of a given curved element (seen as a patch) of a mesh. This is achieved after writing the patch in a Bézier setting (Bernstein polynomials and control points). In addition, we discuss the case of patch derived from a transfinite interpolation and it is proved that only some of them are Serendipity elements indeed, we return to the same elements as above

We also give a method to constructing Lagrange Serendipity (or reduced) simplices with a detailed description of the triangles of degree 3 and 4. We indicate that higher order triangles are not candidate apart if we impose a restricted polynomial space. We show that a tetrahedron of degree 3 is a candidate while high order elements are not candidate even if a restriction in the polynomial space is considered. In addition, we propose a method for the validation of such elements, in a given mesh, where the validation means the positiveness of the jacobian.

5.2. Validity of transfinite and Bézier-Serendipity patches

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

We define generalized transfinite patches for quads and hexes with full symmetry properties. We give a way of constructing those patches by considering the Bézier setting using linear combinations of tensor-product patches of various degree. Those patches are exactly the Bézier-Serendipity patches recently introduced

ASsfor reduced quadrilateral patches, we introduce the so called "Bézier-Serendip" patches. After some recalls about standard Bézier patches, we propose a method to constructing those reduced patches. The corresponding Bernstein polynomials are written by means of linear combinations of the standard Bernstein polynomials. We give a full description of the patches of degree 2, 3, 4 and 5. Since degree 5, the location of the control points is no longer symmetric and to remedy this problem, we propose adding a number of control points which results in *extended* Bézier-Serendip patches. Those reduced patches are in the Bézier framework what the Serendipity elements are in the finite element framework.

A technical report and a paper have been published [16].

5.3. Meshing Strategies and the Impact of Finite Element Quality on the Velocity Field in Fractured Media

Participants: Patrick Laug [correspondant], Géraldine Pichot.

For calculating flow in a fracture network, the mixed hybrid finite element (MHFE) method is a method of choice as it yields a symmetric, positive definite linear system. However, a drawback to this method is its sensitivity to bad aspect ratio elements. For poor-quality triangles, elementary matrices are ill-conditioned, and inconsistent velocity vectors are obtained by inverting these local matrices. In this work, different strategies have been proposed for better reconstruction of the velocity field.

5.4. Automatic Mesh Generation of Multiface Models on Multicore Processors

Participant: Patrick Laug [correspondant].

This work started in September 2014, as part of a sabbatical year at Polytechnique Montréal. In a previous study, a parallel version of an indirect approach for meshing composite surfaces – also called multiface models – was developed. However, this methodology could be inefficient in practice, as the memory management of most existing CAD (computer aided design) systems use static global caches to save information. In a first approach, CAD queries are fully parallelized, using the Pirate library from Polytechnique Montréal (this library provides a set of C++ classes that implement STEP-compliant B-Rep geometric and topological entities, as well as classes to represent meshes and solutions). In a second approach, the CAD system is completely disconnected from the mesh generator, using a discrete geometric support.

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

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

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

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

La seconde classe de générateurs porte sur le développement de méthodes avancées et est basée sur l'exploitation de fonctions chaotiques en utilisant les sorties de ces fonctions comme indice de permutation sur un vecteur initial. Ce projet s'intéresse également aux systèmes de chiffrement pour la protection des données et deux algorithmes de chiffrement d'images utilisant des fonctions chaotiques sont développés et analysés. Ces Algorithmes utilisent un processus de permutation-substitution sur les bits de l'image originale. Une analyse statistique approfondie confirme la pertinence des cryptosystèmes développés.

5.6. Développement de méthodes avancées et maillages appliqués à l'étude de la nanomorphologie des nanotubes-fils en suspension liquide

Participants: Thomas Grosges [correspondant], Dominique Barchiesi, Abel Cherouat, Houman Borouchaki, Laurence Giraud-Moreau, Anis Chaari.

Ce projet de recherche (NANOMORPH) a pour objet principal le développement et la mise au point d'une instrumentation optique pour déterminer la distribution en tailles et le coefficient de forme de nanofils (NF) ou de nanotubes (NT) en suspension dans un écoulement. Au cours de ce projet, deux types de techniques optiques complémentaires sont développées. La première, basée sur la diffusion statique de la lumière, nécessite d'étudier au préalable la physico-chimie de la dispersion, la stabilisation et l'orientation des nanofils dans les milieux d'étude. La seconde méthode, basée sur une méthode opto-photothermique pulsée, nécessite en sus,

la modélisation de l'interaction laser/nanofils, ainsi que l'étude des phénomènes multiphysiques induits par ce processus. L'implication de l'équipe-projet GAMMA3 concerne principalement la simulation multiphysique de l'interaction laser-nanofils et l'évolution temporelle des bulles et leurs formations. L'une des principales difficultés de ces problématiques est que la géométrie du domaine est variable (à la fois au sens géométrique et topologique). Ces simulations ne peuvent donc être réalisées que dans un schéma adaptatif de calcul nécessitant le remaillage tridimensionnel mobile, déformable avec topologie variable du domaine (formation et évolution des bulles au cours du temps et de l'espace).

5.7. Applications du maillage à des problèmes multi-physiques, développement de méthodes de résolutions avancées et modélisation électromagnetisme-thermique-mécanique á l'échelle mesoscopique

Participants: Dominique Barchiesi [correspondant], Abel Cherouat, Thomas Grosges, Houman Borouchaki, Laurence Giraud-Moreau, Sameh Kessentini, Anis Chaari, Fadhil Mezghani.

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

Le travail de l'année 2014 a constitué en la poursuite de l'étude des spécificités de ce type de problème multiphysique pour des structures de forme simple et la mise en place de fonctions test, de référence, pour les développements de maillage adaptatifs pour les modèles multiphysiques éléments finis. Nous espérons pouvoir proposer un projet ANR couplant les points de vue microscopiques et macroscopiques dans les deux années qui viennent.

5.8. Visualization and modification of high-order curved meshes

Participants: Alexis Loyer, Adrien Loseille [correspondant].

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

5.9. Mesh adaptive ALE numerical simulation

Participants: Frédéric Alauzet [correspondant], Nicolas Barral, Adrien Loseille.

Running highly accurate numerical simulations with moving geometries is still a challenge today due to their prohibitive cost in CPU time. Using anisotropic mesh adaptation is one way to drastically reduce the size of the problem and to reach the desired accuracy. Previously, we have developed an ALE formulation using mesh connectivity change in order to achieve any complex displacement. Then, this method has been coupled with the unsteady anisotropic mesh adaptation using the fixed-point algorithm. The key point of this work is the use of an ALE metric that takes into account the mesh motion in the metric field definition.

5.10. Mesh adaptation for Navier-Stokes Equations

Participants: Frédéric Alauzet, Victorien Menier, Adrien Loseille [correspondant].

Adaptive simulations for Navier-Stokes equations require to propose accurate error estimates and design robust mesh adaptation algorithms (for boundary layers).

For error estimates, we design new estimates suited to accurately capture the speed profile in the boundary layers. For mesh adaptation, we design a new method to generate structured boundary layer meshes which are mandatory to accurately compute compressible flows a high Reynolds number (several millions). It couple the specification of the optimal boundary layer from the geometry boundary and moving mesh techniques to extrude the boundary layer in an already existing mesh. The main advantage of this approach is its robustness, *i.e.,* at each step of the algorithm we have always a valid mesh [23].

5.11. Adaptive multigrid strategies

Participants: Frédéric Alauzet [correspondant], Victorien Menier, Adrien Loseille.

Multigrid is a well known technique used to accelerate the convergence of linear system solutions. Using a multigrid strategy to solve non-linear problems improves the robustness and the convergence of each Newton step, the accelerating overall the whole process. In particular, larger time step can be considered. This of main importance when solving turbulent Navier-Stokes equations on complex geometries. First, we developed the classical multigrid method on non-nested meshes. Then, we have pointed out the similarity between the Full MultiGrid (FMG) algorithm and the mesh adaptation algorithm. We have proposed a new Adaptive Full MultiGrid algorithm which improve the overall robustness of the adaptive process and its overall efficiency [23].

5.12. Metric-orthogonal and metric-aligned mesh adaptation

Participants: Frédéric Alauzet, Victorien Menier, Adrien Loseille [correspondant].

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

5.13. Parallel mesh adaptation

Participants: Frédéric Alauzet, Victorien Menier, Adrien Loseille [correspondant].

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

5.14. Unsteady adjoint computation on dynamic meshes

Participants: Eléonore Gauci, Frédéric Alauzet [correspondant].

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

5.15. Line solver for efficient stiff parse system resolution

Participants: Loïc Frazza, Frédéric Alauzet [correspondant].

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

5.16. Error estimate for high-order solution field

Participants: Olivier Coulaud, Adrien Loseille [correspondant].

Afin de produire des solveurs d'ordre élevé, et ainsi répondre aux exigences inhérentes à la résolution de problèmes physiques complexes, nous développons une méthode d'adaptation de maillage d'ordre élevé. Celle-ci est basée sur le contrôle par une métrique de l'erreur d'interpolation induite par le maillage du domaine. Plus précisément, pour une solution donnée, l'erreur d'interpolation d'ordre k est paramétrée par la différentielle kè de cette solution, et le problème se réduit à trouver la plus grande ellipse incluse dans une ligne de niveau de cette différentielle. S'il reste encore quelques difficultés techniques à résoudre avant l'exploitation numérique de notre méthode, les résultats sont très encourageants, tant en terme d'optimalité de la métrique obtenue que de temps de calcul. Il n'y a que peu de doutes sur le fait que ce projet aboutisse prochainement.

IPSO Project-Team

5. New Results

5.1. Uniformly accurate numerical schemes for highly-oscillatory Klein-Gordon and nonlinear Schrödinger equation

The work [20] is devoted to the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called “Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. The method is based on two main ingredients. First, we embed our problem in a suitable “two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

5.2. Higher-order averaging, formal series and numerical integration III: error bounds

In earlier works, it has been shown how formal series like those used nowadays to investigate the properties of numerical integrators may be used to construct high- order averaged systems or formal first integrals of Hamiltonian problems. With the new approach the averaged system (or the formal first integral) may be written down immediately in terms of (i) suitable basis functions and (ii) scalar coefficients that are computed via simple recursions. In [21], we show how the coefficients/basis functions approach may be used advantageously to derive exponentially small error bounds for averaged systems and approximate first integrals.

5.3. Stroboscopic averaging for the nonlinear Schrödinger equation

In [18], we are concerned with an averaging procedure, -namely Stroboscopic averaging-, for highly-oscillatory evolution equations posed in a (possibly infinite dimensional) Banach space, typically partial differential equations (PDEs) in a high-frequency regime where only one frequency is present. We construct a high-order averaged system whose solution remains exponentially close to the exact one over long time intervals, possesses the same geometric properties (structure, invariants,...) as compared to the original system, and is non-oscillatory. We then apply our results to the nonlinear Schrdinger equation on the d-dimensional torus T^d, or in R^d with a harmonic oscillator, for which we obtain a hierarchy of Hamiltonian averaged models. Our results are illustrated numerically on several examples borrowed from the recent literature.

5.4. Uniformly accurate time-splitting schemes for NLS in the semiclassical limit

In [42], we construct new numerical methods for the nonlinear Schrödinger equation in the semiclassical limit. We introduce time-splitting schemes for a phase-amplitude reformulation of the equation where the dimensionless Planck constant is not a singular parameter anymore. Our methods have an accuracy which is spectral in space, of second or fourth-order in time, and independent of the Planck constant before the formation of caustics. The scheme of second-order preserves exactly the L^2 norm of the solution, as the flow of the nonlinear Schrödinger equation does. In passing, we introduce a new time-splitting method for the eikonal equation, whose precision is spectral in space and of second or fourth-order in time.

5.5. Gyroaverage operator for a polar mesh

In [33], we are concerned with numerical approximation of the gyroaverage operators arising in plasma physics to take into account the effects of the finite Larmor radius corrections. This work extended a previous approach to polar geometries. A direct method is proposed in the space configuration which consists in integrating on the gyrocircles using interpolation operator (Hermite or cubic splines). Numerical comparisons with a standard method based on a Padé approximation are performed: (i) with analytical solutions, (ii) considering the 4D drift-kinetic model with one Larmor radius and (iii) on the classical linear DIII-D benchmark case. In particular, we show that in the context of a drift-kinetic simulation, the proposed method has similar computational cost as the standard method and its precision is independent of the radius.

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

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

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

In [44], we propose some numerical schemes for linear kinetic equations in the diffusion and anomalous diffusion limit. When the equilibrium distribution function is a Maxwellian distribution, it is well known that for an appropriate time scale, the small mean free path limit gives rise to a diffusion type equation. However, when a heavy-tailed distribution is considered, another time scale is required and the small mean free path limit leads to a fractional anomalous diffusion equation. Our aim is to develop numerical schemes for the original kinetic model which works for the different regimes, without being restricted by stability conditions of standard explicit time integrators. First, we propose some numerical schemes for the diffusion asymptotics; then, their extension to the anomalous diffusion limit is studied. In this case, it is crucial to capture the effect of the large velocities of the heavy-tailed equilibrium, so that some important transformations of the schemes derived for the diffusion asymptotics are needed. As a result, we obtain numerical schemes which enjoy the Asymptotic Preserving property in the anomalous diffusion limit, that is: they do not suffer from the restriction on the time step and they degenerate towards the fractional diffusion limit when the mean free path goes to zero. We also numerically investigate the uniform accuracy and construct a class of numerical schemes satisfying this property. Finally, the efficiency of the different numerical schemes is shown through numerical experiments.

5.8. Comparison of numerical solvers for anisotropic diffusion equations arising in plasma physics

In [25], we are concentrated to the comparison of numerical schemes to approximate anisotropic diffusion problems arising in tokamak plasma physics. We focus on the spatial approximation by using finite volume method and on the time discretization. This latter point is delicate since the use of explicit integrators leads to a severe restriction on the time step. Then, implicit and semi-implicit schemes are coupled to finite volumes space discretization and are compared for some classical problems relevant for magnetically confined plasmas.

It appears that the semi-implicit approaches (using ARK methods or directional splitting) turn out to be the most efficient on the numerical results, especially when nonlinear problems are studied on refined meshes, using high order methods in space.

5.9. Hamiltonian splitting for the Vlasov-Maxwell equations

In [23], a new splitting is proposed for solving the Vlasov-Maxwell system. This splitting is based on a decomposition of the Hamiltonian of the Vlasov–Maxwell system and allows for the construction of arbitrary high order methods by composition (independent of the specific deterministic method used for the discretization of the phase space). Moreover, we show that for a spectral method in space this scheme satisfies Poisson's equation without explicitly solving it. Finally, we present some examples in the context of the time evolution of an electromagnetic plasma instability which emphasizes the excellent behavior of the new splitting compared to methods from the literature.

5.10. Multiscale numerical schemes for kinetic equations in the anomalous diffusion limit

In [24], we construct numerical schemes to solve kinetic equations with anomalous diffusion scaling. When the equilibrium is heavy-tailed or when the collision frequency degenerates for small velocities, an appropriate scaling should be made and the limit model is the so-called anomalous or fractional diffusion model. Our first scheme is based on a suitable micro-macro decomposition of the distribution function whereas our second scheme relies on a Duhamel formulation of the kinetic equation. Both are Asymptotic Preserving (AP): they are consistent with the kinetic equation for all fixed value of the scaling parameter $\varepsilon > 0$ and degenerate into a consistent scheme solving the asymptotic model when epsilon tends to 0. The second scheme enjoys the stronger property of being uniformly accurate (UA) with respect to epsilon. The usual AP schemes known for the classical diffusion limit cannot be directly applied to the context of anomalous diffusion scaling, since they are not able to capture the important effects of large and small velocities. We present numerical tests to highlight the efficiency of our schemes.

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

In [40], we consider the Vlasov-Poisson equation in a Hamiltonian framework and derive new time splitting methods based on the decomposition of the Hamiltonian functional between the kinetic and electric energy. Assuming smoothness of the solutions, we study the order conditions of such methods. It appears that these conditions are of Runge-Kutta-Nyström type. In the one dimensional case, the order conditions can be further simplified, and efficient methods of order 6 with a reduced number of stages can be constructed. In the general case, high-order methods can also be constructed using explicit computations of commutators. Numerical results are performed and show the benefit of using high-order splitting schemes in that context. Complete and self-contained proofs of convergence results and rigorous error estimates are also given.

5.12. Asymptotic Preserving numerical schemes for multiscale parabolic problems

In [45], we consider a class of multiscale parabolic problems with diffusion coefficients oscillating in space at a possibly small scale ε. Numerical homogenization methods are popular for such problems, because they capture efficiently the asymptotic behaviour as $\varepsilon \to 0$, without using a dramatically fine spatial discretization at the scale of the fast oscillations. However, known such homogenization schemes are in general not accurate for both the highly oscillatory regime $\varepsilon \to 0$ and the non oscillatory regime $\varepsilon \to 1$. In this paper, we introduce an Asymptotic Preserving method based on an exact micro-macro decomposition of the solution which remains consistent for both regimes.

5.13. Parallelization of an advection-diffusion problem arising in edge plasma physics using hybrid MPI/OpenMP programming

In [35], we present a hybrid MPI/OpenMP parallelization strategy for an advection-diffusion problem, arising in a scientific application simulating tokamak's edge plasma physics. This problem is the hotspot of the system of equations numerically solved by the application. As this part of the code is memory-bandwidth limited, we show the benefit of a parallel approach that increases the aggregated memory bandwidth in using multiple computing nodes. In addition, we designed some algorithms to limit the additional cost, induced by the needed extra inter nodal communications. The proposed solution allows to achieve good scalings on several nodes and to observe 70% of relative efficiency on 512 cores. Also, the hybrid parallelization allows to consider larger domain sizes, unreachable on a single computing node.

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

In [43], which is the continuation of [44], we propose numerical schemes for linear kinetic equation which are able to deal with the fractional diffusion limit. When the collision frequency degenerates for small velocities it is known that for an appropriate time scale, the small mean free path limit leads to an anomalous diffusion equation. From a numerical point of view, this degeneracy gives rise to an additional stiffness that must be treated in a suitable way to avoid a prohibitive computational cost. Our aim is therefore to construct a class of numerical schemes which are able to undertake these stiffness. This means that the numerical schemes are able to capture the effect of small velocities in the small mean free path limit with a fixed set of numerical parameters. Various numerical tests are performed to illustrate the efficiency of our methods in this context.

5.15. Analysis of the Monte-Carlo error in a hybrid semi-Lagrangian scheme

In [17] we consider Monte-Carlo discretizations of partial differential equations based on a combination of semi-lagrangian schemes and probabilistic representations of the solutions. The goal of this paper is twofold. First we give rigorous convergence estimates for our algorithm: In a simple setting, we show that under an anti-CFL condition on the time-step δt and on the mesh size δx and for a reasonably large number of independent realizations N, we control the Monte-Carlo error by a term of order $\mathcal{O}(\sqrt{\delta t/N})$. Then, we show various applications of the numerical method in very general situations (nonlinear, different boundary conditions, higher dimension) and numerical examples showing that the theoretical bound obtained in the simple case seems to persist in more complex situations.

5.16. Resonant time steps and instabilities in the numerical integration of Schrödinger equations

In [30], we consider the linear and non linear cubic Schrödinger equations with periodic boundary conditions, and their approximations by splitting methods. We prove that for a dense set of arbitrary small time steps, there exists numerical solutions leading to strong numerical instabilities preventing the energy conservation and regularity bounds obtained for the exact solution. We analyze rigorously these instabilities in the semi-discrete and fully discrete cases.

5.17. Collisions of almost parallel vortex filaments

In [38], we investigate the occurrence of collisions in the evolution of vortex filaments through a system introduced by Klein, Majda and Damodaran, and by Zakharov. We first establish rigorously the existence of a pair of almost parallel vortex filaments, with opposite circulation, colliding at some point in finite time. The collision mechanism is based on the one of the self-similar solutions of the model, described in our previous work. In the second part of this paper we extend this construction to the case of an arbitrary number of filaments, with polygonal symmetry, that are perturbations of a configuration of parallel vortex filaments forming a polygon, with or without its center, rotating with constant angular velocity.

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

In [49] we consider time discretizations of the Vlasov-HMF (Hamiltonian Mean-Field) equation based on splitting methods between the linear and non-linear parts. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that the numerical solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping. Moreover, we prove that the modified state is close to the continuous one and provide error estimates with respect to the time stepsize.

5.19. A kinetic model for the transport of electrons in a graphen layer

In [50], a kinetic model for the transport of electrons in graphene is derived with the tools of semiclassical analysis. The underlying quantum model is a massless Dirac equation, whose eigenvalues display a conical singularity responsible for non adiabatic transitions between the two modes. Our kinetic model takes the form of two Boltzmann equations coupled by a collision operator modeling these transitions. This collision term includes a Landau-Zener transfer term and a jump operator whose presence is essential in order to ensure a good energy conservation during the transitions. We propose an algorithmic realization of the semi-group solving the kinetic model, by a particle method. In the last section, a series of numerical experiments are given in order to study the influences of the various sources of errors between the quantum and the kinetic models.

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

In [39], we study dimension reduction for the three-dimensional Gross-Pitaevskii equation with a long-range and anisotropic dipole-dipole interaction modeling dipolar Bose-Einstein condensation in a strong interaction regime. The cases of disk shaped condensates (confinement from dimension three to dimension two) and cigar shaped condensates (confinement to dimension one) are analyzed. In both cases, the analysis combines averaging tools and semiclassical techniques. Asymptotic models are derived, with rates of convergence in terms of two small dimensionless parameters characterizing the strength of the confinement and the strength of the interaction between atoms.

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

The "interaction picture" (IP) method studied in [13] is a very promising alternative to Split-Step methods for solving certain type of partial differential equations such as the nonlinear Schrödinger equation used in the simulation of wave propagation in optical fibers. The method exhibits interesting convergence properties and is likely to provide more accurate numerical results than cost comparable Split-Step methods such as the Symmetric Split-Step method. In this work we investigate in detail the numerical properties of the IP method and carry out a precise comparison between the IP method and the Symmetric Split-Step method.

5.22. Nonlinear stability criteria for the HMF Model

In [52], we study the nonlinear stability of a large class of inhomogeneous steady state solutions to the Hamiltonian Mean Field (HMF) model. Under a simple criterion, we prove the nonlinear stability of steady states which are decreasing functions of the microscopic energy. To achieve this task, we extend to this context the strategy based on generalized rearrangement techniques which was developed recently for the gravitational Vlasov-Poisson equation. Explicit stability inequalities are established and our analysis is able to treat non compactly supported steady states to HMF, which are physically relevant in this context but induces additional difficulties, compared to the Vlasov-Poisson system.

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

In [54], we consider the three-dimensional time-dependent Gross-Pitaevskii equation arising in the description of rotating Bose-Einstein condensates and study the corresponding scaling limit of strongly anisotropic confinement potentials. The resulting effective equations in one or two spatial dimensions, respectively, are rigorously obtained as special cases of an averaged three dimensional limit model. In the particular case where the rotation axis is not parallel to the strongly confining direction the resulting limiting model(s) include a negative, and thus, purely repulsive quadratic potential, which is not present in the original equation and which can be seen as an effective centrifugal force counteracting the confinement.

5.24. Dimension reduction for anisotropic Bose-Einstein condensates in the strong interaction regime

In [14], we study the problem of dimension reduction for the three dimensional Gross-Pitaevskii equation (GPE) describing a Bose-Einstein condensate confined in a strongly anisotropic harmonic trap. Since the gas is assumed to be in a strong interaction regime, we have to analyze two combined singular limits: a semi-classical limit in the transport direction and the strong partial confinement limit in the transversal direction. We prove that both limits commute together and we provide convergence rates. The by-products of this work are approximated models in reduced dimension for the GPE, with a priori estimates of the approximation errors.

5.25. Models of dark matter halos based on statistical mechanics: I. The classical King model

In [22], we consider the possibility that dark matter halos are described by the Fermi-Dirac distribution at finite temperature. This is the case if dark matter is a self-gravitating quantum gas made of massive neutrinos at statistical equilibrium. This is also the case if dark matter can be treated as a self-gravitating collisionless gas experiencing Lynden-Bell's type of violent relaxation. In order to avoid the infinite mass problem and carry out a rigorous stability analysis, we consider the fermionic King model. In this paper, we study the non-degenerate limit leading to the classical King model. This model was initially introduced to describe globular clusters. We propose to apply it also to large dark matter halos where quantum effects are negligible. We determine the caloric curve and study the thermodynamical stability of the different configurations. Equilibrium states exist only above a critical energy E_c in the microcanonical ensemble and only above a critical temperature T_c in the canonical ensemble.

5.26. Numerical study of a quantum-diffusive spin model for two-dimensional electron gases

In [15], we investigate the time evolution of spin densities in a two-dimensional electron gas subjected to Rashba spin-orbit coupling on the basis of the quantum drift-diffusive model. This model assumes the electrons to be in a quantum equilibrium state in the form of a Maxwellian operator. The resulting quantum drift-diffusion equations for spin-up and spin-down densities are coupled in a non-local manner via two spin chemical potentials (Lagrange multipliers) and via off-diagonal elements of the equilibrium spin density and spin current matrices, respectively. We present two space-time discretizations of the model, one semi-implicit and one explicit, which comprise also the Poisson equation in order to account for electron-electron interactions. In a first step pure time discretization is applied in order to prove the well-posedness of the two schemes, both of which are based on a functional formalism to treat the non-local relations between spin densities. We then use the fully space-time discrete schemes to simulate the time evolution of a Rashba electron gas confined in a bounded domain and subjected to spin-dependent external potentials. Finite difference approximations are first order in time and second order in space. The discrete functionals introduced are minimized with the help of a conjugate gradient-based algorithm, where the Newton method is applied in

order to find the respective line minima. The numerical convergence in the long-time limit of a Gaussian initial condition towards the solution of the corresponding stationary Schrödinger- Poisson problem is demonstrated for different values of the numerical parameters. Moreover, the performances of the semi-implicit and the explicit scheme are compared.

5.27. Numerical analysis of the nonlinear Schrödinger equation with white noise dispersion

In [16], we focus to the numerical study of a nonlinear Schrödinger equation in which the coefficient in front of the group velocity dispersion is multiplied by a real valued Gaussian white noise. We first perform the numerical analysis of a semi-discrete Crank-Nicolson scheme in the case when the continuous equation possesses a unique global solution. We prove that the strong order of convergence in probability is equal to one in this case. In a second step, we numerically investigate, in space dimension one, the behavior of the solutions of the equation for different power nonlinearities, corresponding to subcritical, critical or supercritical nonlinearities in the deterministic case. Numerical evidence of a change in the critical power due to the presence of the noise is pointed out.

5.28. A regularity result for quasilinear stochastic partial differential equations of parabolic type

In [27], we consider a quasilinear parabolic stochastic partial differential equation driven by a multiplicative noise and study regularity properties of its weak solution satisfying classical a priori estimates. In particular, we determine conditions on coefficients and initial data under which the weak solution is Hölder continuous in time and possesses spatial regularity that is only limited by the regularity of the given data. Our proof is based on an efficient method of increasing regularity: the solution is rewritten as the sum of two processes, one solves a linear parabolic SPDE with the same noise term as the original model problem whereas the other solves a linear parabolic PDE with random coefficients. This way, the required regularity can be achieved by repeatedly making use of known techniques for stochastic convolutions and deterministic PDEs.

5.29. Diffusion limit for the radiative transfer equation perturbed by a Wiener process

The aim of [28] is the rigorous derivation of a stochastic non-linear diffusion equation from a radiative transfer equation perturbed with a random noise. The proof of the convergence relies on a formal Hilbert expansion and the estimation of the remainder. The Hilbert expansion has to be done up to order 3 to overcome some difficulties caused by the random noise.

5.30. Invariant measure of scalar first-order conservation laws with stochastic forcing

In [29], under an hypothesis of non-degeneracy of the flux, we study the long-time behaviour of periodic scalar first-order conservation laws with stochastic forcing in any space dimension. For sub-cubic fluxes, we show the existence of an invariant measure. Moreover for sub-quadratic fluxes we show uniqueness and ergodicity of the invariant measure. Also, since this invariant measure is supported by L^p for some p small, we are led to generalize to the stochastic case the theory of L^1 solutions developed by Chen and Perthame in 2003.

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

In [46], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove an integral inequality for the invariant measure ν of a stochastic reaction-diffusion equation. Then we discuss some consequences as an integration by parts formula which extends to ν a basic identity of the Malliavin Calculus. Finally, we prove the existence of a surface measure for a ball and a half-space of H.

5.32. Estimate for P_tD for the stochastic Burgers equation

In [47], we consider the Burgers equation on $H = L^2(0,1)$ perturbed by white noise and the corresponding transition semigroup P_t. We prove a new formula for P_tD_φ (where $\varphi : H \to \mathbb{R}$ is bounded and Borel) which depends on φ but not on its derivative. Then we deduce some new consequences for the invariant measure ν of P_t as its Fomin differentiability and an integration by parts formula which generalises the classical one for gaussian measures.

5.33. Existence of the Fomin derivative of the invariant measure of a stochastic reaction-diffusion equation

In [48], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove existence of the Fomin derivative of the corresponding transition semigroup P_t. The main tool is a new estimate for $P_tD\varphi$ in terms of $\|\varphi\|_{L^2(H,\nu)}$, where ν is the invariant measure of P_t.

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

In [19], we study the following problem. For a large class of models involving several species competing for a single resource in a *homogeneous* environment, it is known that the competitive exclusion principle holds: only one species survives eventually. Various works indicate though that coexistence of many species is possible when the competition occurs in a *heterogeneous* environment. We propose here a spatially heterogeneous system modeling several species competing for a single resource, and migrating in the spatial domain. For this model, it is known, at least in particular cases, that if migrations are *slow* enough, then coexistence occurs. In this paper we show at variance that if the spatial migrations are *fast* enough, then our system can be approximated by a spatially homogeneous system, called aggregated model, which can be explicitly computed, and we show that if the competitive exclusion principle holds for the aggregated model, then it holds as well for the original, spatially heterogeneous model. In other words, we show the persistence of the competitive exclusion principle in the spatially heterogeneous situation when migrations are fast. As a consequence, for fast migrations only one species may survive, namely the best competitor *in average*. We last study which is the best competitor *in average* on some examples, and draw some ecological consequences.

5.35. Randomized message-passing test-and-set

In [37] and [34], we present a solution to the well-known Test&Set operation in an asynchronous system prone to process crashes. Test&Set is a synchronization operation that, when invoked by a set of processes, returns yes to a unique process and returns no to all the others. Recently many advances in implementing Test&Set objects have been achieved, however all of them target the shared memory model. In this paper we propose an implementation of a Test&Set object in the message passing model. This implementation can be invoked by any number $p \leq n$ of processes where n is the total number of processes in the system. It has an expected individual step complexity in $O(\log p)$ against an oblivious adversary, and an expected individual message complexity in $O(n)$. The proposed Test&Set object is built atop a new basic building block, called selector, that allows to select a winning group among two groups of processes. We propose a message-passing implementation of the selector whose step complexity is constant. We are not aware of any other implementation of the Test&Set operation in the message passing model.

MATHERIALS Project-Team

6. New Results

6.1. Electronic structure calculations

Participants: Eric Cancès, Virginie Ehrlacher, David Gontier, Claude Le Bris, Gabriel Stoltz.

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

E. Cancès and N. Mourad have clarified the mathematical framework underlying the construction of norm-conserving semilocal pseudopotentials for Kohn-Sham models, and have proved the existence of optimal pseudopotentials for a family of optimality criteria [34].

E. Cancès and R. Scott (University of Chicago) have examined a technique of Slater and Kirkwood which provides an exact resolution of the asymptotic behavior of the van der Waals attraction between two hydrogen atoms. They have modified their technique to make the problem more tractable analytically and more easily solvable by numerical methods [35].

In [33], E. Cancès, D. Gontier and G. Stoltz analyze the GW method for finite electronic systems. This method allows to compute excited states. To understand it, a first step is to provide a mathematical framework for the usual one-body operators that appear naturally in many-body perturbation theory. It is then possible to study the GW equations which construct an approximation of the one-body Green's function, and give a rigorous mathematical formulation of these equations. With this framework, results can be established for the well-posedness of the GW_0 equations, a specific instance of the GW model. In particular, the existence of a unique solution to these equations is proved in a perturbative regime.

D. Gontier extended his last-year result on N-representability by including the characterization of representable paramagnetic currents [42]. Together with Salma Lahbabi (former student of E. Cancès, University Hassan II Casablanca, ENSEM), he proved the exponential convergence rates of the uniform sampling of the Brillouin zone for the calculation of crystalline structure properties, in linear and nonlinear settings [43].

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

E. Cancès has pursued his long-term collaboration with Y. Maday (Paris 6) on the numerical analysis of electronic structure models. Together with G. Dusson (Paris 6), B. Stamm (Paris 6), and M. Vohralík (Inria), they have designed a new postprocessing method for planewave discretizations of nonlinear Schrödinger equations, and used it to compute sharp *a posteriori* error estimators for both the discretization error and the algorithmic error (convergence threshold in the iterations on the nonlinearity). They have then extended this approach to the Kohn-Sham model. In parallel, they have derived a posteriori error estimates for conforming numerical approximations of the Laplace eigenvalue problem with a homogeneous Dirichlet boundary condition [32]. In particular, upper and lower bounds for the first eigenvalue are given. These bounds are guaranteed, fully computable, and converge with the optimal speed to the exact eigenvalue.

Implicit solvation models aim at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous medium accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. In collaboration with F. Lipparini (Paris 6), B. Mennucci (Department of Chemistry, University of Pisa) and J.-P.

Picquemal (Paris 6), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). E. Cancès, Y. Maday, F. Lipparini and B. Stamm have also extended this approach to the more complex polarizable continuum model (PCM).

C. Le Bris, in collaboration with P. Rouchon (École des Mines de Paris) and with J. Roussel, in the context of an internship at École des Ponts, has pursued the study of a new efficient numerical approach, based on a model reduction technique, to simulate high dimensional Lindblad type equations at play in the modelling of open quantum systems. The added value of the most recent contribution with respect to the previous studies lies in two different aspects. First, the rank of the reduced model used as surrogate for the full model can now be dynamically adjusted, in an adaptive strategy. Second, a variance reduction approach based on the technique of control variate has been developed. The noise intrinsically present in the Monte-Carlo simulation of the underlying stochastic dynamics may indeed be reduced by using the deterministic reduced model as control variate. A publication collects these two aspects and reports on the results achieved [19].

6.2. Complex fluids

Participant: Sébastien Boyaval.

The aim of the research performed in the project-team about complex fluids is mainly focused on the mathematical modelling and numerical simulation of i) non-Newtonian rheologies, with application to geophysical fluids such as mudflows, or the solid transport in rivers, and ii) stratified flows, in particular free-surface flows, which naturally occur in the geophysical context under gravity influence.

The need for reduced models is crucial for numerical computations at the large geophysical scale. S. Boyaval has therefore pursued his research about a systematic asymptotic reduction technique for thin-layers of non-Netwonian fluids with a near hydrostatic pressure [11]. On the other hand, accurate numerical simulations (for benchmark purposes at least) require a full 3D model mainly based on Stokes-like equations, and there is a constant need for better computation methods in that field too. With a view to *condensed* high-order approximations of elliptic PDEs like the Stokes equation on generic meshes (obtained by refinement or agglomeration of a simplicial initial mesh), S. Boyaval has participated in a joint work about hybridization of a mixed-dual generic approach [8]. On the hydraulic applications side, the studies initiated at CEMRACS 2013 about a stochastic representation of fluctuations in the transport of river sediments by bed-load have been published [9].

6.3. Homogenization

Participants: Michael Bertin, Ludovic Chamoin, Virginie Ehrlacher, Thomas Hudson, Marc Josien, Claude Le Bris, Frédéric Legoll, Simon Lemaire, François Madiot, William Minvielle.

6.3.1. Deterministic non periodic systems

The homogenization of (deterministic) non periodic systems is a well known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc (Paris 7) and P.-L. Lions (Collège de France), C. Le Bris has introduced a possible theory, giving rise to a numerical approach, for the simulation of multiscale nonperiodic systems. The theoretical considerations are based on earlier works by the same authors (derivation of an algebra of functions appropriate to formalize a theory of homogenization). The numerical endeavor is completely new. The theoretical results obtained to date are being collected in a series of manuscripts that will be available shortly. The publications [30] and [10] specifically address the issues related to a local perturbation of the periodic problem and the challenging, practically relevant problem of interfaces between periodic structures of different nature (the celebrated "twin boundaries" problem in materials science). Some related problems will now be addressed in the context of the PhD thesis of M. Josien.

6.3.2. Stochastic homogenization

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

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

In [47], C. Le Bris, F. Legoll and W. Minvielle have investigated the possibility to use a variance reduction technique based on computing the corrector equation *only for selected environments*. These environments are chosen based on the fact that their statistics in the finite supercell matches the statistics of the materials in the infinite supercell. This method yields an approximation of the homogenized matrix with an error smaller than standard approximations. The efficiency of the approach has been demonstrated for various types of random materials, including composite materials with randomly located inclusions.

In addition, M. Bertin and F. Legoll, in collaboration with S. Brisard (École des Ponts), have investigated the possibility to use the Hashin-Shtrikman bounds as control variables in a control variate approach. The Hashin-Shtrikman bounds are often used in the computational mechanics community as approximations of the homogenized quantities. Our aim is use them to improve the efficiency of the reference computations, somewhat in the spirit of a preconditionner. Preliminary encouraging numerical results have been obtained.

Over the past years, the project-team has proposed several variance reduction techniques, see e.g. [21] for a method using antithetic variables (in a nonlinear context) and [20] for a control variate approach using a surrogate model based on a defect-type theory. These various approaches have been reviewed and compared to one another in [29].

In collaboration with B. Stamm (Paris 6), E. Cancès, V. Ehrlacher and F. Legoll have proposed in [13] a new approach to approximate the homogenized coefficients of a random stationary material. This method is an alternative to that proposed e.g. by A. Bourgeat and A. Piatniski in [Approximations of effective coefficients in stochastic homogenization, Annales de l'Institut Henri Poincaré 40, 2004] which consists in solving a corrector problem on a bounded domain. The method introduced in [13] is based on a new corrector problem, which is posed on the entire space, but which is simpler than the standard corrector problem in that the coefficients of the equation are uniform outside some ball of finite radius. This implies that, in some cases (including the case of randomly located spherical inclusions), this new corrector problem can be recast as an integral equation posed on the surface of the inclusions. The problem can then be efficiently solved via domain decomposition and using spherical harmonics.

6.3.3. Multiscale Finite Element approaches

From a numerical point of view, 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 an accurate enough approximation).

The MsFEM has been introduced more than 10 years ago. However, even in simple deterministic cases, there are still some open questions, for instance concerning multiscale advection-diffusion equations. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interacts with the multiscale character of the equation is an unsolved mathematical question worth considering for numerical purposes. In that spirit, C. Le Bris, F. Legoll and F. Madiot have studied in [46] several variants of the Multiscale Finite Element Method (MsFEM), specifically designed to address multiscale advection-diffusion problems in the convection-dominated regime. Generally speaking, the idea of the MsFEM is to perform a Galerkin approximation of the problem using specific basis functions, that are precomputed (in an offline stage) and adapted to the problem considered. Several possibilities for the basis functions have been examined (for instance, they may or may not encode the convection field). Depending on how basis functions are defined, stabilization techniques (such as SUPG) may be required. Another option to handle such problems is to use a splitting approach, with two legacy codes, one solving a purely diffusive multiscale equation, the other one solving a single scale, convection-dominated advection-diffusion equation. In [46], these various approaches have been compared in terms of accuracy and computational costs.

In the context of the PhD thesis of F. Madiot, current efforts are focused on the study of an advection-diffusion equation with a dominating convection in a *perforated domain*. The multiscale character of the problem here stems from the geometry of the domain. A paramount difference with the case considered in [46] is that boundary layers may appear throughout the domain (i.e. in the neighborhood of each perforation). The accuracy of the numerical approaches in the boundary layers thus becomes critical.

Most of the numerical analysis studies of the MsFEM are focused on obtaining *a priori* error bounds. In collaboration with L. Chamoin, who is currently in delegation in the project-team for the second year (from ENS Cachan, since September 2014), members of the project-team have been working on *a posteriori* error analysis for MsFEM approaches, with the aim to develop 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 do all the expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach thus needs to be adapted to that context, in order to keep that feature that makes it adapted to a multiscale, multi-query context. The proposed approach yields very interesting results, and provide an accurate and robust estimation of the global error.

Current efforts are targeted towards the design of adaptive algorithms for specific quantities of interest (in the so-called "goal-oriented" setting), and the design of model reduction approaches (such as the Proper Generalized Decomposition, or PGD) in the specific context of multiscale problems.

6.3.4. Coarse approximation of an elliptic problem with oscillatory coefficients

Still another question investigated in the project-team is to find an alternative to standard homogenization techniques when the latter are difficult to use in practice. Consider a linear elliptic equation, say in divergence form, with a highly oscillatory matrix coefficient, and assume that this problem is to be solved for a large number of right-hand sides. If the coefficient oscillations are infinitely rapid, the solution can be accurately approximated by the solution to the homogenized problem, where the homogenized coefficient has been evaluated beforehand by solving the corrector problem. If the oscillations are moderately rapid, one can think instead of MsFEM-type approaches to approximate the solution to the reference problem. However, in both cases, the complete knowledge of the oscillatory matrix coefficient is required, either to build the average model or to compute the multiscale basis. In many practical cases, this coefficient is often only partially known, or merely completely unavailable, and one only has access to the solution of the equation for some loadings. This observation has led to think about alternative methods, in the following spirit. Is it possible to approximate the reference solution by the solution to a problem with a *constant* matrix coefficient? How can this "best" constant matrix approximating the oscillatory problem be constructed in an efficient manner?

A preliminary step, following discussion and interaction with A. Cohen (Paris 6), has been to cast the problem as a convex optimization problem. We have then shown that the "best" constant matrix defined as the solution of that problem converges to the homogenized matrix in the limit of infinitely rapidly oscillatory coefficients. Furthermore, the optimization problem being convex, it can be efficiently solved using standard algorithms. C. Le Bris, F. Legoll and S. Lemaire have comprehensively explored that problem. The algorithm can be made very efficient, and it yields accurate approximation of the homogenized matrix. We have also shown that it is possible to construct, in a second stage, approximations to the correctors, in order to recover an approximation of the *gradient* of the solution.

6.3.5. Optimization of a material microstructure

A project involving V. Ehrlacher and F. Legoll, in collaboration with G. Leugering and M. Stingl (Cluster of Excellence, Erlangen-Nuremberg University), aims at optimizing the shape of some materials (modeled as structurally graded linear elastic materials) in order to achieve the best mechanical response at the minimal cost. As is often the case in shape optimization, the solution tends to be highly oscillatory, hence the need for homogenization techniques. Materials under consideration are being thought of as microstructured materials composed of steel and void and whose microstructure patterns are constructed as the macroscopic deformation

of a reference periodic microstructure. The optimal material (i.e. the best macroscopic deformation) is the deformation achieving the best mechanical response.

For a given deformation, one can first compute the mechanical response using a *homogenized model*. This is the first variant that has been followed. Model reduction techniques are then required, in order to expedite the resolution of the corrector problem needed to identify the homogenized coefficient at each loop of the optimization algorithm. In that context, a PGD-type approach has been proposed.

A second variant is to compute the mechanical response at the *microscale*, using the highly oscillatory model. Preliminary results have been obtained. Current efforts are focused towards choosing an appropriate model reduction strategy.

6.3.6. Discrete systems and their thermodynamic limit

We conclude this section by describing works of the project-team on discrete models with highly oscillatory coefficients.

Dislocations are geometric line defects which interact via long-range stress fields in crystalline solids. In [45], T. Hudson has studied the thermally-driven motion of dislocations in a discrete Monte Carlo model, showing that over long observation times at low temperature in a large body, the most probable trajectory of straight dislocation lines lie close to the solution of an explicit deterministic evolution equation.

Another work is related to the understanding of the origin of hysteresis in rubber-made materials. When submitted to cyclic deformations, the strain-stress curve of these materials indeed shows a hysteresis behavior, which seems to be independent of the speed of loading. Some years ago, members of the project-team have suggested a model, at a mesoscale, to explain this behavior. This model was written in terms of a system made of a finite number of particles. F. Legoll, T. Lelièvre and T. Hudson are currently studying whether a thermodynamic limit of the model previously proposed can be identified. In order to simplify the setting, the reference discrete model has been replaced by a continuum model with highly oscillatory coefficients. This model is nonlinear and time-dependent. The question is now to identify (e.g. using two-scale convergence arguments) its homogenized limit, first in a periodic setting, second in a stochastic setting.

6.4. Computational Statistical Physics

Participants: Giacomo Di Gesù, Thomas Hudson, Dorian Le Peutrec, Frédéric Legoll, Tony Lelièvre, Antoine Levitt, Boris Nectoux, Julien Roussel, Mathias Rousset, Gabriel Stoltz, Pierre Terrier, Pierre-André Zitt.

The work of the project-team in this area is concentrated on two new directions: the sampling of reactive trajectories (where rare events dictate the dynamics of the system), and the computation of average properties of nonequilibrium systems (which complements the more traditional field of techniques to compute free energy differences).

6.4.1. Sampling of reactive trajectories

Finding trajectories for which the system undergoes a significant change is a challenging task since the transition events are typically very rare. Several methods have been proposed in the physics and chemistry literature, and members of the project-team have undertaken their study in the past years.

A first class of techniques are the accelerated dynamics introduced by A. Voter (Los Alamos National Lab) and his collaborators. A short review on the mathematical analysis of these dynamics was written by T. Lelièvre, see [48]. In [23], T. Lelièvre and F. Nier (Paris 13) analyze the low temperature asymptotics for Quasi-Stationary Distributions in a bounded domain. The objective of this analysis is to justify mathematically the validity of hyperdynamics.

Another class of techniques to compute reactive trajectories is based on splitting techniques. After the first result obtained in [12], C.E. Bréhier, T. Lelièvre and M. Rousset pursued their analysis of the Adaptive Multilevel Splitting algorithm, which is a rare event simulation method. In [31], a generalization of the method is proposed, and it is shown how to make the estimator unbiased in a discrete-in-time setting (which is generically the setting encountered in practice). Numerical experiments illustrate the performance of the method.

6.4.2. Nonequilibrium systems and non-reversible dynamics

In [38], T. Lelièvre has studied with A. Duncan and G.A. Pavliotis nonreversible diffusion processes to sample a probability measure. It is shown that nonreversible dynamics are always better in terms of the asymptotic variance (statistical error), but the efficiency of the whole algorithm sensitively depends on the time discretization algorithm, which may induce some bias (deterministic error).

T. Lelièvre together with R. Assaraf, B. Jourdain and R. Roux, have analyzed in [27] the validity of non equilibrium molecular dynamics techniques to compute the derivative of an observable with respect to a parameter-dependent probability measure. The probability measure is defined as the stationary state of a non-reversible stochastic dynamics (in particular no analytical formula for this measure is available). Such computations are at the basis of the numerical approximation of transport coefficients in molecular dynamics.

6.4.3. Numerical analysis of simulation techniques

In [44], G. Stoltz, together with A.-A. Homman (École des Ponts) and J.-B. Maillet (CEA/DAM), present new parallelizable numerical schemes for the integration of Dissipative Particle Dynamics with Energy conservation. So far, no numerical scheme was able to correctly preserve the energy over long times and give rise to small errors on average properties for moderately small timesteps, while being straightforwardly parallelizable. Two new methods are proposed, both of them straightforwardly parallelizable, and allowing to correctly preserve the total energy of the system. The accuracy and performance of these new schemes are illustrated both on equilibrium and nonequilibrium parallel simulations.

The discretization of overdamped Langevin dynamics, through schemes such as the Euler-Maruyama method, may lead to numerical methods which are unstable when the forces are non-globally Lipschitz. One way to stabilize numerical schemes is to superimpose some acceptance/rejection rule, based on a Metropolis-Hastings criterion for instance. However, rejections perturb the dynamical consistency of the resulting numerical method with the reference dynamics. G. Stoltz and M. Fathi (Berkeley) present in [40] some modifications of the standard stabilization of discretizations of overdamped Langevin dynamics by a Metropolis-Hastings procedure, which allow to either improve the strong order of the numerical method, or to decrease the bias in the estimation of transport coefficients characterizing the effective dynamical behavior of the dynamics. The latter approach relies on modified numerical schemes together with a Barker rule for the stabilization.

A. Levitt, in collaboration with C. Ortner (University of Warwick), has worked on the numerical analysis of saddle point search, an important step in the computation of reaction rates. While the convergence theory of minimization algorithms, such as the gradient method, is well-understood and standard, no such theory exists for saddle point algorithms such as the dimer method. Their work reveals a major obstruction to convergence: for some systems, the dimer method can oscillate indefinitely. This shows that there is no Lyapunov function for the associated flow, and highlights the fundamental difference between minimization and saddle search. Further work focuses on improving the reliability and convergence speed of such methods.

6.4.4. Free energy computations

The topic of free energy computations is still a significant research area of the project-team. T. Lelièvre has co-authored a review article [14] on the adaptive biasing force (ABF) method.

In addition, two new results have been obtained on the ABF method by H. Al Rachid (École des Ponts) in collaboration with T. Lelièvre: a numerical result concerning a projected version of the ABF algorithm, which enables to reduce the variance, see [25] ; and a theoretical result on the existence of a solution to the non linear Fokker Planck equation associated to the ABF process, see [49].

T. Lelièvre and G. Stoltz, together with G. Fort (Télécom Paris) and B. Jourdain (École des Ponts), have studied the Self-Healing Umbrella Sampling (SHUS) method in [16]. This method is an adaptive biasing method to compute free energies on the fly by appropriately penalizing already visited regions. The convergence of the method relies on a rewriting as a stochastic approximation method with random steps, and can therefore be seen as a variation of the Wang-Landau method.

6.4.5. Convergence of processes

D. Le Peutrec and G. Di Gesù have studied in [37] the rate of convergence to equilibrium at low temperature of a stochastic interacting large particle system which can be seen as a spatially discrete approximation of the stochastic Allen-Cahn equation on the one-dimensional torus. Upper and lower bounds for the leading term of the associated spectral gap in the small temperature regime are proven, uniformly in the system size. It is also shown that the upper bound is sharp under a suitable control of the growth of the system size by the temperature.

The article [17] by B. Jourdain (École des Ponts), T. Lelièvre and B. Miasojedow (Warsaw) on the mean-field limit for the transient phase of the random walk Metropolis algorithm in the infinite dimension limit has been published in Annals of Applied Probability. In this article, the authors prove that the Metropolis Hastings algorithm converges to a nonlinear stochastic differential equation in the infinite dimensional limit.

6.4.6. Force fields and modeling

In [41], G. Stoltz, together with G. Ferré (École des Ponts) and J.B Maillet (CEA/DAM), has presented a distance between atomic configurations, which is invariant with respect to permutations of the atoms. This distance is defined through a functional representation of atomic positions. It allows to directly compare different atomic environments with an arbitrary number of particles without going through a space of reduced dimensionality (i.e. fingerprints) as an intermediate step. Moreover, this distance is naturally invariant through permutations of atoms and through global rotations. This distance provides an important building block for the construction of accurate force-fields using machine learning techniques.

E. Cancès has contributed to the development of more efficient algorithms for polarizable force field molecular dynamics, which have been implemented and successfully tested on massively parallel computers [18].

During the post-doctoral position of I.G. Tejada, G. Stoltz, F. Legoll and E. Cancès studied in collaboration with L. Brochard (École des Ponts) the derivation of a concurrent coupling technique to model fractures at the atomistic level by combining a reactive potential with a harmonic approximation; see [50].

6.5. Various topics

A. Bakhta (École des Ponts) and V. Ehrlacher [28] have studied a system of PDEs modeling the cross-diffusion of different atomic species in a crystalline solid thin film during a Physical Vapor Deposition process, coupled with the evolution of the domain as external chemical species fluxes are absorbed at the surface of the solid layer. This model leads to a system of degenerate elliptic cross-diffusion equations. They proved the existence of a global weak solution to this system in arbitrary dimension in the case of a constant domain using analysis tools from gradient flow theory. The existence of a global weak solution in a one-dimensional case with external fluxes was also proved. Under the assumption that this solution is unique, the existence of optimal external fluxes in order to achieve desired concentration profiles of the different species in the thickness of the solid layer at the end of the process was also obtained.

Numerical simulations of crystal defects are necessarily restricted to finite computational domains, supplying artificial boundary conditions that emulate the effect of embedding the defect in an effectively infinite crystalline environment. V. Ehrlacher, in a joint work with C. Ortner (U. of Warwick) and A. Shapeev (Skolkovo Institute of Science and Technology) [39] have studied a mathematical framework within which the accuracy of different types of boundary conditions can be precisely assessed.

T. Lelièvre together with F. Casenave (Safran) and A. Ern (École des Ponts) have proposed in the short note [36] an analysis of the Empirical Interpolation Method which highlights the symmetry played by the two variables (parameter and space variable). A variant of the Empirical Interpolation Method is introduced in order to deal with situations where some observations have to be discarded, and the number of observed values is thus different for the two variables.

In collaboration with P.-L. Lions (Collège de France), C. Le Bris has written an extensive set of lecture notes on parabolic equations with irregular data (initial conditions and parameter coefficients). These lecture notes correspond to joint works between the two authors and to an expanded version of the works by P.-L. Lions specifically exposed in his lectures delivered at Collège de France in 2012–2013. The application of the theory to the specific context of stochastic differential equations with irregular coefficients is also examined.

MEMPHIS Team

7. New Results

7.1. Plastic impact of iron on aluminium

A new model for plasticity has been developed this year. An iron projectile is impacting an aluminium plate immersed in air. The initial horizontal velocity of the iron is $1000m.s^{-1}$. The computation is performed on a 2000×1600 mesh with 144 processors. Homogeneous Neumann conditions are imposed on the left and right borders and embedded on the top and bottom.

The results are presented in Fig 6 with a schlieren image (bottom) and the von Mises criteria (top) at different time steps. A log scale is used and the minimum value is fixed to 10^9. We can see that the plate is strongly deformed and form at the end a filament. The projectile is flattened but not as much as in the literature because the yield plastic limit is higher. We see a longitudinal wave propagating in the plate followed by a shear wave that causes the plasticity of the material.

7.2. Air-helium shock-bubble interaction

A three-dimensional hyperelastic model has been developed. It can deal with multi-fluid and solids. Here we show the propagation in air of a Mach 1.22 shock through an helium bubble. The computation is performed on a $1000 \times 400 \times 400$ mesh and lasts for 50h on 300 processors. The zero iso-value of the level set function and schlieren on the horizontal plane through the center of the bubble are presented at different times on Fig. 7 .

7.3. Particles flowing in a fluid

A new type of algorithm is designed to enable contacts efficiently between particles immersed in a fluid by adding a short range repulsive force. The algorithm is derived from the multi geometric deformable model introduced for image segmentation. It can handle multiple deforming bodies and avoid collision using a short range repulsive force depending on the distance to the closest interface. The main advantages of this method is it requires only five fields (three label maps and two distance functions) and one level set function to capture an arbitrary number of cells and it can, at the same time, deal with collisions.

7.4. Inertial Sea Wave Energy Converter (ISWEC)

The ISWEC is a floater and was design by Wave For Energy (http://www.waveforenergy.com) to extract the energy of typical waves in the Mediterranean Sea. The energy is extracted using a mechanical system based on a gyroscope activated by the motion of the floater generated by sea waves. This is a complex system coupling Fluid/Fluid/structure interfaces, computation of the rigid motion of the floater and computation of the power extraction. The problem is solved using in-house numerical solver (NaSCar) developed in MEMPHIS team. The interfaces are tracked using level se functions. The bi fluid interface is computed using Continuous Surface Force method (CSF), the motion of the floater imposed by penalization is computed using the forces and the torques exerted by the flow, and finally this motion activates the gyroscope for power extraction. The gyroscope model was developed by the Politecnico di Torino. Figure 1 shows a numerical simulation of the iswec (see http://www.math.u-bordeaux1.fr/ mbergman/ for a movie)

7.5. Flow with many particles

A version of the code NaSCar has been developed to simulated the flow around particules with high volume fraction (see figure 10). The standard central lubrification forces are used to computed the interaction between spherical particules. Ongoing project will deal with non spherical particules (Lisl Weynans and PhD Baptiste Lambert).

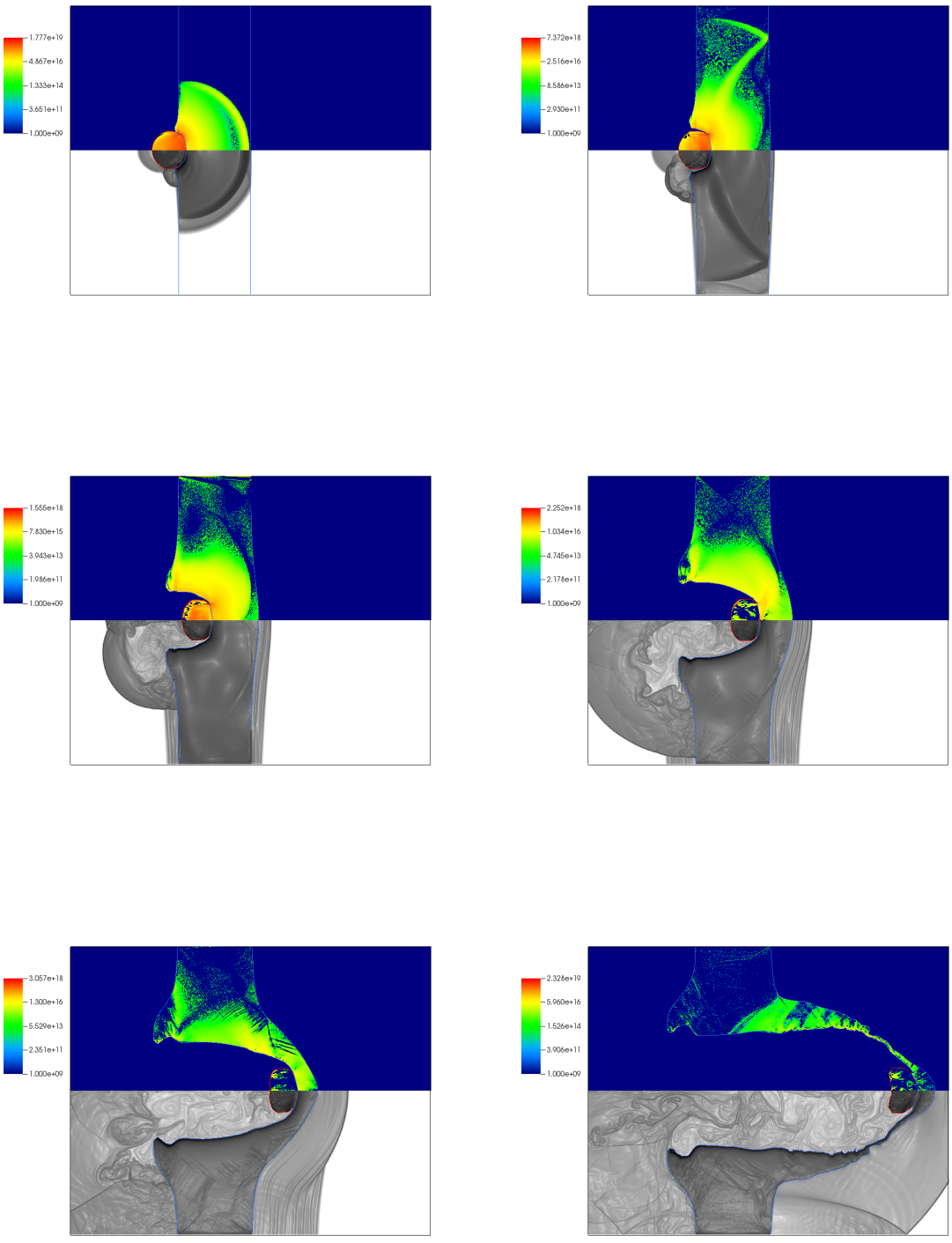


Figure 6. Impact of Iron on Aluminium TC2. Schlieren image and von Mises criteria at $t = 0.03ms$, $0.06ms$, $0.13ms$, $0.26ms$, $0.53ms$ *and* $t = 1.04ms$ *from left to right, top to bottom*

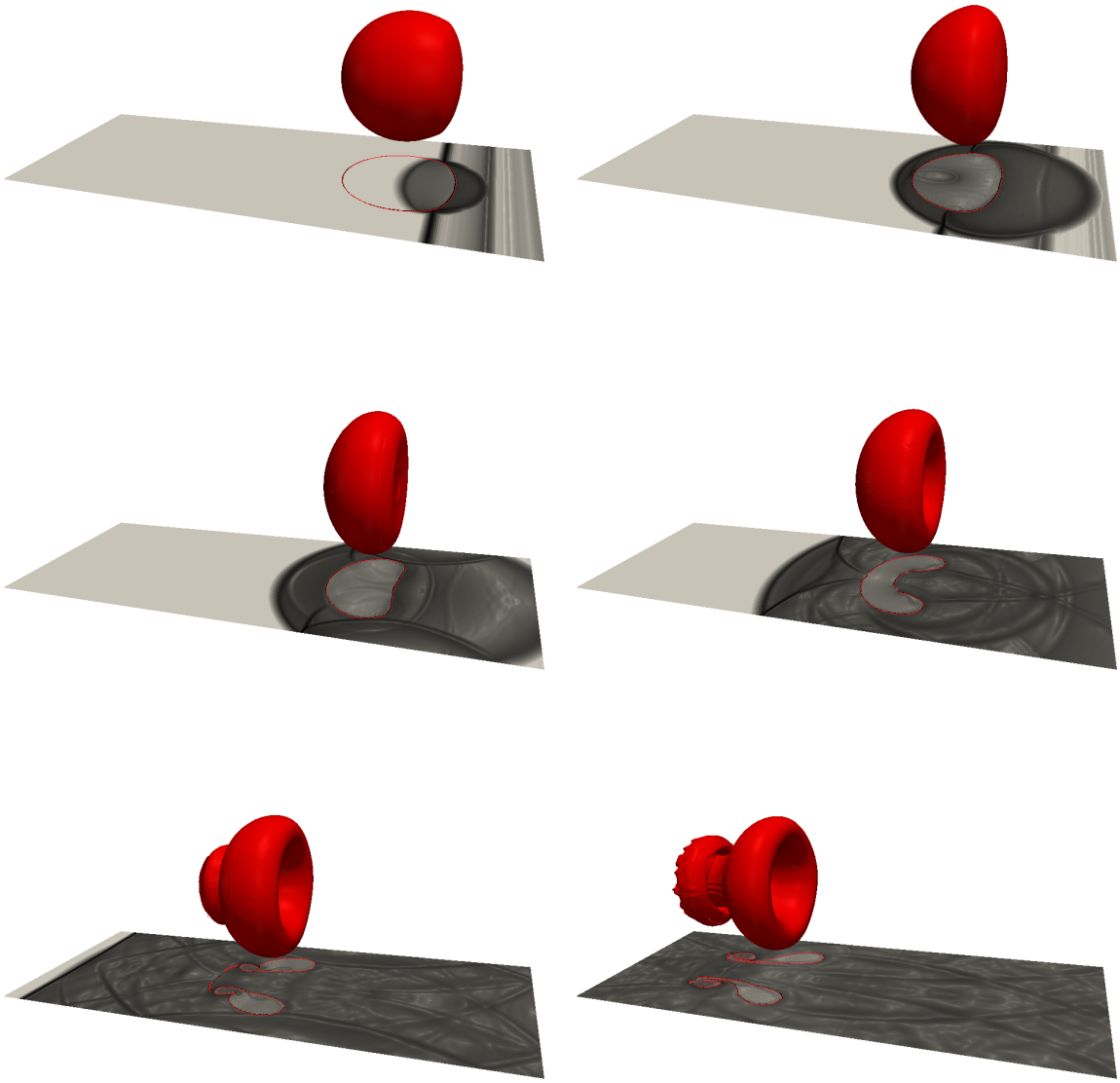


Figure 7. Interaction of a Mach 1.22 shock propagating in air through an helium bubble (TC1). Pictures at $t = 62\mu s,\ 110\mu s,\ 163\mu s,\ 264\mu s,\ 471\mu s,\ 735\mu s$. *From left to right, top to bottom.*

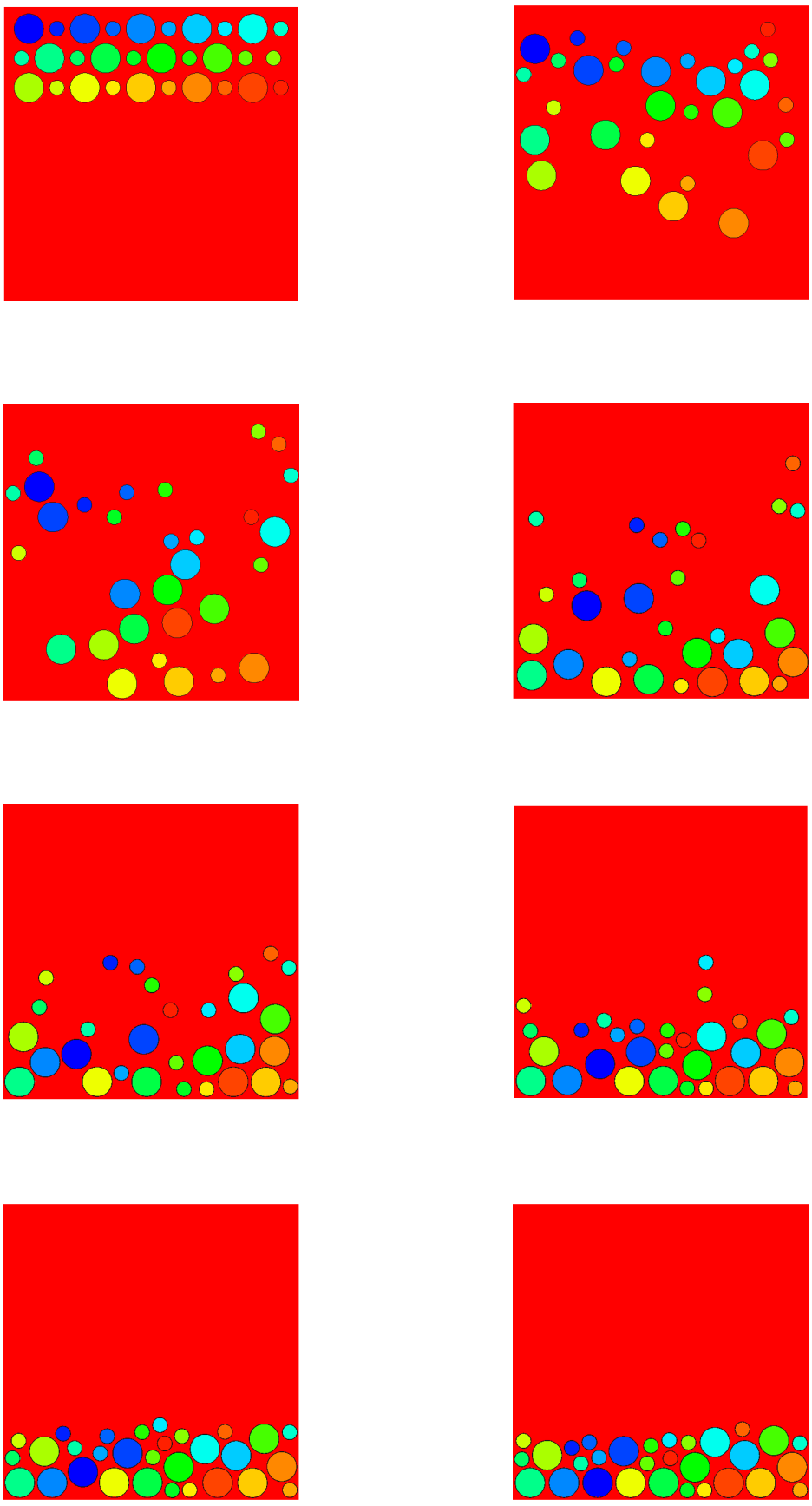


Figure 8. Simulation of 30 rigid bodies of different radii (R = 0.05 or R = 0.025) falling under gravity. The colors indicate the values of the first label map from dark blue for the first body to dark orange for the 30th body and red for the fluid that is the 31st object.

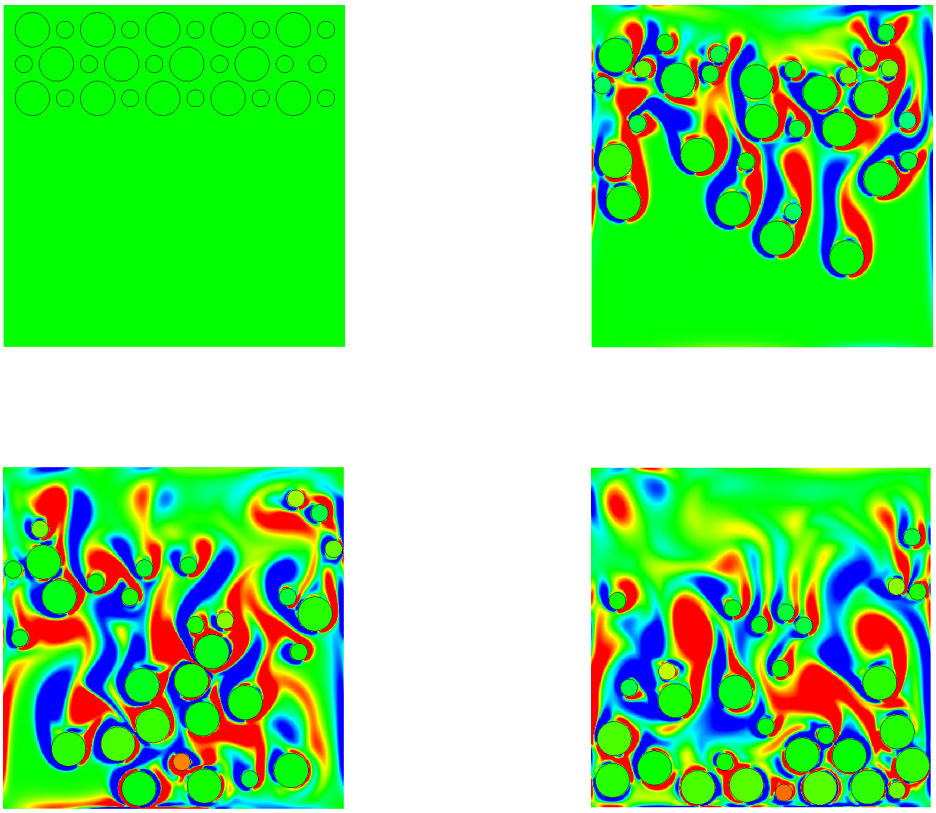


Figure 9. Simulation of 30 rigid bodies of different radii (R = 0.05 or R = 0.025) falling under gravity. The colors indicate the vorticity levels from dark blue for -200 and dark red for 200.

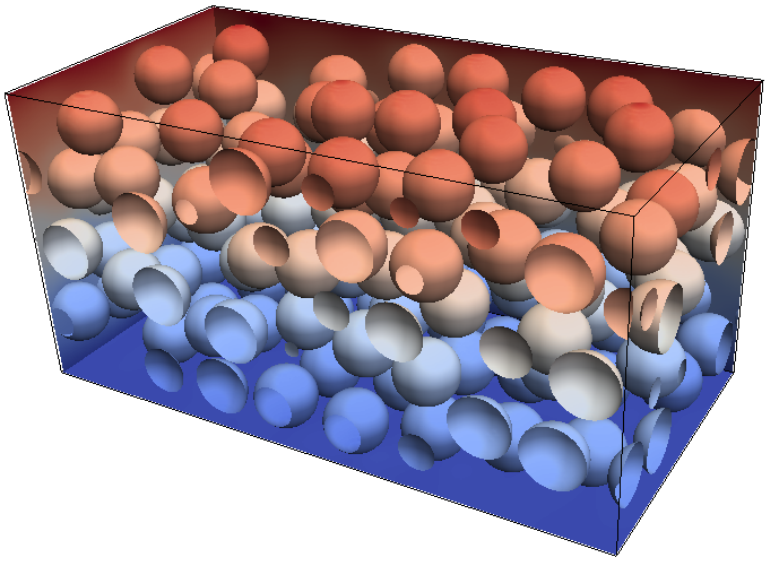


Figure 10. Rheology of a Couette flow with solid particles.

7.6. Overset method

With Valeol (Cifre PhD Claire Morel) we are developing an Overapping grids approach coupling a background cartesian grid with a body fitted grid around wind turbine blades. This method allows us to push away the limit of the numerical simulation on octree grids when small boundary layers play an important role. The generation of overset grids is based on level set functions (post doc AMIES by Franck Luddens). This method has been implemented for two dimensional test cases using the Schwartz method to deal with the domain decomposition. In the same time, we are also building the global operators onto the whole domain, i.e. without Schwartz iterations (PhD Federico Tesser).

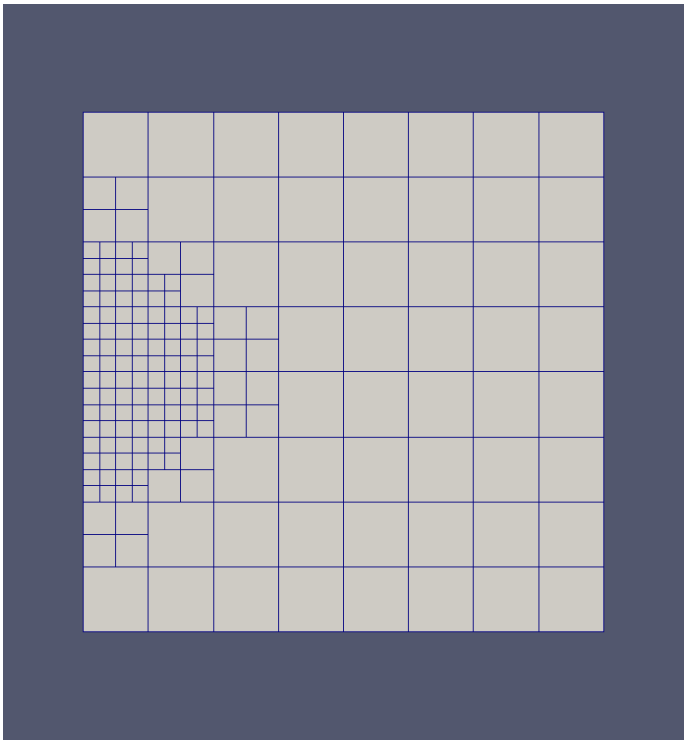
7.7. Electrostrictive materials: modelling and simulation

In this work, a result of the collaboration between physicists, chemists (Annie Colin and Philippe Poulin, CRPP Bordeaux) and applied mathematicians, we deal with mathematical modelling and simulation of electrostrictive materials. These kinds of materials are composed by a polymeric matrix with carbon nanotubes embedded in and this structure gives them interesting electrical properties. Their dielectric constant varies as a function of the mechanical deformation. Housed in a capacitor, they show variable capacity when subjected to vibration and they can generate potential differences from mechanical deformations. Because of their composition, their structure involves different physical scales, from the small nanotube dimension, through the scale of nanotube clusters, to the large dimension of the sample. Our purpose is to provide physicists and chemists with a tool to test in silico several material configurations and to have a deeper insight into the features of these materials, developing numerical models which can predict their steady and unsteady behaviour. We propose to model the physical problem by reducing the nanotubes to dipoles and solving a Gauss equation for the electrical potential equation informed of the presence of nanotubes with zero electrical field conditions on the centres of the nanotubes. We started considering the steady problem, which is interesting for the purpose

of understanding the basic electrical properties of different nanotube configurations and of designing of the material. In order to discretize and simulate the mathematical problem, we chose parallel linear octree-based adaptive meshes and we developed an original hybrid Finite Volume/Finite Difference second-order scheme for 2D and 3D elliptic problems on this kind of mesh. A convergence analysis of the numerical scheme has been developed and validating test cases have been performed. Good qualitative agreement between numerical and real experiments has been observed for the steady model. In the future we aim to quantitatively compare the numerical results and the real material behaviour, to model the unsteady problem and to deal with electrical consequences of mechanical deformations.

7.8. Development of a sharp cartesian method for the simulation of flows with high density ratios

We have developed a sharp cartesian method for the simulation of incompressible flows with high density and viscosity ratios, like air-water interfaces. This method is inspired from a second-order cartesian method for elliptic problems with immersed interfaces (Cisternino-Weynans 2012). A classical predictor-corrector algorithm is used to solve the fluid equations, in a non-incremental version, which means that the guess value for the pressure is zero. This choice avoids instability issues due to the discontinuous pressure values when the interface moves. We take into account the viscous forces by regularizing the density and viscosity values. This approach allows for a more straightforward and robust treatment, and has been proven to provide satisfactory accuracies for high Reynolds numbers. To compute the pressure, it is necessary to solve an elliptic problem. This elliptic problem with discontinuous values across an interface is solved with the second order method cited above. The originality of this method lies in the use of unknowns located at the interface. These interface unknowns are used to discretize the flux jump conditions and the elliptic operator accurately enough to get a second order convergence in maximum norm.



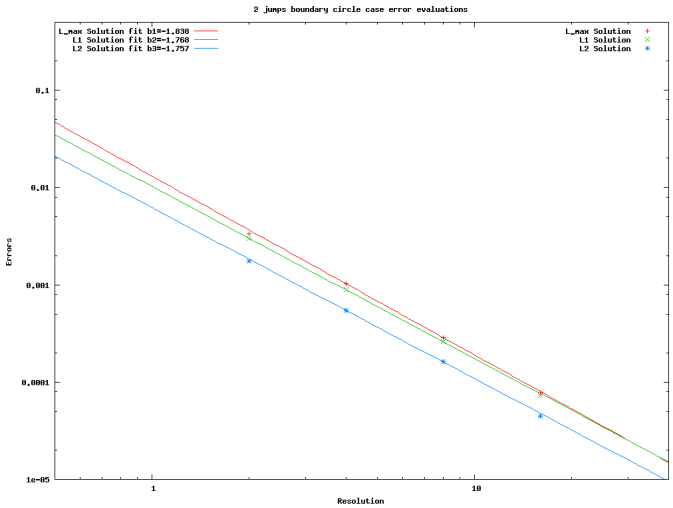


Figure 11. Electrostrictive materials: Mesh and convergence results for the solver.

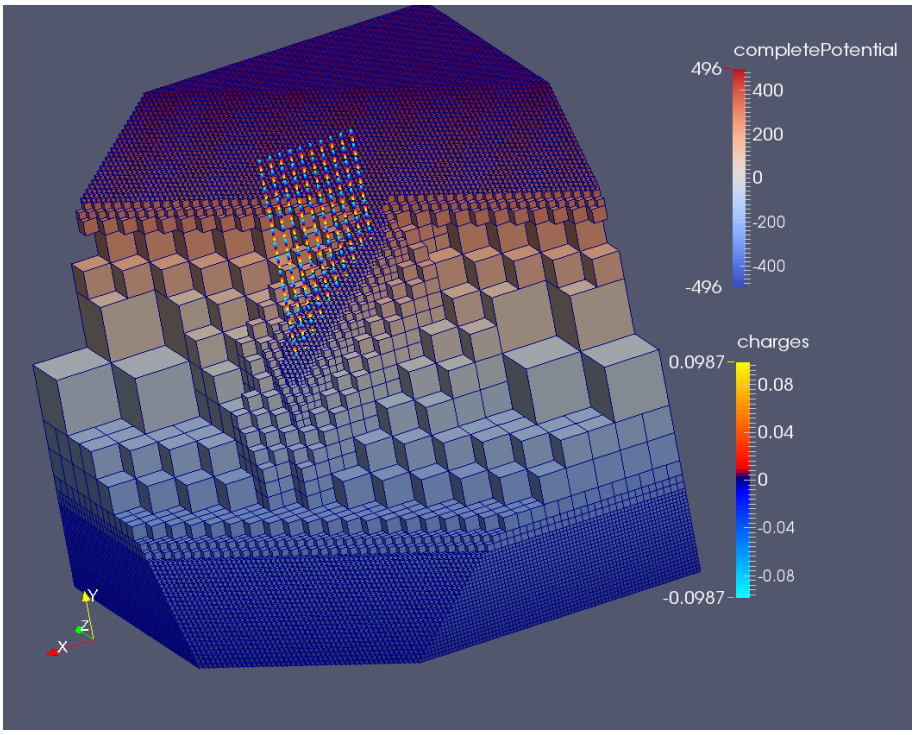


Figure 12. Electrostrictive materials: 3D configuration with nanotubes

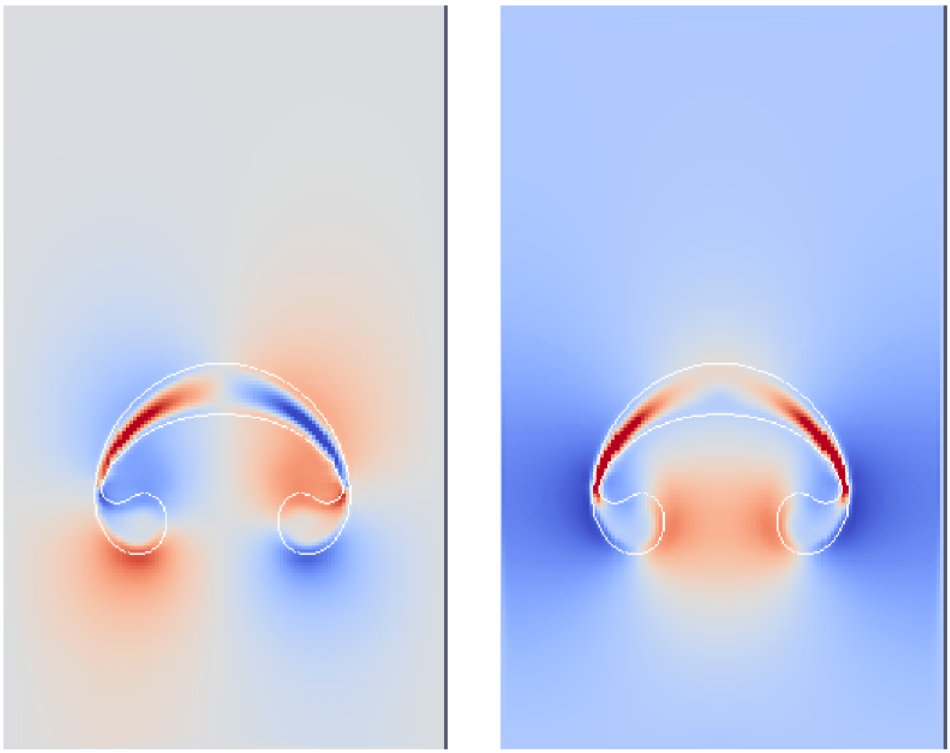


Figure 13. Horizontal et vertical velocity profile of an air bubble rising into water.

MEPHYSTO Team

7. New Results

7.1. Quantitative stochastic homogenization

7.1.1. Discrete equations

7.1.1.1. Decay of the semi-group

A. Gloria, S. Neukamm (Univ. Dresden), and F. Otto (MPI for mathematics in the sciences, Leipzig) developed in [15] a general approach to quantify ergodicity in stochastic homogenization of scalar discrete elliptic equations. Using a parabolic approach, they obtained optimal estimates on the time-decay of the so-called environment seen from the particle. This allowed them to prove optimal bounds on the corrector gradient and the corrector itself in any dimension (thus improving on [5]). They also obtained the first error analysis of the popular periodization method to approximate the homogenized coefficients.

7.1.1.2. Quantitative CLT

In [16], A. Gloria and J. Nolen (Duke Univ.) proved a quantitative central limit theorem for the effective conductance on the discrete torus. In particular, they quantified the Wasserstein distance between a normal random variable and the CLT-like rescaling of the difference between the approximation of the effective conductance by periodization and the effective conductance. Their estimate is sharp and shows that the Wasserstein distance goes to zero (up to logarithmic factors) as if the energy density of the corrector was iid (which it is not). This completes and settles the analysis started in [15] on the approximation of homogenized coefficients by periodization by characterizing the limiting law in addition to the scaling.

7.1.2. Continuum equations

7.1.2.1. Scalar equations with random coefficients

In [17], A. Gloria and F. Otto extended their results [4] , [5] on discrete elliptic equations to the continuum setting. They treated in addition the case of non-symmetric coefficients, and obtained optimal estimates in all dimensions by the elliptic approach (whereas [4],[5] were suboptimal for $d = 2$).

In [14], A. Gloria and D. Marahrens (MPI for mathematics in the sciences, Leipzig) extended the annealed results [14] on the discrete Green function by D. Marahrens and F. Otto to the continuum setting. As a by-product of their result, they obtained new results in uncertainty quantification by estimating optimally the variance of the solution of an elliptic PDE whose coefficients are perturbed by some noise with short range of dependence.

7.1.2.2. Systems with random coefficients

In a revised version of [58], A. Gloria, S. Neukamm, and F. Otto developed a regularity theory for random elliptic operators inspired by the contributions of Avellaneda and Lin [43] in the periodic setting and of S. Armstrong with C. Smart [42]. This allowed them to consider coefficients with arbitrarily slow decaying correlations in the form of a family of correlated Gaussian fields, and obtain (in the new version of this paper) a family of estimates with optimal rates and exponential-type integrability.

In [35], A. Gloria and F. Otto obtained the first nearly-optimal estimates with optimal stochastic integrability on the corrector for linear elliptic systems whose coefficients satisfy a finite range of dependence assumption (thus avoiding the functional inequalities they considered so far).

7.1.2.3. Systems with almost periodic coefficients

In [23], S. Armstrong, A. Gloria and T. Kuusi (Aalto University) obtained the first improvement over the thirty year-old result by Kozlov [60] on almost periodic homogenization. In particular they introduced a class of almost periodic coefficients which are not quasi-periodic (and thus strictly contains the Kozlov class) and for which almost periodic correctors exist. Their approach combines the regularity theory developed by S. Armstrong and C. Smart in [42] and adapted to the almost periodic setting by S. Armstrong and Z. Shen [41], a new quantification of almost-periodicity, and a sensitivity calculus in the spirit of [4].

7.1.3. Clausius-Mossotti formulas

In the mid-nineteenth century, Clausis, Mossotti and Maxwell essentially gave a first order Taylor expansion for (what is now understood as) the homogenized coefficients associated with a constant background medium perturbed by diluted spherical inclusions. Such an approach was recently used and extended by the team MATHERIALS to reduce the variance in numerical approximations of the homogenized coefficients, cf. [39], [38], [62]. In [12], M. Duerinckx and A. Gloria gave the first rigorous proof of the Clausius-Mossotti formula and provided the theoretical background to analyze the methods introduced in [62].

7.2. Derivation of nonlinear elasticity from polymer-physics

7.2.1. Reconstruction of analytical constitutive laws

In [10], M. de Buhan (CNRS, Univ. Paris Descartes), A. Gloria, P. Le Tallec and M. Vidrascu proposed a numerical method to produce analytical approximations (that can be used in practical nonlinear elasticity softwares) of the numerical approximations obtained in [57] of the discrete-to-continuum energy density derived theoretically in [1]. This numerical method is based on the parametrization of the set of polyconvex Ogden laws and on the combination of a least square method and a genetic algorithm (cf. CMA-ES, https://www.lri.fr/ hansen/cmaesintro.html).

7.2.2. Stochastic homogenization of unbounded integral functionals

In [34], M. Duerinckx and A. Gloria succeeded in relaxing one of the two unphysical assumptions made in [1] on the growth of the energy of polymer chains. In particular, [34] deals with the case when the energy of the polymer chain is allowed to blow up at finite deformation.

7.3. Numerical methods

7.3.1. Numerical homogenization

Inspired by the quantitative analysis of [15] and [17], Z. Habibi (former SIMPAF post-doctoral fellow) and A. Gloria introduced in [13] a general method to reduce the so-called resonance error in numerical homogenization, both at the levels of the approximation of the homogenized coefficients and of the correctors. This method significantly extends [2]. The method relies on the introduction of a massive term in the corrector equation and of a systematic use of Richardson extrapolation. In the three academic examples of heterogeneous coefficients (periodic, quasiperiodic, and Poisson random inclusions), the method yields optimal theoretical and empirical convergence rates, and outperforms most of the other existing methods.

7.3.2. Numerical methods for evolution equations

In [11], G. Dujardin and P. Lafitte (ECP) published a result on the asymptotic behavior of splitting schemes applied to multiscale systems which have strongly attracting equilibrium states. They proposed a definition of the asymptotic order of such schemes and proved on examples of ODEs and PDEs systems that one can achieve high asymptotic order with such schemes, provided sufficient conditions are fulfilled.

In [25], G. Dujardin proposed to use high order methods for the numerical simulation of rotating Bose-Einstein condensates. With his co-authors, he developed exponential Runge-Kutta methods and Lawson method for this problem and he analyzed the convergence order of these methods. In particular, they proved that one can achieve maximal order $2s$ with methods with s-stages. They also supported their analysis with numerical experiments carried out in physically realistic simulations.

7.4. Schrödinger equations

7.4.1. Nonlinear optic fibers

In [18], S. De Bièvre, G. Dujardin, and S. Rota-Noradi, in collaboration with physicists of the PhLAM laboratory in Lille, developed an analysis of the phenomenon of modulational instability in dispersion-kicked optical fibers. They proposed a genuine analysis of the phenomenon, together with estimates on physical properties such as the gain along the fibers, and they showed that their analysis actually fits both numerical and physical experiments.

In [20], S. De Bièvre and G. Dujardin, in collaboration with physicists of the PhLAM laboratory in Lille, developed an analysis of the propagation along a periodically-modulated optic fiber of generalized Peregrine rogue waves. In particular, they provided a full analysis of the multiple compression points appearing in such waves.

In D. Bonheure and R. Nascimento [21] obtained new results on the existence and qualitative properties of waveguides for a mixed-diffusion NLS. They provided a full qualitative description of the waveguides when the fourth order dissipation is small.

7.4.2. Nonlinear Schrödinger equations

S. De Bièvre, S. Rota Nodari, and F. Genoud (CEMPI visitor, September 2013) have explained the geometry underlying the so-called energy-momentum method for proving orbital stability in infinite dimensional Hamiltonian systems. Applications include the orbital stability of solitons of the NLS and Manakov equations. This work appeared as a chapter (120p) in the first volume of the CEMPI Lecture Notes in Mathematics, cf. [48].

In [26], Bonheure, S. Cingolani and M. Nys obtained new striking results on stationary solutions of the 3D NLS driven by an exterior magnetic field. They construct a new class of cylindrical solutions in the energy class which concentrate, in the semi-classical limit, on a circle of the plane through the equator. In contrast with the case of solutions localized around a single point, the concentration is driven by the electrical field as well as the magnetic field

7.5. Stochastic acceleration and approach to equilibrium

S. De Bièvre and E. Soret rigorously proved the growth rate of the energy in a Markovian model for stochastic acceleration of a particle in a random medium, cf. [67] and [7].

S. De Bièvre, Carlos Mejia-Monasterio (Madrid) and Paul E. Parris (Missouri) [49] studied thermal equilibration in a two-component Lorentz gas, in which the obstacles are modeled by rotating disks. They show that a mechanism of dynamical friction leads to a fluctuation-dissipation relation that is responsible for driving the system to equilibrium.

Stephan De Bièvre, JeremyFaupin (Metz) and Schuble (Metz) [32] studied a related model quantum mechanically. Here a quantum particle moves through a field of quantized bose fields, modeling membranes that exchange energy and momentum with the particle. They establish a number of spectral properties of this model, that will be essential to study the time-asymptotic behavior of the system.

7.6. Miscellaneous results

In [24] A. Benoit proved that for linear hyperbolic systems of equations in the quarter space a violent instability can be caused by the accumulation of an arbitrary large number of weak instabilities. The proof of this result is based on the construction of the WKB expansions for hyperbolic corner problems with self-interacting phases and is a continuiation of [45].

In [9], C. Cancès, T. Gallouët, and L. Monsaingeon gave a gradient flow interpretation for incompressible immiscible two-phase flows in porous media. With C. Chainais-Hillairet, T. Gallouët characterized the pseudo-stationary state for a corrosion model in [31].

In [8], D. Bonheure, E. Moreira dos Santos, M. Ramos and H. Tavares construct least energy nodal solutions of Hamiltonian elliptic systems. The construct is tricky since the functional associated to Hamiltonian elliptic systems is strongly indefinite. The proof uses a dual variational argument and an approximation scheme with some ideas of Gama-convergence type.

In [27], D. Bonheure, P. D'Avenia and A. Pomponio aim to derive rigorously the PDE formulation of the Born-Infeld model in the electrostatic case. This nonlinear model of electromagnetism was introduced by Born and Infeld who proposed a new Lagrangian which theoretically assumes the existence of a maximal field intensity, likewise Einstein's Lagragian of special relativity opposed to Newton's Lagrangian of classical mechanics. The paper contains new results and new insights on the model. It covers several relevant particular cases but we are still far from the full understanding of the problem.

In [29] and [30], D. Bonheure and coauthors study patterns and phase transitions in a fourth order extension of the famous Allen-Cahn model. In [29], some rigidity results à la Gibbons are proved while [30] concerns qualitative properties of positive patterns with Navier boundary conditions. A conjecture related to De Giorgi's famous one concerning the one dimensionality of monotone phase transition in the classical Allen Cahn model is proposed in [29].

In [28], D. Bonheure and collaborators study multi-layer solutions of the Lin-Ni-Takagi model, which comes from the Keller-Segel model of chemotaxis in a specific case. A remarkable feature of the results is that the layers do not accumulate to the boundary of the domain but satisfy an optimal partition problem contrary to the previous type of solutions constructed for this model.

In [53], M. Duerinckx proved a new mean-field limit result for the gradient flow evolution of particle systems with pairwise Riesz interactions, in dimensions 1 and 2, in cases for which this problem was still open. The proof is based on a method introduced by Serfaty [66] in the context of the Ginzburg-Landau vortices, using regularity and stability properties of the limiting equation.

MOKAPLAN Project-Team

7. New Results

7.1. Numerical methods for JKO Gradient Flows

J-D. Benamou, G. Carlier, M. Laborde, G. Peyré, B. Schmitzer, V. Duval

Taking advantage of the Benamou-Brenier dynamic formulation of optimal transport, we propose in [28], 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.

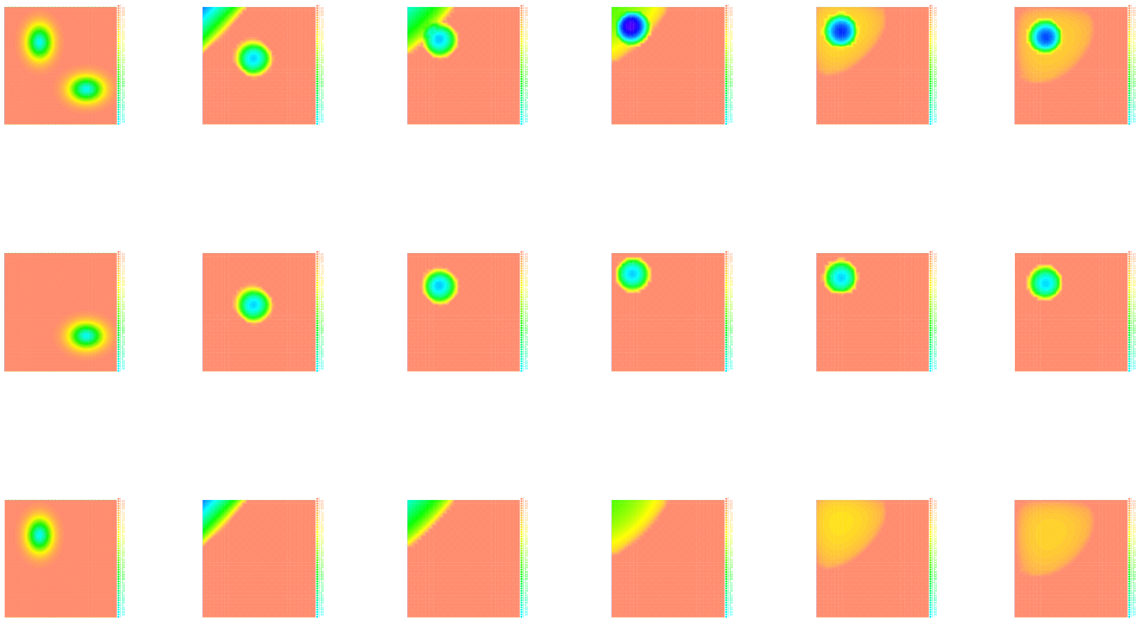


Figure 12. Evolution of two species where the first one is attracted by the other and the second one is repelled by the first one. Top row: display of $\rho_1 + \rho_2$. Middle row: display of ρ_1. Bottom row: display of ρ_2.

We have also investigated the entropy-regularization of the Wasserstein metric to compute gradient flows [19], [34]. This entropic regularization trades the usual Wasserstein fidelity term for a Kullback-Leibler divergence term. Adapting first-order proximal methods to this framework, we have developed numerical schemes which dramatically reduce the computational load needed to simulate the evolution of a mass density through a JKO flow. By construction, the entropy regularization yields an additional diffusion effects to the evolution, but we have proved that a careful choice of the regularization parameter with respect to the timestep yields the convergence of the scheme towards the solutions of the continuous PDE.

A novel Lagrangian method using a discretization of the Monge-Ampère operator for JKO has been developed in [13]. Not only convergence of the scheme has been established but also one advantage of this method is that it makes it possible to use a Newton's method .

7.2. Density Functional Theory

J-D. Benamou Luca Nenna, G. Carlier

In [41] is presented the state of art and recent developments of the optimal transportation theory with many marginals for a class of repulsive cost functions. We introduce some aspects of the Density Functional Theory (DFT) from a mathematical viewpoint, and revisit the theory of optimal transport from its perspective. Moreover, in the last three sections, we describe some recent and new theoretical and numerical results obtained for the Coulomb cost, the repulsive harmonic cost and the determinant.

In [29] we present a numerical method, based on iterative Bregman projections, to solve the optimal transport problem with Coulomb cost. This is related to the strong interaction limit of Density Functional Theory. The first idea is to introduce an entropic regularization of the Kantorovich formulation of the Optimal Transport problem. The regularized problem then corresponds to the projection of a vector on the intersection of the constraints with respect to the Kullback-Leibler distance. Iterative Bregman projections on each marginal constraint are explicit which enables us to approximate the optimal transport plan. We validate the numerical method against analytical test cases.

7.3. Stability for inverse problems with sparsity prior

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

In [42], we have analyzed the recovery performance of two popular finite dimensional approximations of the sparse spikes deconvolution problem over Radon measures, namely the LASSO, and the Continuous Basis-Pursuit. The LASSO is the de-facto standard for the sparse regularization of inverse problems in imaging. It performs a nearest neighbor interpolation of the spikes locations on the sampling grid. The C-BP method, introduced by Ekanadham, Tranchina and Simoncelli, uses a linear interpolation of the locations to perform a better approximation of the infinite-dimensional optimization problem, for positive measures. We have proved that, in the small noise regime, both methods estimate twice the number of original spikes, and we have provided an explicit formula which allows to predict the locations and amplitudes of the spurious spikes. All those properties are in fact connected to an intrinsinc property of the signal: the source condition [16], [24].

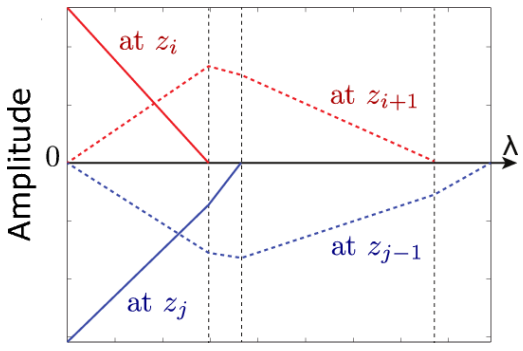


Figure 13. The solution path of the discrete LASSO (as a function of λ) for some discrete measure m_0 (the noise w is set to zero). This shows the amplitudes of the coefficients at $z_i = ih$, resp. $z_j = jh$, (continuous line) and at the next, resp. previous, point of the grid (dashed line) as λ varies.

Those effects are typically due to the use of a discrete grid in the reconstruction process. Several authors have recently proposed algorithms to tackle the problem directly in a continuous setting [75], [92]. As we have shown in [16], the method fails when the distance between spikes with opposite signs are below a certain threshold. However, when all the spikes have the same sign, the LASSO on a continuous domain works for arbitrarily close spikes, being all the more sensitive to noise. In [40], we have given a detailed analysis of the noise sensitivity of the method: if t denotes the minimum separation of the input measure (the minimum distance between two spikes), w refers to the noise and λ is the regularization parameter, when $\|w\|_{L^2}/\lambda$, $\|w\|_{L^2}/t^{2N-1}$ and λ/t^{2N-1} are small enough (where N is the number of spikes), there exists a unique solution to the BLASSO program with exactly the same number of spikes as the original measure. We show that the amplitudes and positions of the spikes of the solution both converge toward those of the input measure when the noise and the regularization parameter drops to zero faster than t^{2N-1}.

7.4. Generalized Solution of Euler

Minimal geodesics along volume preserving maps, through semi-discrete optimal transport

Q. Mérigot and J.-M. Mirebeau introduced a numerical method for extracting minimal geodesics along the group of volume preserving maps, equipped with the L^2 metric, which as observed by Arnold solve Euler's equations of inviscid incompressible fluids. The method relies on the generalized polar decomposition of Brenier, numerically implemented through semi-discrete optimal transport. It is robust enough to extract non-classical, multi-valued solutions of Euler's equations, for which the dimension of the support of the flow is higher than the dimension of the domain, a striking and unavoidable consequence of this model. Our convergence results encompass this generalized model, and our numerical experiments illustrate it for the first time in two space dimensions (see Figure 14).

7.5. Principal Agent Problem

J-D. Benamou, Xavier Dupuis, G. Carlier An alternated projection numerical scheme for the more general c-concavity constraint using Dykstra's algorithm has been recently developed in [33] but being able to handle realistic principal-agent problems remains a challenging issue. Investigating the structure of equilibria in matching problems with non-transferable utilities is also one of our objectives, together with numerical methods in the spirit of the IPFP algorithm.

A semi-discrete approach to the PA problem is investigated. The range of products is discrete and leads to a non convex problem. Non-linear optimization methods are tested. See https://mathmarx.paris.inria.fr:8080.

7.6. Unbalanced Optimal Transport

G. Carlier, F-X. Vialard, B. Schmitzer, L. Chizat Classical optimal transport theory and algorithms assume that the input measures are normalized, i.e. that their total mass is 1. This is an important limitation for many problems in imaging sciences and machine learning, where input data are typically not normalized, and where one should enables local creation or destruction of mass. Handling such "unbalanced" transportation problem is also relevant for applications in biological modeling, for instance to take into account cellular growth through optimal transport gradient flows.

Recently, several researchers of MOKAPLAN made important progress on this problem, by deriving a general framework extending optimal transport to this "unbalanced" setting. In [38] we derived a dynamic optimal transport formulation that enables a source term in the initial formulation of Benamou and Brenier [55]. We proved that it defines a distance on positive measures, enjoy many important properties (dual formulation) and can be computed using fast first order convex optimization methods. We then provided in [39] an even larger class of "unbalanced" optimal transport optimization problems, that are obtained via a static formulation, and show that one can recovers the dynamic formulation in some specific cases. Similar models were derived independently and at the same time by two other international teams [143], [137], which shows the timeliness of our research. We believe these new theoretical and numerical findings will have a strong impact on the developpement of optimal transport methods in imaging sciences and machine learning.

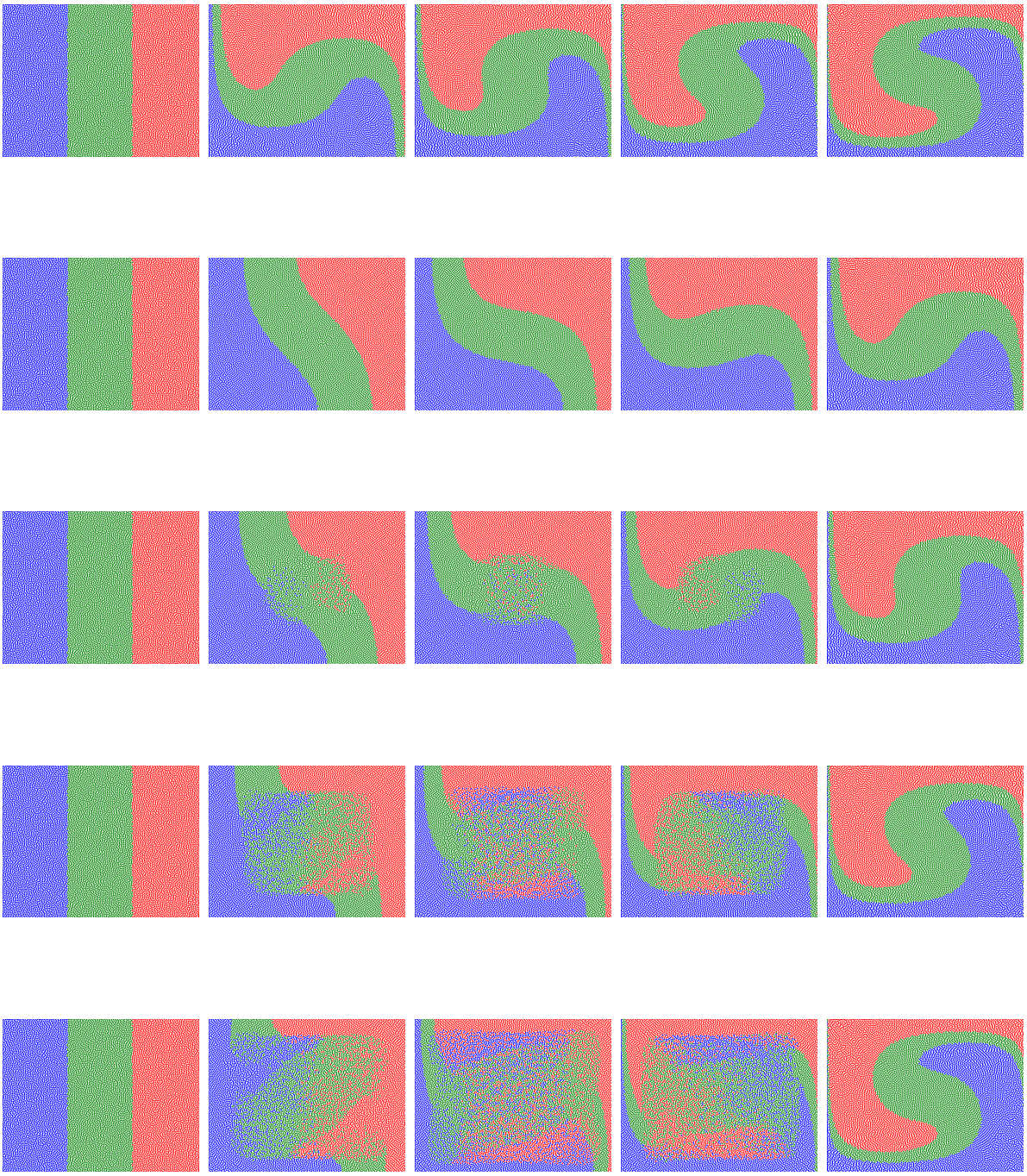


Figure 14. (First row) Beltrami flow in the unit square at various timesteps, a classical solution to Euler's equation. The color of the particles depend on their initial position. (Second to fifth row) Generalized fluid flows that are reconstructed by our algorithm, using boundary conditions displayed in the first and last column. When $t_{\max} < 1$ we recover the classical flow, while for $t_{\max} \geq 1$ the solution is not classical any more and includes some mixing.

NACHOS Project-Team

6. New Results

6.1. Electromagnetic wave propagation

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

Participants: Loula Fezoui, Stéphane Lanteri.

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

6.1.2. High order geometry conforming DGTD method for nanophotonics

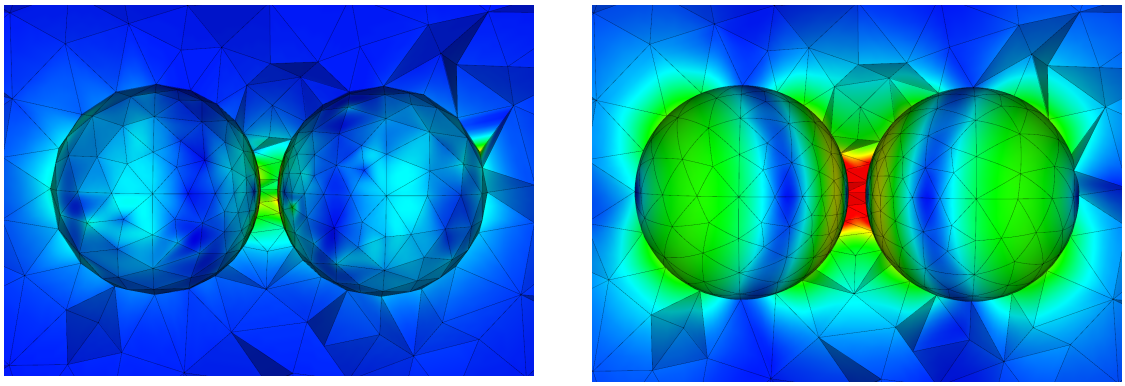
Participants: Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

Usually, unstructured mesh based methods rely on tessellations composed of straight-edged elements mapped linearly from a reference element, on domains which physical boundaries are indifferently straight or curved. Such meshes represent a serious hindrance for high order finite element (FE) methods since they limit the accuracy to second order in the spatial discretization. Thus, exploiting an enhanced representation of physical geometries is in agreement with the natural procedure of high order FE methods, such as the DG method. There are several ways to account for curved geometries. One could choose to incorporate the knowledge coming from CAD in the method to design the geometry and the approximation. These methods are called *isogeometric*, and have received a lot of attention recently. This naturally implies to have access to CAD models of the geometry. On the other hand, *isoparametric* usually rely on a polynomial approximation of both the boundary and the solution. This can be added fairly easily on top of existing implementations. In the present study we focus on the latter type of method, since our goal is first to envisage the benefit of curvilinear meshes for light/matter interaction with nanoscale structures.

6.1.3. Local approximation order DGTD method for nanophotonics

Participants: Stéphane Lanteri, Jonathan Viquerat.

High order DGTD methods for the numerical modeling of light/matter interactions on the nanoscale often assume a uniform distribution of the polynomial order to the cells of the underlying mesh. However, in the case of a mesh showing large variations in cell size, the time step imposed by the smallest cells can be a serious hindrance when trying to exploit high approximation orders. Indeed, a potentially large part of the CPU time is spent in the update of the physical field inside small cells where high polynomial orders might not be essential, while they are necessary in the larger cells. In this study, we consider the possibility of using a non-uniform distribution of the polynomial order in the framework of a global time step DGDT method. By imposing low orders in small cells and high orders in large cells, it is possible to significantly alleviate both the global number of degrees of freedom and the time step restriction with a minimal impact on the method accuracy. Strategies exploiting locally adaptive (LA) formulations usually combine both h- and p-adaptivity (where h denotes the discretization parameter in space and p the degree of the interpolation of the field components) in



Mesh with affine elements Mesh with curvilinear elements

Figure 4. Near-field visualization of the amplitude of the electric field Fourier transformed for a gold nanosphere dimer. Surface-to-surface distance is set to 4 nm. Calculations are based on a DGTD-$\mathbb{P}_4$ method.

order to concentrate the computational effort in the areas of high field variations. Here, the adopted point of view is quite different: starting from a given mesh and a uniform distribution of the polynomial order k, the LA strategy exploits all the polynomial orders p with $p \leq k$ to obtain a solution of similar accuracy with a reduced computational cost.

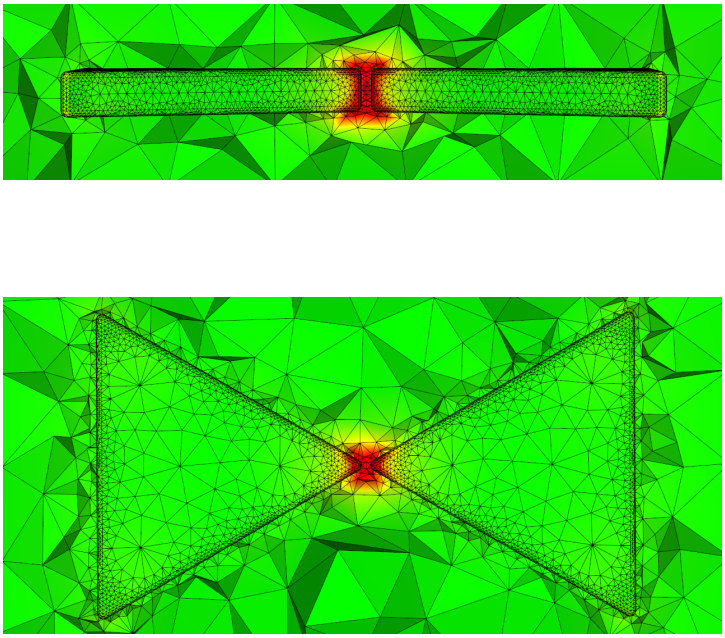


Figure 5. Near-field plasmonic interaction with a bowtie nanoantenns: contour line the amplitude of the discrete Fourier transform of the electric field.

6.1.4. Numerical treatment of non-local dispersion for nanoplasmonics

Participants: Stéphane Lanteri, Claire Scheid, Colin Vo Cong Tri.

When metallic nanostructures have sub-wavelength sizes and the illuminating frequencies are in the regime of metal's plasma frequency, electron interaction with the exciting fields have to be taken into account. Due to these interactions, plasmonic surface waves can be excited and cause extreme local field enhancements (surface plasmon polariton electromagnetic waves). Exploiting such field enhancements in applications of interest requires a detailed knowledge about the occurring fields which can generally not be obtained analytically. For the numerical modeling of light/matter interaction on the nanoscale, the choice of an appropriate model is a crucial point. Approaches that are adopted in a first instance are based on local (no interaction between electrons) dispersion models e.g. Drude or Drude-Lorentz. From the mathematical point of view, these models lead to an additional ordinary differential equation in time that is coupled to Maxwell's equations. When it comes to very small structures in a regime of 2 nm to 25 nm, non-local effects due to electron collisions have to be taken into account. Non-locality leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. In this work, we study a DGTD method able to solve the system of Maxwell equations coupled to a linearized non-local dispersion model relevant to nanoplasmonics. While the method is presented in the general 3d case, in this preliminary stdudy, numerical results are given for 2d simulation settings.

6.1.5. Corner effects in nanoplasmonics

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

The starting point of this ongoing work is the theoretical and numerical study of nanoplasmonic structures with corners. This is the central subject of the PhD thesis of Camille Carvalho. In the latter, the focus is made on a lossles Drude dispersion model with a frequency domain approach. Several well posedness problems arise due to the presence of corners and are addressed in the PhD thesis. A time domain approach in this context can also be investigated with the techniques developed in our project-team. Even if both approaches (time domain and frequency domain) represent similar physical phenomena, problems that arise are different and they appear as complementary; it is thus worth bridging the gap between the two frameworks. We propose to perform a thorough comparison in the case of structures with corners. Several extensions to other models are also envisaged, especially concerning the non local dispersion model.

6.1.6. DGTD method for nanoplasmonics based on generalized dispersion model

Participants: Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

In this work, we are concerned with the numerical modelling of the propagation of electromagnetic waves in dispersive materials for nanophotonics applications. We focus on a generalized model that allows for the description of a wide range of dispersive media. The underlying differential equations are recast into a generic form and we establish an existence and uniqueness result. We then turn to the numerical treatment and propose an appropriate DGTD framework. We obtain the semi-discrete convergence and prove the stability (and to a large extent, the convergence) in the fully discrete case when time integration is achieved with a 4 steps low storage Runge-Kutta scheme, *via* a technique relying on energy principles. Finally, we validate our results through the numerical simulation of two nanophotonics test cases.

6.1.7. Travelling waves for the non-linear Schrödinger equation in 2d

Participants: David Chiron [J.A. Dieudonné Laboratory, University of Nice-Sophia Antipolis], Claire Scheid.

We are interested in the numerical study of the two-dimensional travelling waves of the non-linear Schrödinger equation for a general non-linearity and with nonzero condition at infinity that can appear in optics. The equation has a variational structure that we propose to exploit to design a numerical method. We characterize the saddle points of the action as minimizers of another functional, allowing us to use a gradient flow. Combining this approach with a continuation method in the speed of the wave, we obtain the numerical

solution for the full range of velocities. We plot the energy-momentum diagrams for different type of non-linearities. Through various examples, we show that even though the non-linearity has the same behaviour as the well-known Gross-Pitaevskii (GP) non-linearity, the qualitative properties of the travelling waves may be extremely different. For instance, we observe cusps, a modified Kadomtsev-Petviashvili I (KP-I) asymptotic in the transonic limit (as the speed of the wave approaches the speed of sound), various multiplicity results.

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

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

Although the DGTD method has already been successfully applied to complex electromagnetic wave propagation problems, its accuracy may seriously deteriorate on coarse meshes when the solution presents multiscale or high contrast features. In other physical contexts, such an issue has led to the concept of multiscale basis functions as a way to overcome such a drawback and allow numerical methods to be accurate on coarse meshes. The present work, which has been initiated in the context of the visit of Frédéric Valentin in the 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 2d case for models problems.

6.1.9. HDG methods for the time-domain Maxwell equations

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

This study is concerned with the development of accurate and efficient solution strategies for the system of 3d time-domain Maxwell equations coupled to local dispersion models (e.g. Debye, Drude or Drude-Lorentz models) in the presence of locally refined meshes. Such meshes impose a constraint on the allowable time step for explicit time integration schemes that can be very restrictive for the simulation of 3d problems. We consider here the possibility of using an unconditionally stable implicit time or a locally implicit time integration scheme combined to a HDG discretization method. In doing so, we extend our former study which was dealing with the 2d time-domain Maxwell equations for non-dispersive media.

6.1.10. HDG methods for the frequency-domain Maxwell equations

Participants: Thomas Frachon, Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Ludovic Moya, Ronan Perrussel [Laplace Laboratory, Toulouse].

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

6.2. Elastodynamic wave propagation

6.2.1. Sesimic wave interaction with viscoelastic media

Participants: Nathalie Glinsky, Stéphane Lanteri, Fabien Peyrusse [Department of Mathematics, Purdue University].

This work is concerned with the development of high order DGTD methods formulated on unstructured simplicial meshes for the numerical solution of the system of time-domain elastodynamic equations. These methods share some ingredients of the DGTD methods developed by the team for the time-domain Maxwell equations among which, the use of nodal polynomial (Lagrange type) basis functions, a second order leap-frog time integration scheme and a centered scheme for the evaluation of the numerical flux at the interface between neighboring elements. A recent novel contribution is the numerical treatment of viscoelastic attenuation. For this, the velocity-stress first order hyperbolic system is completed by additional equations for the anelastic functions including the strain history of the material. These additional equations result from the rheological model of the generalized Maxwell body and permit the incorporation of realistic attenuation properties of viscoelastic material accounting for the behaviour of elastic solids and viscous fluids. In practice, we need solving 3L additional equations in 2d (and 6L in 3d), where L is the number of relaxation mechanisms of the generalized Maxwell body. This method has been implemented in 2d and 3d.

6.2.2. DG method for arbitrary heterogeneous media

Participants: Nathalie Glinsky, Diego Mercerat [CETE Méditerranée].

We have recently devised an extension of the DGTD method for elastic wave propagation in arbitrary heterogeneous media. In realistic geological media (sedimentary basins for example), one has to include strong variations in the material properties. Then, the classical hypothesis that these properties are constant within each element of the mesh can be a severe limitation of the method, since we need to discretize the medium with very fine meshes resulting in very small time steps. For these reasons, we propose an improvement of the DGTD method allowing non-constant material properties within the mesh elements. A change of variables on the stress components allows writing the elastodynamic system in a pseudo-conservative form. Then, the introduction of non-constant material properties inside an element is simply treated by the calculation, via convenient quadrature formulae, of a modified local mass matrix depending on these properties. This new extension has been validated for a smoothly varying medium or a strong jump between two media, which can be accurately approximated by the method, independently of the mesh.

6.2.3. HDG method for the frequency-domain elastodynamic equations

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

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

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

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

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

6.3. High performance numerical computing

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

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

We are concerned here with the porting of a Discontinuous Galerkin Time-Domain solver for computational bioelectromagnetics to the novel heterogeneous architecture proposed in the DEEP-ER european project on exascale computing. This architecture is based on a Cluster/Booster division concept (see Fig. 6). The Booster nodes are based on the Intel Many Integrated Core (MIC) architecture. Therfore, one objective of our efforts is the algorithmic adaptation of the DG kernels in order to leverage the vectorizing capabilities of the MIC processor. The other activities that are undertaken in the context of our contribution to this project aim at exploiting the software environments and tools proposed by DEEP-ER partners for implementing resiliency strategies and high performance I/O operations. In particular, the Cluster nodes are used for running some parts of the pre- and post-processing phases of the DGTD solver which do not lend themselves well to multithreading, as well as I/O intensive routines. One possibility to achieve this is to consider a model in which these less scalable and I/O phases are reverse-offloaded from Booster processes to Cluster processes in a one-to-one mapping. This is achieved by exploiting the OmpSs offload functionality, developed at Barcelona Supercomputing Center for the DEEP-ER platform. In future work, the OmpSs framework will also be leveraged to expose task-based parallelism and exploit task-based resilience.

6.3.2. Hybrid MIMD/SIMD high order DGTD solver for nanophotonics

Participants: Tristan Cabel, Gabriel Hautreux [CINES, Montpellier], Stéphane Lanteri, Raphaël Léger, Claire Scheid, Jonathan Viquerat.

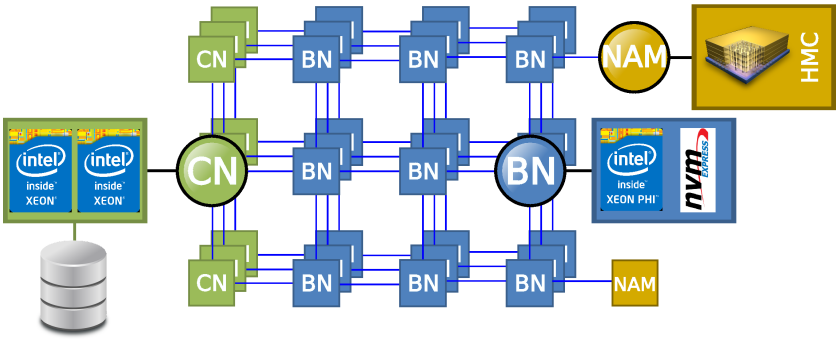


Figure 6. DEEP-ER hardware architecture sketch.

This work is concerned with the development of a scalable high order finite element type solver for the numerical modeling of light interaction with nanometer scale structures. From the mathematical modeling point of view, one has to deal with the differential system of Maxwell equations in the time domain, coupled to an appropriate differential model of the behavior of the underlying material (which can be a dielectric and/or a metal) at optical frequencies. For the numerical solution of the resulting system of differential equations, we adopt the high order DGTD (Discontinuous Galerkin Time-Domain) solver described in [21]. A hybrid MIMD/SIMD parallelization of this DGTD solver has been developed by combining the MPI and OpenMP parallel programming models. The performances of the resulting parallel DGTD solver have been assessed on the Curie system of the PRACE research infrastructure. For that purpose, we selected a use case typical of optical guiding applications. A Y-shaped waveguide is considered which consists in nanosphere embedded in vacuum (see Fig. 7). The constructed tetrahedral mesh consists of 520,704 vertices and 2,988,103 elements. The high order discontinuous finite element method designed for the solution of the system of time-domain Maxwell equations coupled to a Drude model for the dispersion of noble metals at optical frequencies is formulated on a tetrahedral mesh.

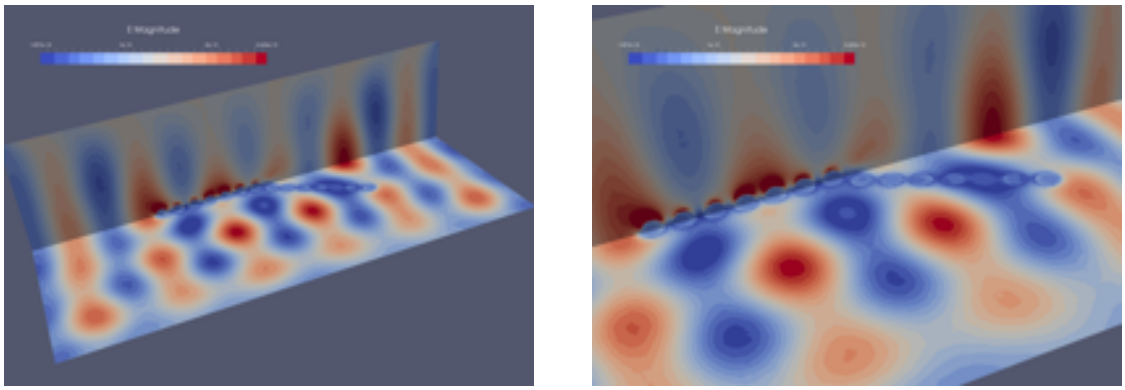


Figure 7. Y-shaped waveguide: contour lines of the amplitude of the discrete Fourier transform of the electric field.

6.4. Applications

6.4.1. Light diffusion in nanostructured optical fibers

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

Optical fibers are the basis for applications that have grown considerably in recent years (telecommunications, sensors, fiber lasers, etc.). Despite these undeniable successes, it is necessary to develop new generations of amplifying optical fibers that will overcome some limitations typical of silica. In this sense, the amplifying Transparent Glass Ceramics (TGC), and particularly the fibers based on this technology, open new perspectives that combine the mechanical and chemical properties of a glass host and the augmented spectroscopic properties of embedded nanoparticles, particularly rare earth-doped oxide nanoparticles. Such rare earth-doped silica-based optical fibers with transparent glass ceramic (TGC) core are fabricated by the Optical Fibers team of the Laboratory of Condensed Matter (LPMC) in Nice. The obejctive of this collaboration with Wilfried Blanc at LPMC is the study of optical transmission terms of loss due to scattering through the numerical simulation of light propagation in a nanostructured optical fiber core using a high order DGTD method developed in the team.

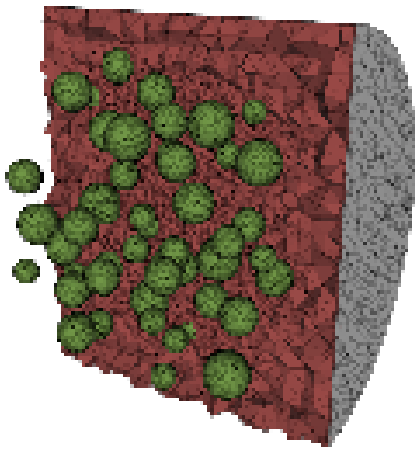


Figure 8. Unstructured tetrahdral mesh of a nanostructured optical fiber core.

6.4.2. Gap-plasmon confinement with gold nanocubes

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

The propagation of light in a slit between metals is known to give rise to guided modes. When the slit is of nanometric size, plasmonic effects must be taken into account, since most of the mode propagates inside the metal. Indeed, light experiences an important slowing-down in the slit, the resulting mode being called *gap-plasmon*. Hence, a metallic structure presenting a nanometric slit can act as a light trap, i.e. light will accumulate in a reduced space and lead to very intense, localized fields. Recently, the chemical production of random arrangements of nanocubes on gold films at low cost was proved possible by Antoine Moreau and colleagues at Institut Pascal. Nanocubes are separated from the gold substrate by a dielectric spacer of variable thickness, thus forming a narrow slit under the cube. When excited from above, this configuration is able to support gap-plasmon modes which, once trapped, will keep bouncing back and forth inside the cavity. At visible frequencies, the lossy behavior of metals will cause the progressive absorption of the trapped electromagnetic field, turning the metallic nanocubes into efficient absorbers. The frequencies at which this

absorption occurs can be tuned by adjusting the dimensions of the nanocube and the spacer. In collaboration with Antoine Moreau, we propose to study numerically the impact of the geometric parameters of the problem on the behaviour of a single nanocube placed over a metallic slab (see Fig. 9). The behavior of single nanocubes on metallic plates has been simulated, for lateral sizes c ranging from 50 to 80 nm, and spacer thicknesses δ from 3 to 22 nm. The absorption efficiency in the cube Q_{cube} at the resonance frequency is retrieved from the results of each computation (see Fig. 10).

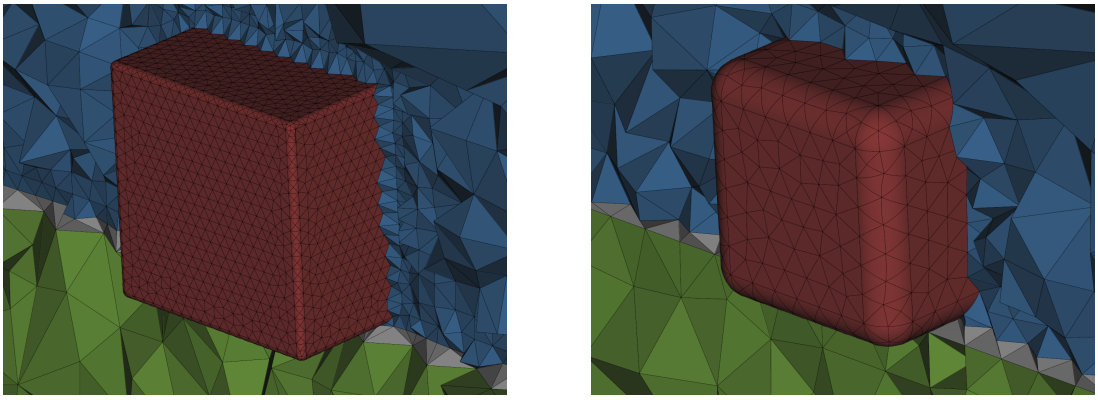
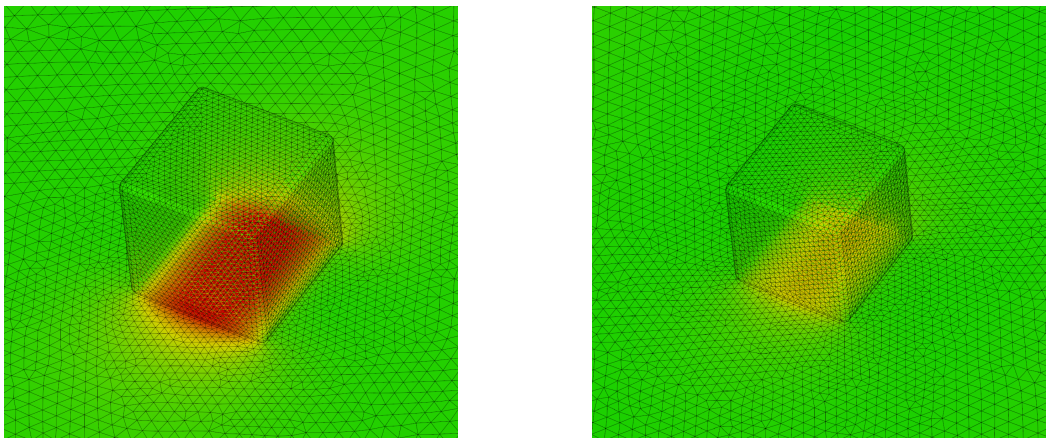


Figure 9. Meshes of rounded nanocubes with rounding radii ranging from 2 to 10 nm. Red cells correspond to the cube. The latter lies on the dielectric spacer (gray cells) and the metallic plate (green). Blue cells represent the air surrounding the device.



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

Figure 10. Amplitude of the discrete Fourier transform of the magnetic field for different nanocube configurations. All field maps are scaled identically for better comparison. The obtained field is more intense for configurations that yield high Q_{cube} values.

6.4.3. Light propagation in power splitters

Participants: Julien Coulet, Carlos Henrique Da Silva Santos [Instituto Federal de Educaçäo, Ciência e Tecnologia de Säo Paulo, Brazil], Hugo Enrique Hernandez Figueroa [Universidade Estadual de Campinas, Faculdade de Engenharia Elétrica e de Computaçäo, Säo Paulo, Brazil], Stéphane Lanteri, Frédéric Valentin [LNCC, Petropolis, Brazil].

Power splitters are passive devices widely used in signal processing, which splits an input signal into two or more output signals. The repartition of the input power over each output is specifc to the required usage. Even if power splitters are common in classical electronics, designing them at the micrometric scale is quietly recent and is an active field of research. The purpose of this study initiated in the framework of a collaboration with researchers at Unicamp in Säo Paulo is to study the electromagnetic wave propagation is such a power splitter geometry using a high order DGTD method developed in the team, see Fig. 11 .

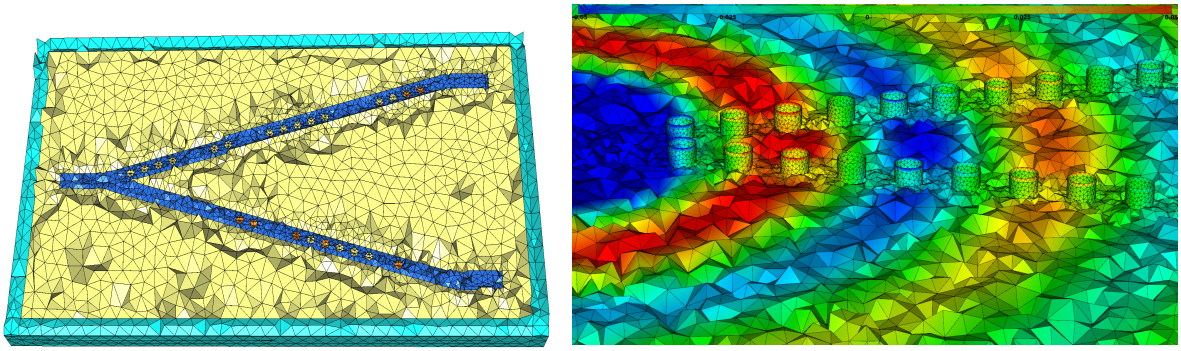
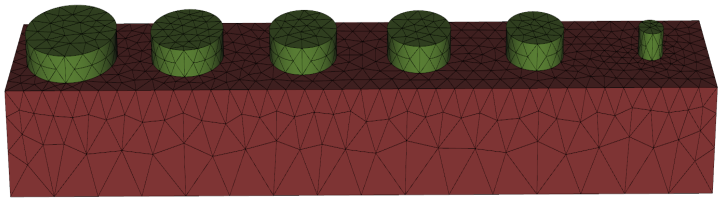


Figure 11. Geomtry of Y-shaped power splitter (left) and contour lines of the amplitude of the electric field (right).

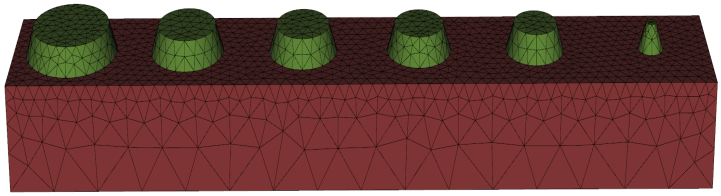
6.4.4. Dielectric reflectarrays

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

In the past few years, important efforts have been deployed to find alternatives to on-chip, low-performance metal interconnects between devices. Because of the ever-increasing density of integrated components, intra- and inter-chip data communications have become a major bottleneck in the improvement of information processing. Given the compactness and the simple implantation of the devices, communications *via* free-space optics between nanoantenna-based arrays have recently drawn more attention. Here, we focus on a specific low-loss design of dielectric reflectarray (DRA), whose geometry is based on a periodic repartition of dielectric cylinders on a metallic plate. When illuminated in normal incidence, specific patterns of such resonators provide a constant phase gradient along the dielectric/metal interface, thus altering the phase of the incident wavefront. The gradient of phase shift generates an effective wavevector along the interface, which is able to deflect light from specular reflection. However, the flaws of the lithographic production process can lead to discrepancies between the ideal device and the actual resonator array. Here, we propose to exploit our DGTD solver to study the impact of the lithographic flaws on the performance of a 1D reflectarray (see Fig. 12). Efficient computations are obtained by combining high-order polynomial approximation with curvilinear meshing of the resonators, yielding accurate results on very coarse meshes (see Fig. 13). The study is continued with the computation of the reflection of a 2D reflectarray. This work constitutes the base of a wider study in collaboration with Maciej Klemm at the Centre for Communications Research, University of Bristol.

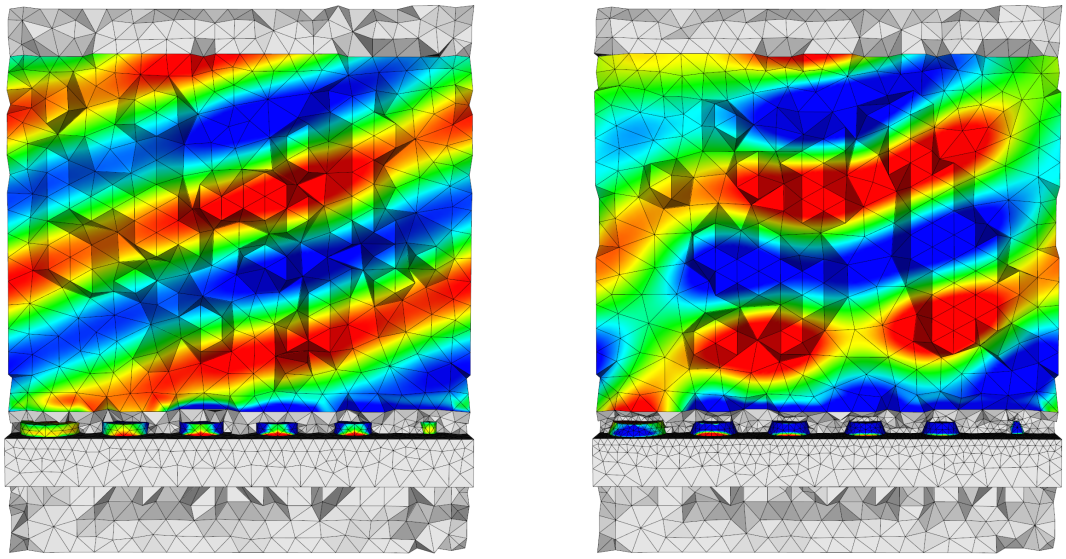


Ideal reflectarray



Realistic reflectarray

Figure 12. Ideal and realistic 1D dielectric reflectarray meshes. The red tetrahedra correspond to silver, while the green ones are made of an anisotropic dielectric material. The device is surrounded by air and terminated by a PML above and below, and by periodic boundary conditions on the lateral sides.



Ideal reflectarray Realistic reflectarray

Figure 13. Time-domain snapshot of E_y component for ideal and realistic 1D dielectric reflectarrays. Solution is obtained in established regime at $t = 0.1$ ps. Fields are scaled to $[-1, 1]$.

NANO-D Project-Team

7. New Results

7.1. Algorithms for Orbital-Free Density Functional Theory

Participants: Francois Rousse, Stephane Redon.

The Schrödinger equation permits, in theory, to model and simulate every molecular systems exactly. Unfortunately it is not computationally doable to solve this equation even on really small systems (2 atoms). Density Functional Theory (DFT) gives a method to solve this equation, find the electronic structure and simulate molecules with the laws of physics on reasonably large system : from 1.000 to 10.000 depending on the basis chosen and the version of DFT used. Unfortunately, the computation of kinetic energy requires the orthogonalization of the basis, which consumes a lot of time and prevents the algorithm from being adaptive : one needs to recompute the whole system if a little change is done in the molecules position. One can deals with this issue by computing the kinetic energy directly with the electronic density and not anymore with the orbitals. That is the idea of Orbital-Free DFT (OF-DFT). It can models great systems (up to 1.000.000 atoms) and be turned adaptive. On the other hand, it looses a lot of accuracy and power to model different kind of systems on the other DFT.

We have already developed our own OF-DFT code. It runs on parallel cores, is implemented in the SAMSON platform as a SAMSON App and gives correct electron's densities. The electronic structures are computed in real space to preserve the possibility of incremental calculations. We are now going to test our implementation, and will then attempt to make the method adaptive. The difficulty will be the determination of the domain that needs to be recomputed when a part of the system has moved, and the criteria that will help to do so.

7.2. Parallel adaptively restrained particle simulations

Participants: Krishna Kant Singh, Stephane Redon.

We have continued our work on the development of parallel adaptively restrained particle simulations. We developed new algorithms for neighbor list and incremental force updates. These algorithms have advantages over the state-of-the-art methods for simulating a system using Adaptively Restrained Molecular Dynamics (ARMD). We have simulated systems with different number (500, 4000 and 108000) of LJ particles using adaptively restrained integrator and Lennard-Jones potential in NVE (constant number of particles, Volume and Energy) and NVT ensemble (constant number of particles, Volume and Temperature). All the particles were placed in an orthogonal box. We used periodic periodic boundary conditions with 8.5 angstrom cut-off for the Lennard-Jones potential. The system was simulated using 2 femtoseconds. We compared the LAMMPS algorithm to adaptive algorithm while using adaptively restrained integrator. Our results show that a significant speed-up can be achieved if more than 60% of the particles are restrained (Figure 4). Figure 5 shows that ARMD in NVT ensemble preserves the average temperature of the system (irrespective of number of restrained particles).

7.3. Incremental algorithms for long-range interactions

Participants: Semeho Edorh, Stephane Redon.

Numerical simulations of molecular dynamics (MD) are very expensive in terms of CPU resources. During Molecular dynamics simulations, the most CPU intensive task is the evaluation of the interaction potential [78]. Due to the large number of particles involved, updating this potential may have, at each time-step, a very high computational cost.

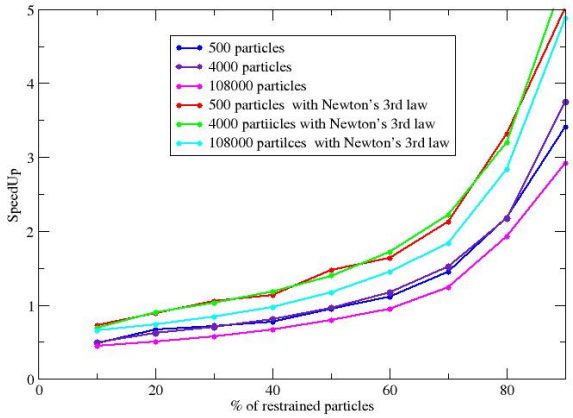


Figure 4. Speedup using ARMD on different benchmark

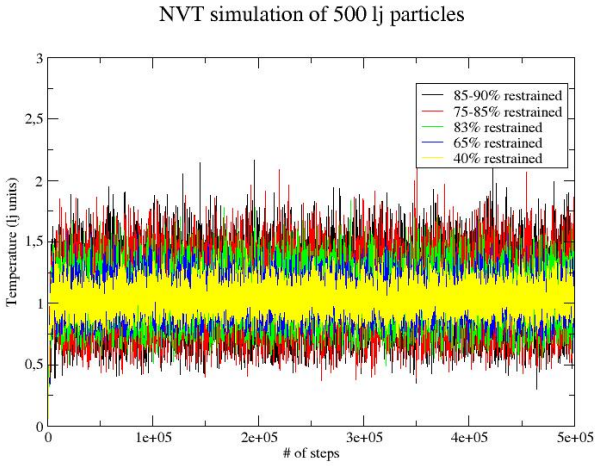


Figure 5. Temperature profile of 500 LJ particles in NVT ensemble using ARMD

In large crystalline ionic system, Ewald summation is the most popular method for computing electrostatic interactions. It rewrites the interaction potential ϕ as the sum of a short-range term and a long-range term. Ewald summation using optimal parameters requires $\mathcal{O}(N^{3/2})$ operations [47], [30] but it can be modified so that it involves only about $\mathcal{O}(N \log N)$ operations [31], [85] by using the Fast Fourier Transform.

We want to develop a new approach that can reduce the computational cost by using incremental algorithms. The key-idea is to use, for each time-step of the simulation, information that we have computed in previous steps.

The Particle Mesh Ewald (PME) algorithm developped by Darden et al. is the most successful approach for computing long range interactions. In the particle mesh method, just as in standard Ewald summation, the generic interaction potential is separated into two terms.The so-called short-range contribution can be easily calculated in a direct space by using truncation methods. Where as the long-range contribution is calculated using two Fast Fourier transforms ($N \log(N)$ algorithm). In pratice, the long range contribution algorithm boil than to [30]:

- Map particle charge density Q to a mesh
- Compute the forward Fast Fourier Transform of the approximation Qm of charge density on the mesh
- Multiply Qm by a green function (related to the choice of the mesh).
- Compute a backward Fast Fourier Transform of the result.
- Retrieve the long-range contribution potential by interpolating the previous result at particles positions.

We modified this algorithm to make it incremental. We started from the PME implementation in LAMMPS. Instead of mapping the charge density to the mesh, we mapped the increment of density dQ to the mesh. The FFT solver KissFFT is based on a divide-and-conquer algorithm. We built a sparse input solver as a modified version of FFT solver which computes only needed (non trivial) operations [74]. We built also a sparse output solver inspired by the algorithm proposed by Katabi et al. [36]. Unfortunately, we did not get significant speed-ups with these modifications.

We decided to compute the increment of the long-range contribution related to the increment of density dQ by using multi-resolution methods. These methods are slower than PME but have better adaptive behavior. The multigrid approach was chosen because of its $\mathcal{O}(N)$ behavior and its good scalability [13]. We are currently developing an adaptive multigrid method.

7.4. Motion planning architecture for nanosystems

Participants: Leonard Jaillet, Stephane Redon.

In the past, we have started the development of original quasi-static simulation methods for nano-scale systems, based on motion planning methods inspired from Robotics. In the continuity of this work, we have proposed an original Motion Planning architecture for nanosystems platform called planning. This platform offers a general framework for motion planning applied to nanosystems. In particular it includes:

- A flexible definition of the degrees of freedom that describe the system, allowing different levels of representation (e.g. Cartesian coordinates, internal coordinates, coarse grain representation, etc.).
- The possibility to define an arbitrary set of initial, final and intermediate states, guiding the search for a solution path.
- The possibility to define an arbitrary set of constraints on the intermediate states of the path (e.g. geometric constraints, energy constraints, etc.)
- Several modular functionalities specific to motion planning (e.g. conformational sampling, exploration strategy, nearest neighbor search, etc.)
- An adapted integration within SAMSON which allows using directly all the existing force fields and state updaters present in the platform.

The planning architecture has been the base of several SAMSON modules. In particular, it led to the Planner-Explore module, which regroups many of the functionalities proposed and that can by combined together through a graphical interface. This module has in particular been used to study two complex problems:

- To capture the transition paths between endiandric acids (see Figure 6).
- To find the global minima of Lennard-Jones clusters, for dimensions up to one hundred.

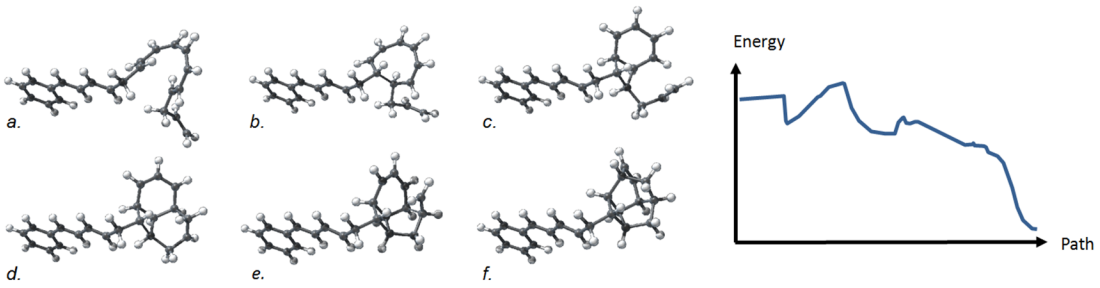


Figure 6. Transition path with its corresponding energy for an homolog of the endiandric acid and produced thanks to the Planner-Explore module.

7.5. Optimization of transition paths

Participants: Leonard Jaillet, Stephane Redon.

Motion planning methods allow producing initial paths which represent transitions from one given conformation to another. However, these paths are typically suboptimal because of the probabilistic nature of the search strategy. Hence, it is necessary to develop tools to locally increase the path quality of the solution generated during the first phase. We have proposed several methods to address such a problem. One method developed is a variant of a state-of-the-art approach called nudged elastic band (NEB). It optimizes a set of intermediate images along the path, such that each image finds the lowest energy possible while maintaining equal spacing to neighboring images. Another technique we proposed is to rely on an equivalent of the shortcutting technique developed in Robotics motion planning, but applied to the context of energy landscape. Finally, we also have complemented these methods with additional tools to do simple path edition such as cutting or thinning paths.

7.6. As-rigid-as-possible shape interpolation for molecular modeling

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

Computer-aided methods play an important role in the study of molecular structures and interactions. Inspired by the as-rigid-as-possible approaches in the field of computer graphics, we created a tool for studying large deformation of molecular structures. This tool generates interpolated structures between two known conformations of a molecule while satisfying physical constraints. The users may use it for exploring, preprocessing, or combining their model with other biological algorithms. The developed method is flexible and can be extended to include physical properties of molecular structures.

We tested our method on a graphene sheet folding into a nanotube (Figure 8) and a few biological molecules, one of which is shown in Figure 9 . The results show realistic transition motions compared to those from the linear interpolation approach.

The ARAP interpolation method has two main advantages: simplicity and preservation of local rigidity. The method is totally geometrical, yet can be extended to include physical or biological properties such as bond strength. It will be proposed as a SAMSON Element for the SAMSON software platform for computational nanoscience.

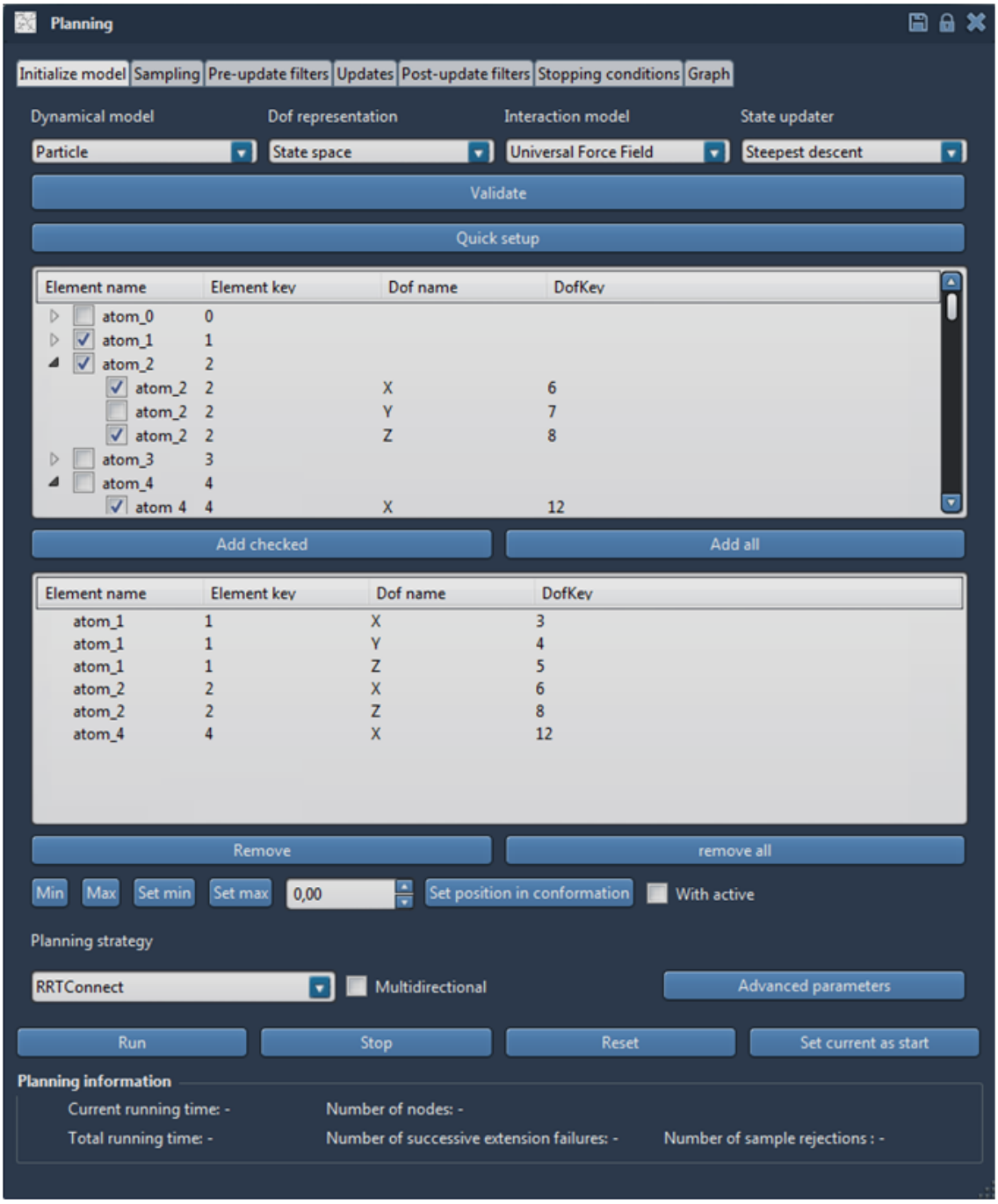


Figure 7. One tab of the graphical interface of the Planner-Explore modules, which allows initializing the model to be simulated.

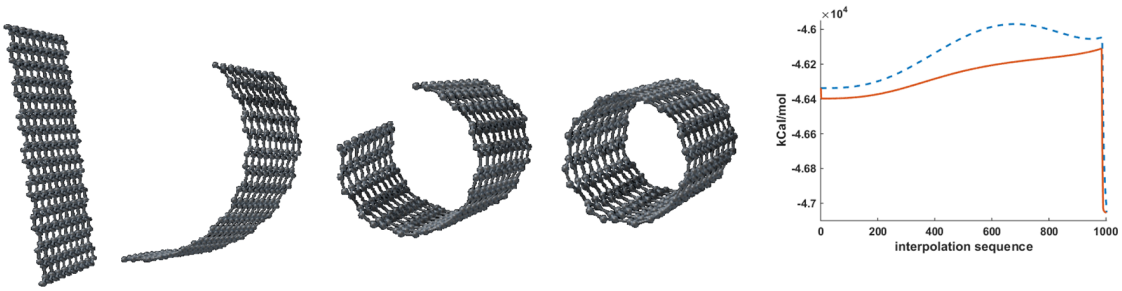


Figure 8. ARAP interpolation to generate graphene sheet folding into a nanotube. The last figure plots the energy for a sequence of 1000 interpolated images. The energy of ARAP interpolation is shown by the dotted blue curve and the optimal energy after applying NEB is shown by the solid red curve.

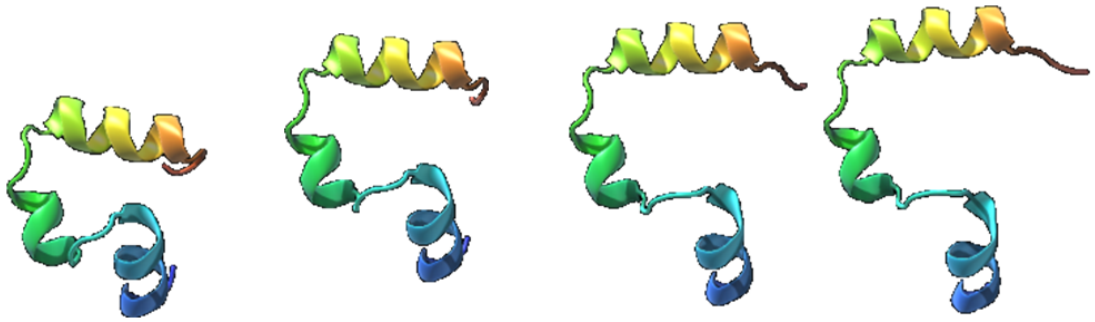


Figure 9. Transition obtained by the ARAP method of a subdomain of the villin headpiece (protein ID: 1YFR) into its distorted shape generated manually.

7.7. Automatic parameterization for the Universal Force Field

Participants: Svetlana Artemova, Leonard Jaillet, Stephane Redon.

We have continued working on the integration of the Universal Force Field in SAMSON. This force field is a classical non-reactive force field that has parameterizations for all atoms of the periodic table with atomic number lower than 103. Our implementation of this force field includes a new automatic perception scheme for molecular systems that is specifically-tailored for UFF, as well as several corrections and refinements that have been lately proposed in the literature. We have tested this implementation on more benchmarks and improved its computational performance. Additionally, we have compared our implementation to that of the OpenBabel toolbox. As a result, our self-contained implementation was integrated in a new module for SAMSON and is now available on SAMSON-Connect website (see Figure 10). The paper describing the obtained results will appear in the Journal of Computational Chemistry.

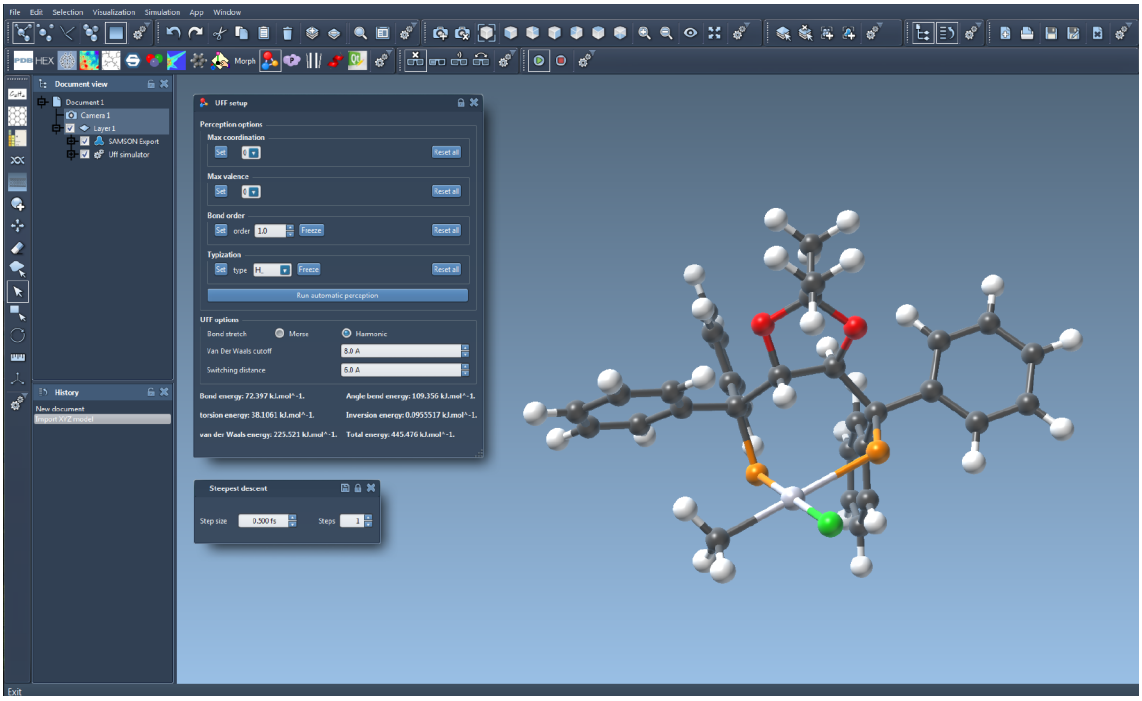


Figure 10. A molecule being interactively manipulated in SAMSON thanks to the UFF module. The interface of the UFF module allows to setup UFF. The upper part of the interface proposes options to manually adjust the perception of the molecular system. The middle part proposes the UFF options. The lower part prints out each energy contribution with the resulting total energy.

7.8. Interactive modeling with the Universal Force Field

Participants: Leonard Jaillet, Svetlana Artemova, Stephane Redon.

In parallel with the classical Universal Force Field, we have continued working on an extension of this force field that we call Interactive Modeling UFF (IM-UFF). In classical UFF topologies and atoms' typizations are set in the initialization phase and remain fixed for the entire simulation. IM-UFF, on the contrary, allows soft transitions for both topologies and atoms' typizations. This new approach, thus, combines the possibility to

significantly modify molecular structures (as with reactive force fields) with a broad diversity of supported systems thanks to the universality of UFF. Such an extension lets the user easily build and edit molecular systems interactively while being guided by physically-based inter-atomic forces. The validity of this extended version of UFF was tested on the same large set of benchmarks as those used to test classical UFF, and the results of both approaches were compared.

7.9. Error Analysis of Modified Langevin Dynamics

Participants: Zofia Trstanova, Gabriel Stoltz, Stephane Redon.

Adaptively Restrained Particles Simulations (ARPS) were recently proposed with the purpose of speeding up molecular simulations. The main idea is to modify the Hamiltonian such that the kinetic energy is set to zero for small velocities, which allows to save computational time since particles do not move and forces need not be updated. ARPS can be combined with Langevin dynamics in order to speed up the computation of macroscopic quantities.

The aim of this work is to understand how simulation errors depend on the parameters of the method. We distinguish the statistical error and the systematic error related to the finiteness of the time step Δt. The statistical error is controlled by variance, that is given by

$$\sigma^2 = -2 \left\langle A - \mu(A), \mathcal{L}^{-1} \left(A - \mu(A) \right) \right\rangle_{L^2(\mu)} \tag{1}$$

where μ is the invariant measure, $\mathcal{L}$ is the generator of the stochastic process and A an observable. First we demonstrate by use of weighted L^∞ estimations that the ARPS-Langevin dynamics are well defined. In the main part of this work, we quantify the increase of variance of the ARPS-Langevin process as a function of the ARPS parameters. For small parameters, we express the generator of the ARPS-Langevin dynamics as a perturbed generator of the Langevin dynamics, and study the asymptotic expansions of the variance (1) in the restrained dynamics parameter ε.

$$\sigma_\varepsilon^2 = \sigma^2 + \mathcal{O}(\varepsilon)$$

For large values of ε, we perform numerical simulations. For a simple 1D system we approximate $\mathcal{L}^{-1}$ by Galerkin approach and for higher-dimensional systems we discretize the stochastic differential equations by a second order method and analyze a model of a dimer surrounded by solvent particles.

7.10. Algorithmic speed up of the ARPS method

Participants: Zofia Trstanova, Gabriel Stoltz, Stephane Redon.

Adaptively Restrained Particles Simulations (ARPS) allow to save computational time at each time step since particles do not move and forces need not be updated. The associated gain can be quantified by an algorithmic speed-up factor $S_{\text{algo}} \geq 1$. Intuitively, freezing more particles leads to larger algorithmic speed-ups, but also larger correlations in time.

We analyzed the algorithmic speed up with respect to the standard methods. Since the ARPS algorithm is based on adding and subtracting of the forces between active particles, the gain with respect to the standard method, where only one complete computation of all interactions is performed at each time step, is achieved only if the percentage of restrained particles is big enough. Hence we studied the necessary conditions, under which the computational complexity of the forces updating in the ARPS method is lower than the one of the standard method. This allows to achieve an algorithmic speed up that is always bigger than one.

We also propose a simple strategy for choosing optimal simulation parameters.

7.11. Numerical analysis for the ARPS method

Participants: Zofia Trstanova, Gabriel Stoltz, Stephane Redon.

Previous works have led to understanding of the choice of optimal parameters for the ARPS dynamics. The interest lies in achieving the highest percentage of restrained particles, while minimizing the modification of the variance and the systematic error. We study discretization schemes of the ARPS-Langevin dynamics, such that the systematic error remains of second order in the time step size and we introduce a Metropolis step in order to stabilize the simulations and hence to allow "a sharper" choice of the ARPS parameters, which lead to better algorithmic speed-ups.

7.12. New rendering algorithm for secondary structures

Participants: Marc Aubert, Stephane Redon.

We developed a new algorithm for rendering secondary structures of proteins (Figure 11). The method relies on the determination of the most probable secondary structure elements (e.g. alpha helices and beta sheets) based on geometrical features of a protein. After construction of control points on the CPU, the method generates triangles directly on the Graphics Processing Unit (GPU) through geometry shaders. The number of generated triangles may be adaptively chosen based on e.g. the camera distance and the desired resolution. The secondary structure algorithm and the rendering algorithm are both fast enough to allow for interactive modification of the protein (e.g. thanks to As-Rigid-As-Possible editing algorithms).

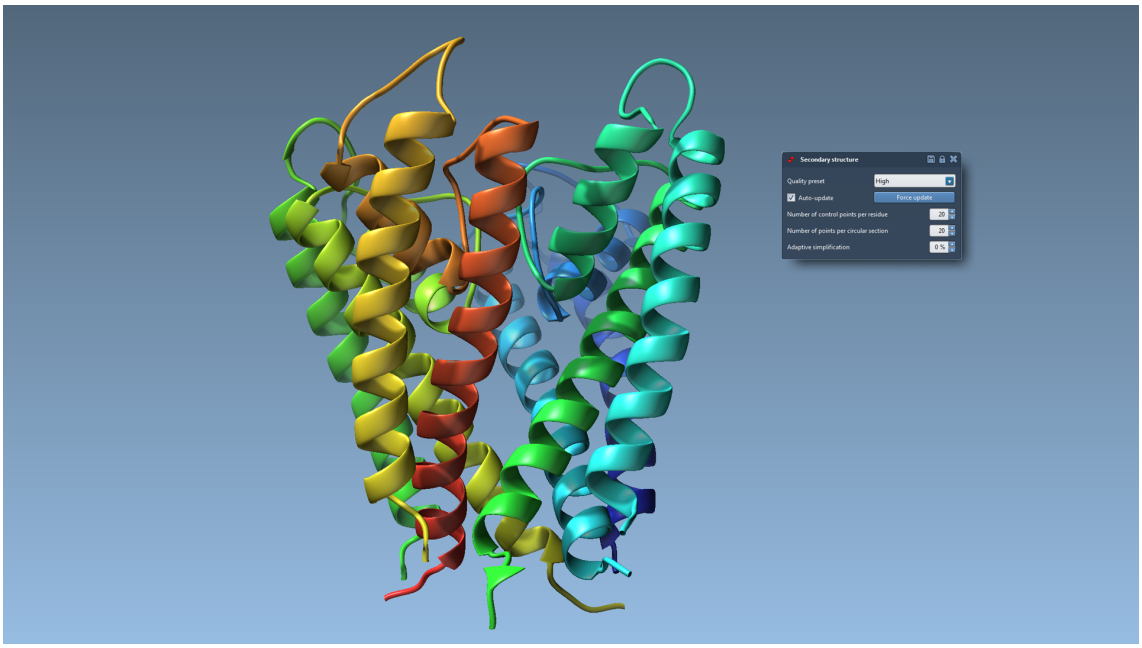


Figure 11. Protein secondary structure rendering on GPUs.

7.13. Property models

Participants: Marc Aubert, Stephane Redon.

We extended the hierarchy of classes in SAMSON for *property models*. Property models are one of the five categories of models in SAMSON, with structural models (for geometry and topology), visual models (for custom graphical representations), dynamical models (to describe degrees of freedom) and interaction models (to represent energies and forces). We have added classes to easily represent in SAMSON various functions, fields (e.g. scalar fields and vector fields), etc. These property models are template classes which may rely on the unit system of SAMSON to perform dimensional analysis at compile time.

7.14. Integration of tools in SAMSON

Participants: Nadhir Abdellatif, Stephane Redon.

Thanks to funding from the Nanosciences Foundation in Grenoble, we developed SAMSON Elements (modules for SAMSON) that integrate existing tools. In particular, we integrated OpenBabel, a tool to convert between numerous molecular formats (Figure 12), ClustalW, a tool for sequence alignment (Figure 13), and Pepsi-SAXS, a tool for SAXS developed in the group (Figure 14).

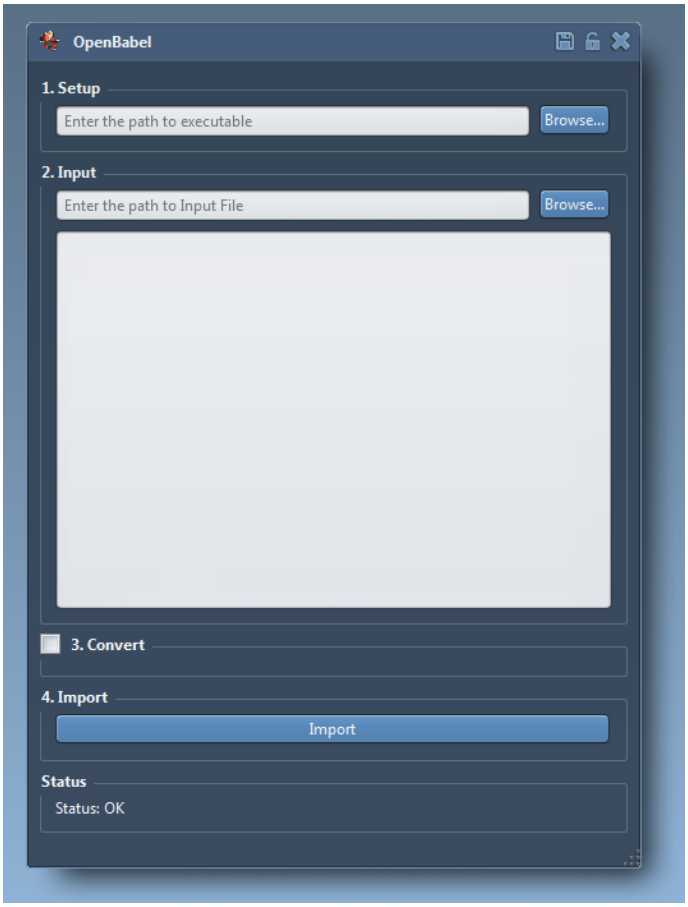


Figure 12. The OpenBabel connector in SAMSON

7.15. Development of SAMSON Connect

Participants: Mohamed Yengui, Jocelyn Gate, Stephane Redon.

We have continued the development of SAMSON Connect (Figure 15 , https://www.samson-connect.net), the online platform for distributing SAMSON and SAMSON Elements (modules for SAMSON). SAMSON Connect is a web application, associated to a database, that functions as the well-known stores for mobile Apps (e.g. Google Play, the Apple App store, etc.). Users may create an account, download SAMSON, and add SAMSON Elements to their configuration based on their needs (Figure 16). Adding a SAMSON Element is performed in just one click (to the Add button of the corresponding SAMSON Element), and the SAMSON

Figure 13. ClustalW in SAMSON

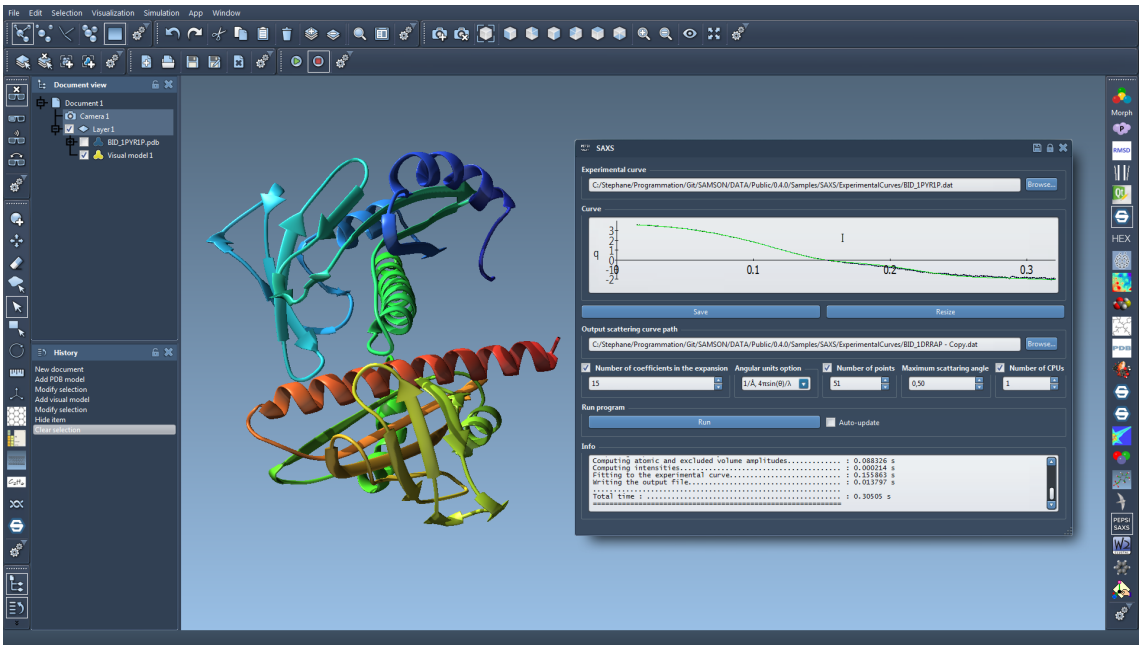


Figure 14. Our Pepsi-SAXS tool integrated in SAMSON

Element is installed when the user restarts SAMSON. Users may also request an upgrade to a Developer status, after which they can download the SAMSON Software Development Kit used to develop SAMSON Elements. They may then upload their SAMSON Elements to SAMSON Connect in order to share them. The platform opened in March 2015 to release the first beta version of SAMSON. We also produced some video tutorials for SAMSON (Figure 17).

On the back-office of SAMSON Connect, we added several functionalities that facilitate publishing new versions of SAMSON and SAMSON Elements (e.g. choosing default SAMSON Elements), email users based on their account type (user, developer, etc.), OS, etc. We also turned to automatic acceptance of new user accounts (once they validate their email address). We also updated the SAMSON web service to enable more message types and retrieve information about the server, the database, etc.

7.16. Documenting the SAMSON Software Development Kit

Participants: Stephane Redon, Jocelyn Gate, Svetlana Artemova.

The SAMSON Software Development Kit (SDK) is at the core of the SAMSON platform and makes it possible to develop SAMSON Elements (modules). The API of SAMSON contains numerous classes and allows for a variety of modules types (e.g. parsers, force fields, visual models, integrators, apps, editors, etc.), and provides several non-elementary mechanisms (e.g. a unit system, a signals and slots mechanism, memory management, data structures for incremental calculations, etc.). We continued writing the SDK documentation accessible to SAMSON Elements developers. The current PDF version for the beta 0.4.0 version has passed 500 pages.

7.17. SAMSON SDK Helpers

Participants: Jocelyn Gate, Stephane Redon.

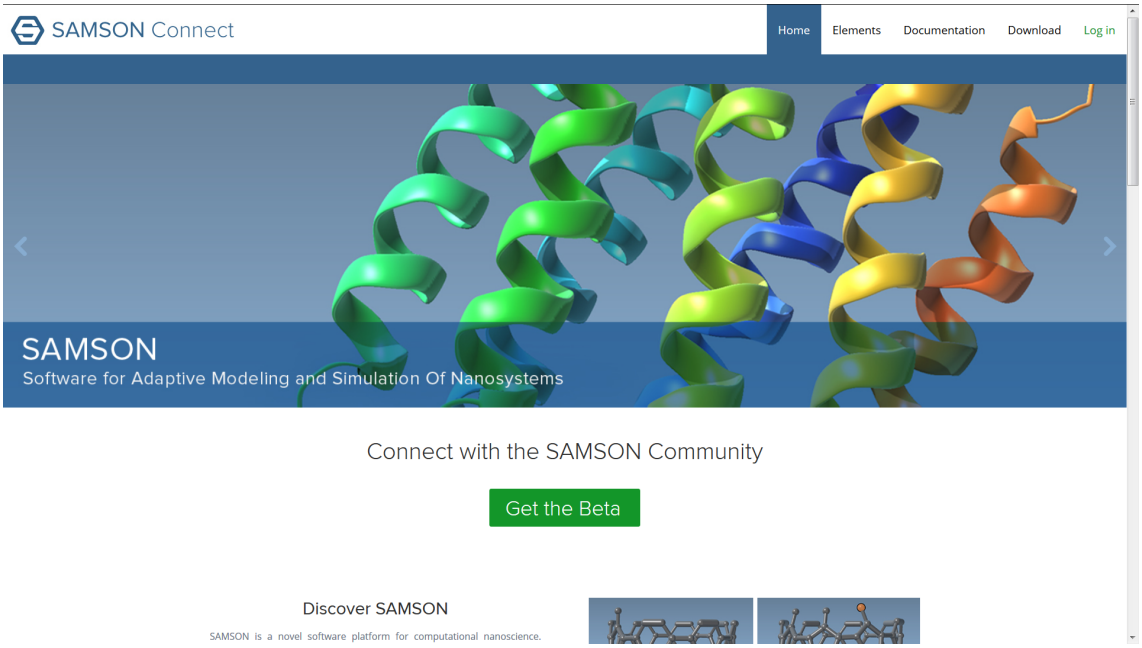


Figure 15. The home page of SAMSON Connect (https://www.samson-connect.net)

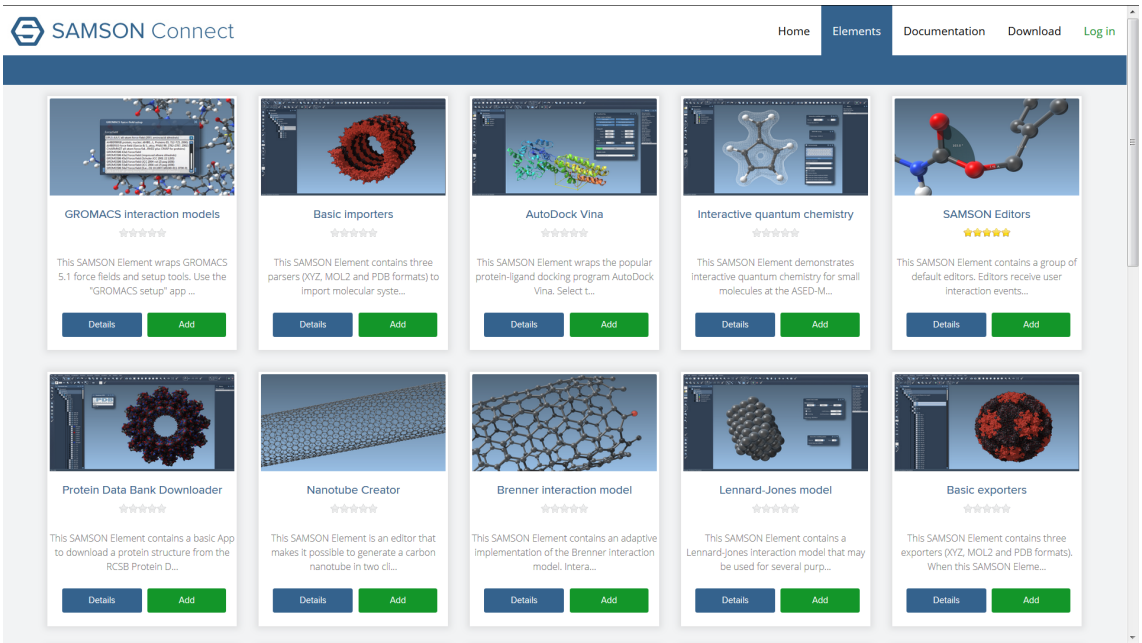


Figure 16. The Elements page, where users may add SAMSON Elements (modules) to their configuration (https://www.samson-connect.net)

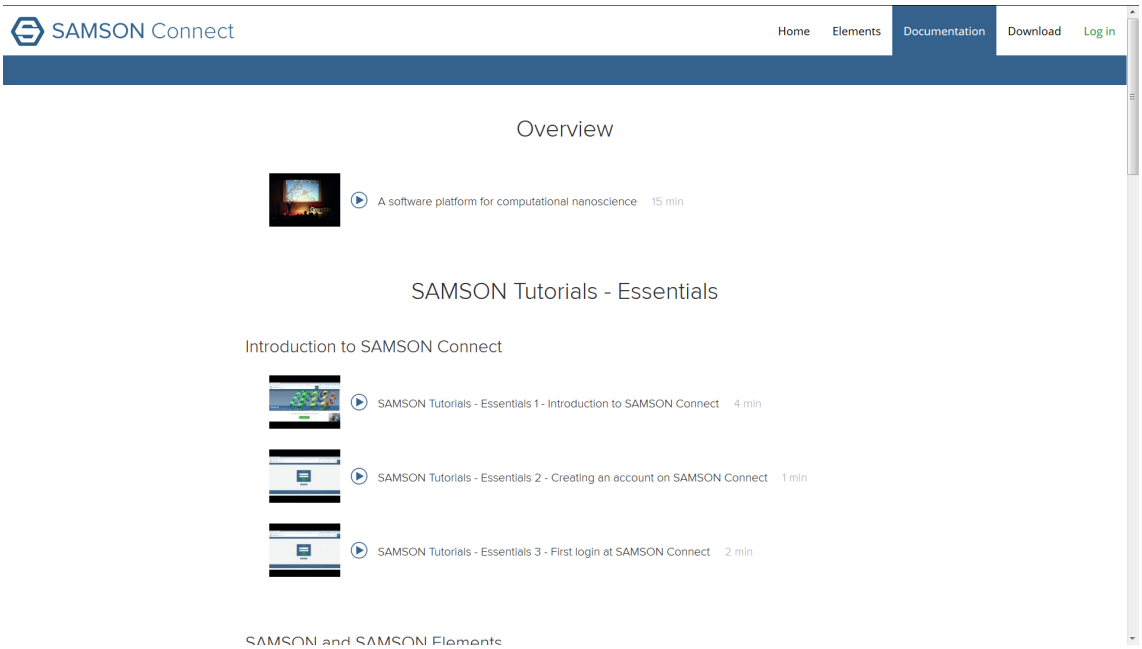


Figure 17. The documentation page on SAMSON Connect (https://www.samson-connect.net)

We have developed a number of Helpers in the SAMSON SDK, in order to facilitate the development of SAMSON Elements (modules for SAMSON). For example, the SAMSON Element generator (Figure 18) generates code that immediately compiles and runs, and that developers may complete, for a number of SAMSON Classes.

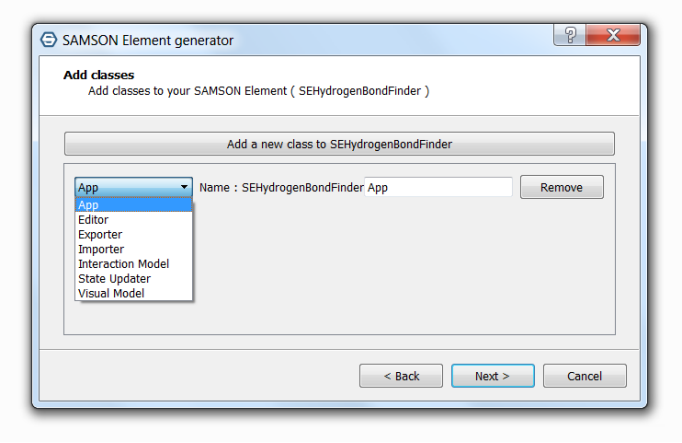


Figure 18. The SAMSON Element Generator makes it easy to develop modules for SAMSON

We have also developed for the group a helper able to upload numerous SAMSON Elements to SAMSON Connect at the same time (Figure 19), which is especially useful given the rapidly growing number of modules being developed in the team.

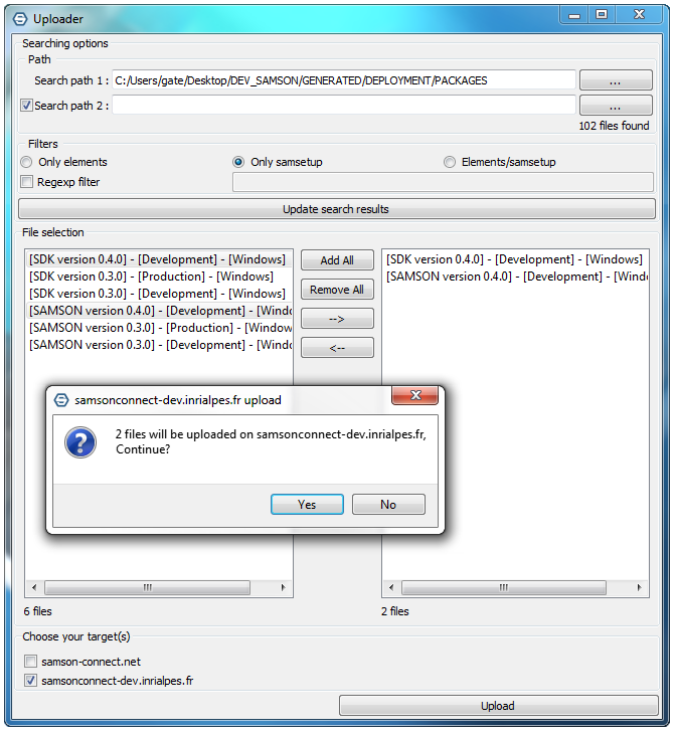


Figure 19. The SAMSON Element uploader eases the transfer of multiple SAMSON Elements to SAMSON Connect

7.18. Pepsi-SAXS : an adaptive method for rapid and accurate computation of small angle X-ray scattering profiles

Participant: Sergei Grudinin.

We developed a new method called Pepsi–SAXS that calculates small angle X-ray scattering profiles from atomistic models. Our method is based on the multipole expansion scheme and is significantly faster and more precise compared to other tested methods. In particular, using the Nyquist–Shannon–Kotelnikov sampling theorem, we adapt the multipole expansion order to the size of the model and the resolution of the experimental data. We argue that using the adaptive expansion order, our method has the same quadratic dependence on the number of atoms in the model as the Debye-based approach, however, with a much smaller prefactor in the computational complexity.

We have systematically validated our method on an excessive set of over fifty models collected from the BioIsis and SASBDB databases. Using a laptop, we demonstrated that Pepsi-SAXS is about 9, 33 and 43 times faster compared to CRYSOL, FoXS and the 3D-Zernike method in SAStbx, correspondingly, when tested on data from the BioIsis database, and is about 5, 18 and 23 times faster compared to CRYSOL, FoXS and SAStbx, correspondingly, when tested on data from SASBDB. On average, Pepsi-SAXS achieves 17% smaller value of χ compared to CRYSOL and 15% smaller value of χ compared to FoXS for BioIsis profiles, and 6% smaller value ofχ compared to CRYSOL and 19% smaller value of χ compared to FoXS for SASBDB profiles.

7.19. Knodle: a Support Vector Machines-based automatic perception of organic molecules from 3D coordinates

Participants: Maria Kadukova, Sergei Grudinin.

We addressed the problem of the assignment of atom types and bond orders in low molecular weight compounds. For this purpose, we developed a prediction model based on nonlinear Support Vector Machines (SVM), implemented in a KNOwledge-Driven Ligand Extractor called *Knodle*, a software library for the recognition of atomic types, hybridization states and bond orders in the structures of small molecules. We trained the model using an excessive amount of structural data collected from the PDBbindCN database. Accuracy of the results and the running time of our method is comparable with other popular methods, such as NAOMI, fconf, and I-interpret. More precisely, on the popular Labute's benchmark set consisting of 179 protein-ligand complexes, *Knodle* makes five to six perception errors, NAOMI makes seven errors, I-interpret makes nine errors, and fconv makes thirteen errors. On a larger set of 3,000 protein-ligand structures collected from the PDBBindCN general data set (v2014), *Knodle* along with NAOMI have a comparable accuracy of approximately 6 % of errors, whereas fconv produces approximately 13 % of errors. Overall, our study demonstrates the efficiency of nonlinear SVM in structure perception tasks.

7.20. Symmetry Detection Method

Participants: Silvia Dias Pinto, Sergei Grudinin.

We developed an algorithm for automatic recognition of the point group symmetry in electron density maps of biological objects. More precisely, the method operates on cryo-Electron Microscopy (cryoEM) data, which typically contain 3D structures of multi-domain proteins and their complexes. We represent the shape using a spherical harmonic decomposition and then operate on the expansion coefficients to quantify the structural symmetry thanks to a mismatch function. Overall, we developed new mathematical and computational frameworks for symmetry detection using the polynomial expansion approach.

7.21. Pepsi-Dock: fast predictions of putative docking poses using accurate knowledge-based potentials functions to describe interactions between proteins

Participants: Emilie Neveu, Sergei Grudinin, David W. Ritchie, Petr Popov.

Many biological tasks involve finding proteins that can act as an inhibitor for a virus or a bacteria, for example. Such task requires knowledge on the structure of the complex to be formed. Protein Data Bank can help but only a small fraction of its proteins are complexes [16]. Therefore, computational docking predictions, being low-cost and easy to perform, are very attractive if they describe accurately the interactions between proteins while being fast to find which conformation will be the most probable. We have been developing a fast and accurate algorithm that combines the FFT-accelerated docking methods [67] with a precise knowledge-based potential functions [58] describing interactions between the atoms in the proteins .

Interactions between proteins follow complex and non-linear laws which computation is time-consuming. It is of common usage to start the predictions with a simple, approximated, expression of these interactions to then reduce the space search in order to use more complex laws. However we think it is important to use the most accurate free energy not to miss some important docking solutions. Thus, our aim is to integrate the very-detailed knowledge-based potentials into the *Hex* code and to take advantage of its exhaustive search, which is by now still the most efficient and reliable search algorithm [67] .

Last year, we adapted the machine learning process so that the knowledge-based potentials describing atom interactions can be translated into the polynomial basis used in *Hex*. The current evaluations of the knowledge-based scores takes more time than a shape+electrostatic representation but is still fast: exploring 10^9 conformations of a complex takes on average 5-10 minutes on a regular laptop computer.

This year, we run cross-validation experiments and tested different data sets in order to improve the predictions. Using bound conformations of each proteins to make the predictions, we retrieve up to 70% correct complexes of about 200 complexes. Results show that the knowledge-based potentials, while being general, correctly predict the interactions. Even better results could be achieved without the limitations in the search range by the spherical sampling grid which lacks of precision far away of its origin. Because many complexes have separation distances greater than 30 Å, we are now working on a multi-centre definition of the potentials in order to correctly predict the structures of protein complexes starting from their unbound structures.

7.22. Pepsi-Piper: rigid docking predictions using Pepsi potentials into Piper code

Participants: Sergei Grudinin, Emilie Neveu, Dima Kozakov, Dzmitry Podgorny.

This work is the continuation of the Pepsi-Dock project that aims to develop fast predictions of putative docking poses using accurate knowledge-based potentials functions to describe interactions between proteins. The goal is to integrate the precise, and yet easy to compute, distance-based pairwise knowledge-based potentials [58] into the Piper search code [48] in order to compare its exhaustive search with the *Hex* one. The former samples the conformations using a cartesian grid while the latter, a spherical one. We proved our potential used in *Hex* can predict the structures of complexes with a really good success rate, the main limitation being the lack of precision of the spherical sampling when the separation distance of the two proteins is too large. We think predicting docking combining our potential and a sampling search based on a cartesian grid as in Piper will achieve greater results, but will require more computational time.
We first adapt our potential to the Piper code and showed that the ranking results on the data set used for training are better than the ranking provided by Piper [25]: when the potential is used to sort the conformations, the correct solution is found in the first ten for 85% cases, while Piper found it in only 25% cases. The next step is to use the cartesian sampling to make docking predictions. When the Piper code will be ready to integrate our potential, we will be able to confront with other knowledge-based potentials such as the one initially used in Piper, DARS.

7.23. Flex-Dock: towards flexible docking predictions using metaheuristics optimisation methods

Participants: Emilie Neveu, Sergei Grudinin, Alexandre Hoffman, Angelo Migliosi, Xavier Besseron, Grégoire Danoy, Pascal Bouvry.

Docking numerical methods are used to predict the preferred location of one molecule with respect to the second when bound to each other. This is particularly useful for the design of drugs that inhibit the effects of viruses or bacteria. However proteins change their conformation upon binding and searching for flexible conformations involves enormous degrees of freedom and complex physics. Thus, the prediction of realistic interactions with full flexibility of the two partners is an intractable global optimisation problem.
There are currently several algorithms that produce high quality predictions of molecular complexes [43]. But very few manages to deal with the flexibility of the proteins. A common method is to refine the most probable predicted rigid complexes with a scoring allowing for flexibility [81]. Here, we want to tackle flexibility and sampling all together. Exhaustive search methods, which were by now the most accurate optimisation method for relatively small molecules [53] will be too time-consuming when it comes to large proteins. There is a strong need to explore and define new optimisation algorithms such as metaheuristic ones that can deal with several local minima and a large minima and a large search space. The main goal of this project is to define the problem and find for the optimisation method that will potentially give better results than the actual reference, SwarmDock [54].
We worked on a first comparison of several evolutionary-based algorithms (Genetic Algorithm [40], Differential Evolution [76], Particle Swarm Optimisation [46]) using rigid proteins only and on the use of multi-objective algorithms when the proteins are flexible.

To take into account flexibility, we approximate large-scale deformations of each proteins using an elastic network model combined with a low-frequency approximation called normal mode analysis such as in [81] or in [54]. Combined with the rigid transformation between the two proteins, it defines a complete while reduced set of degrees of freedom to search for.
The scoring function has to discriminate correct conformations from impossible ones. Our scoring is the main difference with SwarmDock. It takes into account the energy gained by docking using the precise knowledge-based potentials derived in [58], whereas only a simple physics-based energy is used in SwarmDock. We also want to explore another scoring that will also add the energetic cost of each moves of the proteins. To do so, we started to develop multi-objective algorithms. Combined with a Pareto Front analysis, this will help us to validate the scoring and to compare different evolutionary-based algorithms.Tests will be directly made on the Protein-Protein Benchmark [42] so that we can compare with other docking methods.

7.24. FastRMS: rapid determination of RMSDs corresponding to macromolecular rigid body motions, adding flexibility via collective motions

Participants: Sergei Grudinin, Petr Popov, Emilie Neveu.

Computing the root mean sum of squared deviations (RMSDs) between two sets of coordinates each describing a different conformation of a macromolecule is a necessary step in many structural bioinformatics and molecular modelling technics to assess structural predictions [43], identify biding sites [49] or structurally classify proteins. A straightforward and universally-used method determines the RMSD with a computational complexity proportional to the number of atoms in the molecule. We recently presented RigidRMSD, a fast algorithm that determines RMSDs corresponding to a set of rigid body motions of a macromolecule in constant time with respect to the number of atoms in the molecule [57]. Here, we extend it to proteins with flexibility modelled with collective motion such as an elastic network model combined with normal mode analysis.
With these new assumptions, the complexity of the algorithm depends linearly or quadratically with the number of collective motion vectors selected to approximate the flexibility. The typical number of vectors needed to have accurate flexible movements being much lower than the number of atoms composing the molecules, we prove our algorithm is still faster than the common method. Our algorithm is particularly useful for rigid body modelling applications such as rigid body docking procedures allowing for flexibility via collective motions: clustering, high-throughput analysis and simulation results [49], [26], [59]. A C++ implementation of our algorithm will be soon available at http://nano-d.inrialpes.fr/software/RigidRMSD.

7.25. SAM : Spherical Polar Fourier Assembly of Protein Complexes with Arbitrary Point Group Symmetry

Participants: David W. Ritchie, Sergei Grudinin.

We presented a novel FFT-based *ab inito* docking algorithm called "SAM" for building perfectly symmetrical models of protein complexes with arbitrary point group symmetry. The basic approach uses a novel and very fast 1D symmetry-constrained spherical polar Fourier search to assemble cyclic C_n systems from a given protein monomer. Structures with higher order (D_n, T, O, and I) point group symmetries may be built using a subsequent symmetry-constrained Fourier domain search to assemble trimeric sub-units. Our results show that the SAM algorithm can correctly assemble monomers of up to around 500 residues to produce a near-native complex structure with the given point group symmetry in 17 out of 18 test cases. The SAM program may be downloaded for academic use at *http://sam.loria.fr/*.

7.26. KSENIA : Knowledge of Native Protein-Protein Interfaces is Sufficient to Construct Predictive Models for the Selection of Binding Candidates

Participants: Petr Popov, Sergei Grudinin.

Selection of putative binding poses is a challenging part of virtual screening for protein-protein interactions. Predictive models to filter out binding candidates with the highest binding affinities comprise scoring functions that assign a score to each binding pose. Existing scoring functions are typically deduced collecting statistical information about interfaces of native conformations of protein complexes along with interfaces of a large generated set of non-native conformations. However, the obtained scoring functions become biased toward the method used to generate the non-native conformations, i.e. they may not recognize near-native interfaces generated with a different method.

Present study demonstrates that knowledge of only native protein-protein interfaces is sufficient to construct well-discriminative predictive models for the selection of binding candidates. Here, we introduce a new scoring method that comprises a knowledge-based potential called *KSENIA* deduced from the structural information about the native interfaces of 844 crystallographic protein-protein complexes. We derive *KSENIA* using convex optimization with a training set composed of native protein complexes and their near-native conformations that are obtained using deformations along the low-frequency normal modes. As a result, our knowledge-based potential has only marginal bias toward a method to generate putative binding poses. Furthermore, *KSENIA* is smooth by construction, which allows to use it along with a rigid-body optimization to refine the binding poses. Using several test benchmarks we demonstrate that our method discriminates well native and near-native conformations of protein complexes from the non-native ones. Our methodology can be easily adapted to the recognition of other types of molecular interactions, such as protein-ligand, protein-RNA, etc. *KSENIA* will be made publicly available as a part of the SAMSON software platform at https://www.samson-connect.net.

7.27. Predicting Binding Poses and Affinities in the CSAR 2013–2014 Docking Exercises Using the Knowledge-Based Convex-PL Potential

Participants: Sergei Grudinin, Petr Popov, Emilie Neveu, Georgy Cheremovskiy.

The 2013–2014 CSAR docking exercise was the opportunity to assess the performance of the novel knowledge- based potential we are developing, named Convex-PL. The data used to derive the potential consists only of structural information from protein-ligand interfaces found in the PDBBind database. As expected, our potential proved to be very efficient in the near- native pose detection exercises, where we correctly predicted two near-native poses in the 2013 exercise and also ranked 22 near- native poses first and 2 second in the 2014 exercise. Somewhat more surprisingly, we obtained a fair performance in some of the CSAR affinity ranking exercises, where the Spearman correlation coefficients between our predictions and the experiments are greater than 0.5 for several protein–ligand sets. Nonetheless, affinity prediction exercises turned out to be a challenge, and significant progress in the development of our method is needed before we can successfully predict binding constants.

7.28. Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: a CASP-CAPRI experiment

Participants: Sergei Grudinin, Petr Popov, Emilie Neveu.

We present the results for CAPRI Round 30, the first joint CASP-CAPRI experiment, which brought together experts from the protein structure prediction and protein-protein docking communities. The Round comprised 25 targets from amongst those submitted for the CASP11 prediction experiment of 2014. The targets included mostly homodimers, a few homotetramers, and two heterodimers, and comprised protein chains that could readily be modeled using templates from the Protein Data Bank. On average 24 CAPRI groups and 7 CASP groups submitted docking predictions for each target, and 12 CAPRI groups per target participated in the CAPRI scoring experiment. In total more than 9500 models were assessed against the 3D structures of the corresponding target complexes. Results show that the prediction of homodimer assemblies by homology modeling techniques and docking calculations is quite successful for targets featuring large enough subunit interfaces to represent stable associations. Targets with ambiguous or inaccurate oligomeric state assignments, often featuring crystal contact-sized interfaces, represented a confounding factor. For those,

a much poorer prediction performance was achieved, while nonetheless often providing helpful clues on the correct oligomeric state of the protein. The prediction performance was very poor for genuine tetrameric targets, where the inaccuracy of the homology-built subunit models and the smaller pair-wise interfaces severely limited the ability to derive the correct assembly mode. Our analysis also shows that docking procedures offer a clear advantage over standard homology modeling techniques and that highly accurate models of the protein components are not always required to identify their association modes with acceptable accuracy.

Most of the targets in Round 30 of CAPRI were homodimers and homotetramers, thus it was a good opportunity to test our novel symmetry assembling docking method. To do so, we imposed C2 symmetry constraints for all the homodimers and we imposed C4 and D2 symmetry constraints for all the homotetramers from the target complexes. Below, we present the new fast multi-resolution method for docking both symmetric and non-symmetric protein complexes that was used in Round 30 of CAPRI. First, the structures of the individual subunits were taken from the stage two predictions of the CASP10 assessment experiment. More precisely, starting from 150 available CASP 3D models of monomers, we predicted models of symmetric multimers using the novel symmetry docking method, which performs symmetry-induced protein docking using the shape-complementarity scoring function computed as spherical polar Fourier correlations. Specifically, this method performs exhaustive search over the available (four in case of cyclic symmetries or six otherwise) degrees of freedom for the given point group symmetry type. For the targets of Round 30 of CAPRI we imposed three types of symmetry, C2, C4, and D2. For the case of heterodimers, we used the standard Hex docking method.

For the input of the docking methods, we generated the scaffolds of initial models of monomers by cutting-off the side chains. More specifically, we mutated all side-chains except for the glycines to alanines. Compared to the standard all-atom rigid-body docking methods, we expect the scaffold docking approach to produce binding poses that are less sensitive to the flexibility of the side-chains. We clustered the solutions with the threshold ligand-RMSD value of 8 Åusing the RigidRMSD library. Finally, we ranked the clusters by the value of the best score and kept 50 best clusters for the refinement stage. In total, for each target we proceeded to the refinement with 7,500 modeled structures of protein complexes.

On the next step, we optimized each putative binding interface of the all-atom representation of a protein complex by means of a rigid-body first-order minimization scheme. Specifically, after each rigid-body minimization step we proceeded with the optimization of side-chains described by the rotameric representation using the SCWRL4 package. We computed the interactions between the subunits in a protein complex using the novel reference state-free knowledge-based scoring function KSENIA, which is smooth by construction and is thus very suitable for a gradient-based minimization protocol. Finally, we ranked the predictions by the value of the KSENIA potential of the optimized structure and selected ten best candidates for the submission.

7.29. Convex relaxation for non-convex quadratic optimization problems with applications to side-chain prediction in protein structures

Participants: Aleksandr Katrutsa, Sergei Grudinin.

The side-chain prediction problem is the major part of the more general protein structure prediction problem, which is very important for drug design and in the prediction of stable protein mutations. Formally, the side-chain prediction problem states in the form of discrete quadratic optimization problem with an indefinite matrix in the quadratic term,

$$\mathbf{x}^\top \mathbf{Q}\mathbf{x} + \mathbf{b}^\top \mathbf{x} \to \min_{\mathbf{x}\in\{0,1\}^n} \tag{2}$$

This problem is NP-hard, so to get a good approximation solution we used convex semidefinite relaxation with different types of constraints. This approach is the powerful optimization technique that helps to reformulate the initial non-convex problem as a convex one and sometimes even gives the exact solution. The important step is to operate with precise energy function, which is used to compute the energy of different interactions

in proteins. To obtain this, we used the machine-learning procedure, which extracts the parameter vector for the potential from the training set of protein structures. After the training step, we used this vector to compute the energy of a protein and to find the side-chains corresponding to the minimal total energy of the protein. The current accuracy in side-chain prediction is about 80%, which is achieved using the spectrum relaxation of the matrix in the quadratic term. Also, this approach is very fast, precisely, it requires less than 1 second per protein to predict the positions of its side-chains.

7.30. Critical assessment of protein-ligand docking methods via Drug Design Data Resource (D3R) Challenge 2015

Participants: Andreas Eisenbarth, Sergei Grudinin.

We participated at the Drug Design Data Resource (D3R) Challenge 2015. In the challenge, we were given protein structures and sets of ligand molecules in order to detect the putative binding poses. The aim was to find the energetically most favourable pose of each ligand relative to a protein. To do so, we first performed the docking simulations using the state-of-the-art software AutoDock Vina, then explored sets of parameters that produced chemically reasonable poses, and finally did the re-scoring using the ComvexPL potential. Later, we critically examined AutoDock Vina sampling method and detected points where it can be improved and also assessed the integration of our inhouse developed ConvexPL scoring algorithm.

7.31. Towards the development of FFT-accelerated flexible fitting methods

Participants: Alexandre Hoffmann, Valerie Perrier, Sergei Grudinin.

We studied a set of new methods for non-rigid molecular fitting. The problem can be formulated as follows : Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be two molecular structures (e.g. proteins). We are given $d_1 : \mathbb{R}^3 \mapsto \mathbb{R}$, the electron density of $\mathcal{P}_1$ and $(Y_k \in \mathbb{R}^3)_{k=1\cdots N_{atoms}}$, the average positions of the atoms of $\mathcal{P}_2$. Assuming we can generate an artificial electron density $d_2 : \mathbb{R}^3 \mapsto \mathbb{R}$ from $(Y_k \in \mathbb{R}^3)_{k=1\cdots N_{atoms}}$, our problem is to find a transformation of the atoms $T : \mathbb{R}^{3N_{atoms}} \mapsto \mathbb{R}^{3N_{atoms}}$ that minimizes the L^2 distance between d_1 and d_2.

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

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

We have developed several algorithms based on the FFT to find T_{rigid} and we have developed two algorithms for flexible molecular fitting that are based on convex and non-convex optimization and the trust region methods. Our tests demonstrate that while one method gives good results for small deformations, the other gives good results for bigger deformations.

We have been also improving the current NMA method (which is essentially a model reduction technique), that is used in other tools such as the flexible fitting to small angle scattering profiles. Finally, we started the development of a method for a harder fitting/docking problem in which only electron density would be known. The basic idea would be to find the C^1-diffeomorphism $T : \mathbb{R}^3 \mapsto \mathbb{R}^3$ that minimizes the L^2 distance between d_1 and d_2.

We developed several stand-alone C++ libraries to solve some of our problems including:

- a non-convex optimization library,
- a normal mode analysis library,
- a fitting library that implements our new methods.

POEMS Project-Team

6. New Results

6.1. Wave propagation in non classical media

6.1.1. Modal analysis of electromagnetic dispersive media

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

Except in vacuum, the velocity of electromagnetic waves generally depends on the frequency. This dispersion plays in particular a vital role in situations where the effective index takes values below unity or negative, which happens with metamaterials or plasmonic devices. However, most of the studies in this domain are considering only the time-harmonic regime, forgetting dispersion, which leads to apparent paradoxes. We have elaborated a project, in collaboration with the Institut Fresnel in Marseille. Our objective is to gather physical and mathematical points of view to explore a frequency-to-time approach for dispersive media. This approach is based on a general technique which allows to hide dispersion in an augmented formulation of Maxwell's equations. Using this tool, our aim is first to carry the spectral analysis of dispersive systems, take advantage of this analysis to predict the time-dependent behaviour of dispersive systems, then design adapted numerical methods for their simulation and finally confirm predictions by real experiments. To begin with, during the internship of Bilal Yezza, a toy problem has been studied, where the presence of accumulation points in the spectrum is due to the dispersion. This project has been submitted to the ANR for the second year and has already led to preliminary common works and discussions, in particular during the workshop *Leaky days* organized by Christophe Hazard in Palaiseau in June 2015.

6.1.2. Perfectly Matched Layers in plasmas and metamaterials

Participants: Eliane Bécache, Patrick Joly, Maryna Kachanovska, Valentin Vinoles.

We work on the stability of Generalized Perfectly Matched Layers (GPMLs) in dispersive media for which classical PMLs are in general unstable. These new PMLs involve, in addition to the absorption parameter $\sigma \geq 0$, a real valued rational function of the frequency $\psi(\omega)$. We first worked on isotropic media and derived, using Fourier analysis methods, a necessary and sufficient condition on the function $\psi(\omega)$ for the stability of the PML model. This result has been presented in several conferences and used to design new stable PMLs for negative index metamaterials and uniaxial anisotropic plasmas (even though this last model is anisotropic, the anisotropy has a structure that permits a special decomposition of vector fields that give a new equivalent model adapted for our GPMLs).

We are currently working on the generalization of this analysis to a class of anisotropic dispersive models using a different approach based on Laplace transform in time.

However, this theory does not apply to more general cold plasma models that we wish to treat. Finding good PMLs in this case still remains a challenging open question. Several attempts, such as radial PMLs (which we discussed about with our visitor Martin Halla from TU Wien), have failed.

6.2. Wave propagation in heterogeneous media

6.2.1. Homogenization of layered media

Participant: Jean-François Mercier.

Metamaterials have revived interest in the theory of homogenization techniques because some standard techniques, based on the Ross Nicholson-Weir method, can lead to unphysical effective parameters, since depending on the incident wave. In collaboration with Agnès Maurel and Abdelkader Ourir from the Langevin Institut and Simon Felix from the LAUM, we have proposed more suitable homogenization methods to describe wave propagation in artificial environments, by considering homogenization of sliced media. When the medium is structured at a sub-wavelength scale, it can be described as a simpler equivalent medium, homogeneous and anisotropic, with a tensor mass density and an effective modulus of elasticity. We considered two cases:

- for a propagating incident wave, we obtained the diffusion properties of the medium and we have shown that the effective medium correctly captures the acoustic properties of the real medium.

- however, in the real problem, evanescent waves are generated and if one of them is resonant, the properties of transmission and reflection of the incident wave are changed: this happens for the electromagnetic waves (Wood anomalies, "spoof plasmon"). To capture these resonance effects, we have considered evanescent incident waves. We then showed that the homogenization predicts the dispersion curves of the resonant waves: in the homogenized problem, they correspond to guided waves by the anisotropic layer.

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

Participants: Sonia Fliss, Valentin Vinoles.

This work is a part of the PhD of Valentin Vinoles, and is done in collaboration with Xavier Claeys (LJLL, Paris VI). It is motivated by the fact that classical homogenization theory poorly takes into account interfaces, which is particularly unfortunate when considering negative materials, because important phenomena arise precisely at their surface (plasmonic waves for instance). To overcome this limitation, we want to construct high order transmission conditions. Using matched asymptotics, we have treated the case of a plane interface between a homogeneous and a homogenized periodic half space. The analysis is based on an original combination of Floquet-Bloch transform and a periodic version of Kondratiev techniques. The obtained conditions involve Laplace- Beltrami operators at the interface and require to solve *cell problems* in infinite strips. The numerical computations are based on specific transparent conditions for periodic media. The error analysis and the numerical study are on-going works.

6.2.3. Scattering by small heterogeneities

Participants: Patrick Joly, Simon Marmorat.

Simon Marmorat has defended his thesis, done in collaboration with the CEA-LIST and with Xavier Claeys (LJLL, Paris VI). The goal was to develop an efficient numerical approach to simulate the propagation of waves in concrete, which is modelled as a smooth background medium, with many small embedded heterogeneities. To do so, one has proposed two reduced models relying on the asymptotic analysis of the problem with respect to the (small) size of the heterogeneities. The first model looks like a fictitious domain method in which the analysis of the near field (closed to the heterogeneities) is exploited. The second one is a method of auxiliary sources, based on the analysis of the far field (far from the heterogeneities). Rigorous error estimates have been established. From the numerical point of view, some points, related to the Galerkin enrichment of standard finite element methods, still need to be completed.

6.2.4. Effective boundary conditions for strongly heterogeneous thin layers

Participants: Mathieu Chamaillard, Patrick Joly.

This topic is the object of the PhD of Mathieu Chamaillard, done in collaboration with Houssem Haddar (Inria, Defi). We are interested in the construction of effective boundary conditions for the diffraction of waves by an obstacle covered with a thin coating whose physical characteristics vary “periodically”. The width of the coating and the period are both proportional to the same small parameter δ.

The results obtained previously on scalar propagation models have been extended to 3D Maxwell's equations resulting in the construction of an effective condition of the form $E \times n = \delta ik \mathcal{Z}_\Gamma (n \times (H \times n))$ where the impedance operator $\mathcal{Z}_\Gamma$, a second order tangential differential operator along Γ, depends on the geometry of the obstacle and of the material properties of the coating. The analysis, which is much more involved than in the scalar case (in particular in what concerns the stability analysis), provides error estimates in $O(\delta^2)$.

The thesis will be defended in the end of January 2016.

6.3. Spectral theory and modal approaches for waveguides

6.3.1. Guided modes in ladder-like open periodic waveguides

Participants: Sonia Fliss, Patrick Joly, Khac Long Nguyen, Elizaveta Vasilevskaya.

The general objective is the study of localized modes in locally perturbed periodic media and of guided modes in periodic media with a lineic perturbation. We investigate the existence theory of such modes as well as their numerical computations.

The problem, that is investigated in the framework of the PhD thesis of E. Vasilevskaya, in collaboration with Bérangère Delourme (Paris 13 University), is the case where the propagation medium is a thin structure whose limit is a periodic graph. We exhibit situations where the introduction of a line defect into the geometry of the domain leads to the appearance of guided modes. From the theoretical point of view, the problem is studied by asymptotic analysis methods, the small parameter being the thickness of the domain, so that when the thickness of the structure is small enough, the domain approaches a graph. The spectral theory of the underlying limit operator defined in the graph plays a key role in the analysis. For 2D configurations, we have shown that for sufficiently thin structures, it suffices to reduce the width of one rung to make appear guided modes. Moreover, using matched asymptotic expansions, we have constructed asymptotic expansions at any order of the corresponding eigenvalues and guided modes. For 3D configurations, the spectral theory of the underlying limit operator was already studied. In a further step, one can expect, again by asymptotic analysis, to get corresponding existence results for the original problem, at least for sufficiently thin structures.

From a numerical point of view, the modes can be computed using non linear eigenvalue problems and specific transparent boundary conditions for periodic media. During his post-doc, Khac Long Nguyen has implemented an exact method based on Dirichlet-to-Neumann operators to compute localized modes in 2D locally perturbed periodic media or guided modes in 3D periodic media with a lineic perturbation. This was already done few years ago for waveguides configurations but here the construction of the transparent boundary conditions are much more involved.

6.3.2. Reduced graph models for networks of thin co-axial electromagnetic cables

Participants: Geoffrey Beck, Patrick Joly.

This work is the object of the PhD of Geoffrey Beck and is done in collaboration with Sébastien Imperiale (Inria, MEDISIM). The general context is the non destructive testing by reflectometry of electric networks of co-axial cables with heterogeneous cross section and lossy materials, which was the subject of the ANR project SODDA. We consider electromagnetic wave propagation in a network of thin coaxial cables (made of a dielectric material which surrounds a metallic inner-wire). The goal is to reduce 3D Maxwell's equations to a 1D like model. During the past two years, we derived and justified generalized telegraphers model for a single cable. This year, we incorporated in our model the losses due to the skin effect induced by the non perfectly conducting nature of the metallic wire. Finally using the method of matched asymptotics, we have derived and justified improved Kirchhoff conditions.

6.3.3. Multimodal methods for the propagation of acoustic and electromagnetic waves

Participant: Jean-François Mercier.

In collaboration with Agnès Maurel from the Langevin Institut and Simon Felix from the LAUM, we have developed fast multimodal methods to describe the acoustic propagation in rigid waveguides or in periodic arrays. An incident wave is scattered by penetrable inclusions or by the succession of different penetrable media separated by interfaces of any shape. The difficulties are: to take into account the modes coupling and to get modes naturally decoupled at the entrance and at the exit of the computational domain. A weak formulation of the problem provides a modal formulation taking exactly into account the matching conditions at the interfaces. A consequence is that the obtained convergence is the best convergence expected, given the regularity of the solution. After the study of isotropic cases, we have generalized this approach to the case of anisotropic media, the difficulty being to take into account a tensor in the propagation equation.

6.3.4. Plasmonic waveguides

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

This work, which is a part of the PhD of Camille Carvalho, is done in collaboration with Lucas Chesnel (Inria, Defi). A plasmonic waveguide is a cylindrical structure consisting of metal and dielectric parts. In a certain frequency range, the metal can be seen as a lossless material with a negative dielectric permittivity. The study of the modes of a plasmonic waveguide is then presented as an eigenvalue problem with a sign-change of coefficients in the main part of the operator. Depending on the values of the contrast of permittivities at the metal / dielectric interface, different situations may occur. In the "good" case, the problem is self-adjoint with compact resolvent and admits two sequences of eigenvalues tending to + and -∞. But when the interface presents corners, for a particular contrast range, the problem is neither self-adjoint nor with compact resolvent. In this case, Kondratiev's theory of singularities allows to build extensions of the operator, with compact resolvent. Finally, we show that the eigenvalues for one of these extensions can be computed by combining finite elements and Perfectly Matched Layers at the corners. The paradox is that a specific treatment has to be done to capture the corners singularities, even to compute regular eigenmodes.

6.4. Inverse problems

6.4.1. Quasi-Reversibility method and exterior approach for evolution problems

Participant: Laurent Bourgeois.

This work is a collaboration with Jérémi Dardé from Toulouse University. We address some linear ill-posed problems involving the heat or the wave equation, in particular the heat/wave equation with lateral Cauchy data. We have introduced several kinds of variational mixed formulations of quasi-reversibility which enable us to solve these ill-posed problems by using classical Lagrange finite elements. We have also designed a new approach called the "exterior approach" to solve inverse obstacle problems with initial condition and lateral Cauchy data for the heat/wave equation. It is based on a combination of an elementary level set method and the quasi-reversibility methods we have just mentioned. Some numerical experiments have proved the feasibility of our strategy to identify obstacles from lateral Cauchy data for the heat equation in 2D and for the wave equation in 1D. Our objective is now to focus on the wave equation in 2D. Firstly we wish to obtain a minimal value of the final time in order to ensure uniqueness of the obstacle from the lateral Cauchy data. Secondly we want to test our exterior approach numerically. We expect better results than with the heat equation.

6.4.2. Higher-order expansion of misfit functional for defect identification in elastic solids

Participants: Marc Bonnet, Rémi Cornaggia.

This work, done in the context of the PhD of Rémi Cornaggia, concerns the identification of scatterers of moderate size, modelled as elastic inhomogeneities embedded in an homogeneous elastic background medium, by time-harmonic elastodynamic measurements. Least-squares functionals, commonly used for defect identification, are expanded in powers of the small characteristic radius a of a trial inhomogeneity. This entails the expansion of the elastodynamic scattering problem, which is needed only on the support of the trial inhomogeneity and is established by means of a Lippmann-Schwinger volume integral equation. This approach generalizes, to higher orders in a, the well-known concept of topological derivative. Such expansion,

whose derivation and evaluation are facilitated by using an adjoint state, provides a basis for the quantitative estimation of flaws whereby a region of interest may be exhaustively probed at reasonable computational cost. So far, the higher-order expansion has been derived under fairly general conditions, mathematically justified, and demonstrated on simple numerical examples involving the identification of a spherical inhomogeneity in an unbounded 3D medium.

6.4.3. Complete transmission invisibility in waveguides

Participant: Anne-Sophie Bonnet-Ben Dhia.

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

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

During the visit of Sergei Nazarov, we found a new approach which allows to build completely invisible perturbations in the mono-mode regime (i.e. when the frequency is chosen below the first cut-off frequency) with no phase shift in transmission. These perturbations include some kinds of thin resonators whose height is adapted to the frequency.

All our results mainly rely on asymptotic theory.

6.4.4. Energy-based cost functional for three-dimensional transient elastodynamic imaging

Participant: Marc Bonnet.

This work is a continuing collaboration with Wilkins Aquino (Duke University, USA). It is concerned with three-dimensional elastodynamic imaging by means of the modified error in constitutive relation (MECR), combining the energy norm of the constitutive residual and a more-classical L^2 norm on the measurement residuals.

We have in particular considered the case of imaging using interior data. The stationarity equations associated with the minimization of a MECR objective function, subject to the conservation of linear momentum, yields a well-posed problem coupling two elastodynamic fields, even in cases where boundary conditions are initially underspecified (making it difficult to define *a priori* a forward problem). Numerical results demonstrate the robust performance of the method in situations where the available measurement data is incomplete and corrupted by noise of varying levels.

In a separate study, elastodynamic imaging using transient data and based on time-domain solvers has been investigated. In this context, each evaluation of a time-domain MECR cost functional entails solving two elastodynamic problems (one forward, one backward), which moreover are coupled (unlike the case of L^2 misfit functionals). This coupling creates a major computational bottleneck, making MECR-based inversion difficult for spatially 2D or 3D configurations. To overcome this obstacle, we propose to (a) set the entire computational procedure in a consistent time-discrete framework that incorporates the chosen time-stepping algorithm, and (b) use an iterative successive over-relaxation-like method for the resulting stationarity equations. The resulting MECR-based inversion algorithm is formulated under quite general conditions, allowing for 3D transient elastodynamics, straightforward use of available parallel solvers, a wide array of time-stepping algorithms commonly used for transient structural dynamics, and flexible boundary conditions and measurement settings. The proposed MECR algorithm is then demonstrated on computational experiments involving 2D and 3D transient elastodynamics and up to over 500 000 unknown elastic moduli.

6.4.5. Linear Sampling Method with realistic data in waveguides

Participants: Laurent Bourgeois, Arnaud Recoquillay.

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

Our strategy consists in transforming the time domain problem into a multi-frequency problem by the Fourier transform. This allows us to take full advantage of the established efficiency of modal frequency-domain sampling methods. We have already proved the feasibility of our approach in the 2D acoustic case. In particular, we have shown how to optimize the number of sources/receivers and the distance between them in order to obtain the best possible identification result. The next steps consist in extending such an approach to the elastic case and trying it experimentally, that is with real data. Experiments will be carried in CEA.

6.5. Integral equations

6.5.1. Fast BEM solvers based on $\mathcal{H}$-matrices for 3-D frequency-domain elastodynamics

Participants: Stéphanie Chaillat, Patrick Ciarlet, Luca Desiderio.

The main advantage of the Boundary Element Method (BEM) is that only the domain boundaries are discretized leading to a drastic reduction of the total number of degrees of freedom. In traditional BE implementation the dimensional advantage with respect to domain discretization methods is offset by the fully-populated nature of the BEM coefficient matrix. Using the $\mathcal{H}$-matrix arithmetic and low-rank approximations (performed with Adaptive Cross Approximation) it is possible to derive fast iterative and direct solvers for the BEM system. We extend the method to 3-D frequency-domain elastodynamics. To this end, the Adaptive Cross Approximation is adapted to deal with vectorial problems. To validate the accuracy of the solution of the LU based direct solver, we derive an error estimate. Finally, we check numerically the theoretical estimate of the storage costs. In particular, we study the efficiency of low-rank approximations when the frequency is increased. This is done in partnership with SHELL company in the framework of the PhD of Luca Desiderio.

6.5.2. OSRC preconditioner for 3D elastodynamics

Participant: Stéphanie Chaillat.

This work is done in collaboration with Marion Darbas from University of Picardie and Frédérique Le Louer from Technological University of Compiègne. The fast multipole accelerated boundary element method (FM-BEM) is a possible approach to deal with scattering problems of time-harmonic elastic waves by a three-dimensional rigid obstacle. In 3D elastodynamics, the FM-BEM has been shown to be efficient with solution times of order $O(N \log N)$ per iteration (where N is the number of BE degrees of freedom). However, the number of iterations in GMRES can significantly hinder the overall efficiency of the FM-BEM. To reduce the number of iterations, we propose a clever integral representation of the scattered field which naturally incorporates a regularizing operator. When considering Dirichlet boundary value problems, the regularizing operator is a high-frequency approximation to the Dirichlet-to-Neumann operator. For a spherical obstacle, the approximation of the DtN is a linear combination of the tangential and normal parts. The numerical efficiency of the preconditioned integral equation (i.e. the independence of the number of iterations from the mesh size and frequency) is verified for spherical obstacles, validating the concept of analytical preconditioners for 3D elastodynamics FM-BEM. For more general shapes, this approximation of the DtN is more complex to derive. As a first step, we construct and validate the approximation in the framework of the On-Surface Radiation Condition (OSRC) method.

6.5.3. A wideband Fast Multipole Method for oscillatory kernels

Participant: Stéphanie Chaillat.

This work is done in collaboration with Francis Collino. We derive a new Fast Multipole Method (FMM) based on plane wave expansions (PWFMM), combining the advantages of the low and high frequency formulations. We revisit the method of Greengard et al. (1998) devoted to the low frequency regime and based on the splitting of the Green's function into a propagative and an evanescent part. More precisely, we give an explicit formula of the filtered translation function for the propagative part, we derive a new formula for the evanescent part and we provide a new interpolation algorithm. At all steps, we check the accuracy of the method by providing error estimates. These theoretical developments are used to propose a wideband FMM based entirely on plane wave expansions. The numerical efficiency and accuracy of this broadband PWFMM are illustrated with a numerical example.

6.5.4. Coupling integral equations and high-frequency methods for ultrasonic NDT modelling

Participants: Marc Bonnet, Laure Pesudo.

This work, in partnership with CEA LIST and in collaboration with Francis Collino, is undertaken in the context of the PhD thesis of Laure Pesudo. Modelling ultrasonic non destructive testing (NDT) experiments simultaneously involves the scattering of waves by defects of moderate size (for which discretization-based methods such as the BEM are appropriate) and propagation over large distances (requiring high-frequency approximations). Those two types of simulation methods are therefore simultaneously needed in NDT modelling but do not lend themselves easily to coupling. The coupling approach proposed here takes advantage of the fact that the far-field asymptotic approximation of integral representation formulas (which accurately account for the scattering by defects) yields a superposition of rays (satisfying the leading-order equations arising from high-frequency asymptotics). This allows to convert incoming rays into plane waves, compute their scattering by obstacles, and convert the scattered field into rays. A defect of given shape and characteristics becomes (approximately) represented as a point-like scatterer with anisotropic reflection properties that are computed (offline) from BEM solutions of near-field problems. Using a partition of unity on the obstacle boundary allows to approximate the obstacle by a set of point-like reflectors, thereby enlarging the size of obstacles amenable to this approach. Preliminary tests on 2D scalar wave propagation problems show that sufficient far-field accuracy is achieved for wavelength-sized defects.

6.5.5. Dynamic soil-structure interaction

Participants: Marc Bonnet, Stéphanie Chaillat, Zouhair Adnani.

This work, undertaken in the context of the PhD thesis of Zouhair Adnani (CIFRE partnership with EDF), concerns the simulation of dynamic soil-structure interaction (SSI) in connection with seismic assessment of civil engineering structures. The main goal is to formulate, implement, and evaluate on realistic test examples, a computational strategy that combines the fast multipole integral equation method for elastic wave propagation in unbounded regions (COFFEE FMM-accelerated BEM solver), and finite elements for modelling civil engineering structures and neighboring soil regions (the EDF in-house code Code_Aster). In a preliminary phase, the evaluation of transient elastodynamic responses via the Fourier synthesis of frequency-domain solutions computed using COFFEE (see Section 5.1) has been studied on several test problems, achieving substantial improvements of computational efficiency for this component of SSI analysis.

6.5.6. Volume Integral Formulations

Participant: Marc Bonnet.

Volume integral equations (VIEs), also known as Lippmann-Schwinger integral equations, arise naturally when considering the scattering of waves by penetrable, and possibly heterogeneous, inhomogeneities embedded in a homogeneous background medium. In contrast with the vast existing literature on boundary integral equations, comparatively few studies are available regarding the mathematical properties of VIEs. In this work, we investigate the solvability of VIE formulations arising in elastodynamic scattering by penetrable obstacles. The elasticity tensor and mass density are allowed to be smoothly heterogeneous inside the obstacle and may be discontinuous across the background-obstacle interface, the background elastic material being homogeneous. Both materials may be anisotropic, within certain limitations for the background medium. The VIE associated with this problem is derived, relying on known properties of the background fundamental tensor.

To avoid difficulties associated with existing radiation conditions for anisotropic elastic media, we propose an alternative definition of the radiating character of transmission solutions. The unique solvability of the volume integral equation (and of the scattering problem) is established. For the important special case of isotropic background properties, our definition of a radiating solution becomes equivalent to the classical Sommerfeld-Kupradze radiation conditions.

6.6. Domain decomposition methods

6.6.1. Transparent boundary conditions with overlap in unbounded anisotropic media

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

We are interested in acoustic or elastic wave propagation in time harmonic regime in a 2D or 3D medium which is a local perturbation of an infinite anisotropic homogeneous medium. We investigate the question of deriving a formulation which is suitable for numerical computations. This question is difficult due to the anisotropy of the surrounding medium. Our approach consists in coupling several plane-waves representations of the solution in half-spaces surrounding the defect with a FE computation of the solution around the defect. The difficulty is to ensure that all these representations match, in particular in the infinite intersections of the half-spaces. It leads to a formulation which couples, via integral operators, the solution in a bounded domain including the defect and its traces on the edge of the half-planes. We have shown that this formulation has good properties from theoretical and numerical points of view.

6.6.2. Electromagnetic scattering by objects with multi-layered dielectric coatings

Participants: Patrick Joly, Matthieu Lecouvez.

The PhD thesis of Matthieu Lecouvez, undertaken in collaboration with the CEA-CESTA and Francis Collino, has been defended in July. It concerned the diffraction of time harmonic electromagnetic waves by perfectly conducting objects covered by multi-layered (possibly thin) dielectric coatings. This idea was to use a domain decomposition method in which each layer would constitute a subdomain. The transmission conditions between the subdomains involve some specific impedance operators in order to achieve a geometric convergence of the method (compared to the slow algebraic convergence obtained with standard Robin conditions). This year, the theoretical aspects of our work have been completed and are the object of an article in preparation.

6.6.3. Domain Decomposition Methods for the neutron diffusion equation

Participants: Patrick Ciarlet, Léandre Giret.

Studying numerically the steady state of a nuclear core reactor is expensive, in terms of memory storage and computational time. In its simplest form, one must solve a neutron diffusion equation with low-regularity solutions, discretized by finite element techniques, totaling millions of unknowns or more, within a loop. Iterating in this loop allows to compute the smallest eigenvalue of the system, which determines the critical, or non-critical, state of the 3D core configuration. This problem fits within the framework of high performance computing so, in order both to optimize the memory storage and to reduce the computational time, one can use a domain decomposition method, which is then implemented on a parallel computer. The definition of an efficent DD method has been addressed for conforming meshes prior to the PhD research of Léandre Giret. The development of non-conforming, hence more flexible, DD methods has recently been finalized.
The optimization of the eigenvalue loop is under way. The current research also focuses on the numerical analysis of the full suite of algorithms to prove convergence for the complete multigroup SPN model (which involves coupled diffusion equations). Realistic computations will be carried out with the APOLLO3 neutronics code.
This topic is developed in partnership with CEA-DEN (Erell Jamelot).

6.7. Aeroacoustics

6.7.1. Time-harmonic acoustic scattering in a vortical flow

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

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

We have proved that the Goldstein equations are well-posed in a domain Ω for a potential flow, or for a vortical flow if the flow is Ω-filling (each point of Ω is reached by a streamline coming from the inflow boundary in a finite time). A non Ω-filling flow corresponds to the presence or recirculations areas and we have shown that, for such flows, some of the closed streamlines can be resonant. To study deeper this phenomenon, we focused on the case of a rotating flow in an annular geometry. We proved that outside the set of resonance frequencies, the radiation problem is well-posed. Work is under progress to determine the solution on a resonant streamline.

6.7.2. Propagation of solitons through Helmholtz resonators

Participant: Jean-François Mercier.

With Bruno Lombard (Laboratoire de Mécanique et Acoustique of Marseille), we studied the propagation of an acoustic solitary wave in a 1D waveguide connected to a periodic array of Helmholtz resonators. Starting from a model of the literature, obtained by approximations, our goal was to provide a numerical modeling, which validates (or not) the underlying model and the assumptions. The model consists of two coupled equations evolution: a nonlinear PDE describing acoustic waves (similar to the Burgers equation), and a linear ODE describing oscillations in the Helmholtz resonators. We have developed a numerical method based on two main ingredients: a diffusive representation of fractional derivatives and a splitting method applied to the evolution equations. The numerical scheme has been validated by comparison with exact solutions. The properties of non-linear solutions have been investigated numerically.

In collaboration with O. Richoux of the LAUM, this work has been extended, comparing to experimental results. Adjustments had to be made, the attenuation of the numerical model being weaker than that observed experimentally. To remedy this, we have incorporated some attenuation mechanisms that we had neglected. One consequence of these additions is that a more sophisticated numerical method had to be developed. A good agreement has been found with experimental results.

RAPSODI Team

7. New Results

7.1. Design and analysis of advanced finite volumes schemes

The fact that a numerical method is able to handle nonlinear test functions in its numerical analysis is crucial in order to ensure its physical relevance, and consequently its good behavior.

In [15], C. Cancès and C. Guichard proposed a first nonlinear numerical method to solve possibly degenerate parabolic equations with anisotropy on general simplicial meshes. The nonlinear control volume finite element (CVFE) scheme is based on P1 finite elements with mass-lumping combined with a tricky upwinding of the mobilities. The method has the remarkable property of preserving the positivity of the solutions. Moreover, it ensures the decay of the physical entropy. Its convergence is proved in [15] and numerical results are exhibited. In particular, they show that the method is first order accurate in space in standard situations, but can lack robustness w.r.t. the anisotropy in some particularly unfavorable situations.

This drawback was corrected by C. Cancès and C. Guichard in [35], where a second order in space method based on the so-called VAG scheme [57] was proposed. This method is able to handle very general grids, heterogeneous data and strong anisotropy ratios. Moreover, it preserves at the discrete level the variational structure of the continuous problem, yielding the nonlinear stability of the scheme. A complete convergence analysis was performed in [35]. The numerical results presented in [35] show that the robustness default of the first nonlinear method [15] has been corrected.

In [36], C. Cancès *et al.* proposed and analyzed a nonlinear CVFE scheme for a degenerate Keller-Segel model with anisotropic and heterogeneous diffusion tensors. The scheme is based on the one proposed in [15]. The convergence of the scheme is proved under very general assumptions. Finally, some numerical experiments are carried out to prove the ability of the scheme to tackle degenerate anisotropic and heterogeneous diffusion problems over general meshes without jeopardizing the positivity of the solutions.

In [17], C. Chainais-Hillairet, A. Jüngel and S. Schuchnigg prove the time decay of fully discrete finite-volume approximations of porous-medium and fast-diffusion equations with Neumann or periodic boundary conditions in the entropy sense. The algebraic or exponential decay rates are computed explicitly. In particular, the numerical scheme dissipates all zeroth-order entropies which are dissipated by the continuous equation. The proofs are based on novel continuous and discrete generalized Beckner inequalities.

In [18], C. Chainais-Hillairet, A. Jüngel and P. Shpartko propose and analyze a numerical scheme for a spinorial matrix-diffusion model for semiconductors. The model consists of strongly coupled parabolic equations for the electron density matrix or, alternatively, of weakly coupled equations for the charge and spin-vector densities, coupled to the Poisson equation for the electric potential. The main features of the numerical scheme are the preservation of nonnegativity and L^∞ bounds of the densities and the dissipation of the discrete free energy. The existence of a bounded discrete solution and the monotonicity of the discrete free energy are proved. The fundamental ideas are reformulations using spin-up and spin-down densities and certain projections of the spin-vector density, free energy estimates, and a discrete Moser iteration. Furthermore, numerical simulations of a simple ferromagnetic-layer field-effect transistor in two space dimensions are presented.

In [32], M. Bessemoulin-Chatard and C. Chainais-Hillairet study the large–time behavior of a numerical scheme discretizing drift–diffusion systems for semiconductors. The numerical method is finite volume in space, implicit in time, and the numerical fluxes are a generalization of the classical Scharfetter–Gummel scheme which allows to consider both linear or nonlinear pressure laws. They study the convergence of approximate solutions towards an approximation of the thermal equilibrium state as time tends to infinity, and obtain a decay rate by controlling the discrete relative entropy with the entropy production. This result is proved under assumptions of existence and uniform-in-time L^∞ estimates for numerical solutions, which are then discussed.

7.2. A posteriori analysis and computational optimization

In 2015, E. Creusé *et al.* have developed a posteriori error estimators for the harmonic potential formulations of the Maxwell system, in order to simulate eddy-current problems arising in the context of quasi-static approximations. The originality of our contribution is to provide estimators with sharp bounds and explicit constants. It was achieved by solving in the same time the so-called "$\mathbf{A}/\varphi$" and "$\mathbf{T}/\Omega$" potential formulations [38]. If this way to proceed was already known and usually used for stationary problems, the extension to harmonic ones constitutes the novelty of our contribution. It was in particular necessary to prove some superconvergence properties of additional terms. The reliability as well as the local efficiency of the derived estimator have been established without any generic constant, and numerical tests clearly illustrate their optimal behavior, from academic benchmarks to more industrial ones.

Another track to optimize the computational effort consists in refining and coarsening the model. This approach is based on the following ansatz : the more the model is complex, the more expensive are the computations. This approach was used by F. Filbet and T. Rey in [23] to simulate kinetic equations, the kinetic equations being replaced by cheaper hydrodynamic limits when it is relevant. The same idea was used in H. Mathis *et al.* [27] in order to simulate complex flows modeled by hyperbolic systems with relaxation. A rigorous error analysis of such a model adaptation procedure was performed on a simplified model by C. Cancès *et al.* in [13].

7.3. Modeling and numerical simulation of complex fluids

Recently, C. Calgaro *et al.* compared some very recent numerical schemes for the resolution of incompressible variable density flows; namely an Hybrid Finite Volume/Finite Element scheme, and a Discrete Duality Finite Volume one [34]. This work was performed in collaboration with the Inria team COFFEE (Inria Nice Sophia-Antipolis). In addition to this original and attentive comparison, our main contribution has been to improve the way to implement the Neumann boundary condition on the density, when a second-order accurate scheme is considered in space. Indeed, for some critical situations such as the simulation of Rayleigh-Taylor instabilities using unstructured meshes, this point is crucial to avoid unphysical numerical instabilities in the vicinity of the boundaries corresponding to symmetric axis. The obtained results are very promising, and constitute an important step towards the simulation of more complex models on which we are working at the moment.

In [25], M. Gisclon and I. Lacroix-Violet consider the barotropic compressible quantum Navier-Stokes equations with a linear density dependent viscosity and its limit when the scaled Planck constant vanish. Following recent works on degenerate compressible Navier-Stokes equations, we prove the global existence of weak solutions by the use of a singular pressure close to vacuum. With such singular pressure, we can use the standard definition of global weak solutions which also allows to justify the limit when the scaled Planck constant denoted by ε tends to 0.

The H-theorem, originally derived at the level of the Boltzmann nonlinear kinetic equation for a dilute gas undergoing elastic collisions, strongly constrains the velocity distribution of the gas to evolve irreversibly towards equilibrium. As such, the theorem could not be generalized to account for dissipative systems: the conservative nature of collisions is an essential ingredient in the standard derivation. The work [24] gives the first strong numerical evidences, along with a proof for a simplified model, of dissipation of the Boltzmann entropy (the so-called H-theorem) for solutions to the granular gases equation. This dissipative kinetic equation describes the non-equilibrium behavior of a gas composed of macroscopic particles, namely complex fluids such as avalanches, pollens flows or planetary rings.

7.4. Theoretical and numerical analysis of corrosion models

The Diffusion Poisson Coupled Model [1] is a model of iron based alloy in a nuclear waste repository. It describes the growth of an oxide layer in this framework. The system is made of a Poisson equation on the electrostatic potential and convection-diffusion equations on the densities f charge carriers (electrons, ferric cations and oxygen vacancies), supplemented with coupled Robin boundary conditions. The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations.

In [19], C. Chainais-Hillairet and I. Lacroix-Violet consider a simplified version of this model, where only two charge carriers are taken into account and where there is no evolution of the layer thickness. They prove the existence of a solution for the time-dependent simplified model.

P.-L. Colin, C.Chainais-Hillairet and I. Lacroix-Violet have performed in [16] the numerical analysis of the numerical scheme presented in [2] for the same model. The scheme is a Euler implicit in time scheme with Scharfetter-Gummel approximation of the convection-diffusion fluxes. They prove existence of a solution to the scheme, a priori estimates satisfied by the solution and convergence of the numerical scheme to a weak solution of the corrosion model.

Numerical experiments done for the simulation of the full DPCM model with moving boundaries shows the convergence in time towards a pseudo-steady-state. C. Chainais-Hillairet and T. O. Gallouët show in [37] the existence of pseudo-stationary solutions for some simplified versions of the DPCM model. They also propose a new scheme in order to compute directly this pseudo-steady-state. Numerical experiments show the efficiency of this method.

7.5. Variational modeling and analysis

Bose-Einstein condensates are a unique way to observe quantum effects at a (relatively) large scale. The fundamental states of such condensates are obtained as minimizers of a Gross-Pitaievskii functional. In [39], M. Goldman and B. Merlet consider the case of a two component Bose-Einstein condensate in the strong segregation regime (the energy favors spatial segregation of the two different Boson species). They identify two different regimes in the strong segregation and small healing length limit. In one of these regimes, the relevant limit is an interesting weighted isoperimetric problem which explains some of the numerical simulations of [63].

In [14], C. Cancès *et al.* show that the equations that are classically used for modeling the motion of two incompressible immiscible phases in a porous medium can be formally reinterpreted as the gradient flow of the free energy in a degenerated geometry closely related to the Wasserstein metric. This extends to realistic models the seminal approach [65] and the more recent one [64].

APICS Project-Team

6. New Results

6.1. Inverse problems for Poisson-Laplace equations

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

This section is concerned with inverse problems for 3-D Poisson-Laplace equations, among which source recovery issues. Though the geometrical settings differ in Sections 6.1.1 and 6.1.2 , the characterization of silent sources (those giving rise to a vanishing field) is one common problem to both which has been resolved in the magnetization setup [33].

6.1.1. Inverse problems in medical imaging

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

In 3-D, functional or clinical 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 [38][5] 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 4.2).

In this connection, a dedicated software FindSources3D (see Section 3.4.2) is being developed, in collaboration with the team Athena and the CMA. We continued this year algorithmic developments, prompted by a fruitful collaboration with the firm BESA, namely automatic detection of the number of sources (which was left to the user until recently). It appears that, in the rational approximation step, *multiple* poles possess a nice behavior with respect to branched singularities. This is due to the very physical assumptions on the model (for EEG data, one should consider *triple* poles). Though numerically observed in [7], there is no mathematical justification so far why multiple poles generate such strong accumulation of the poles of the approximants. This intriguing property, however, is definitely helping source recovery. It is used in order to automatically estimate the "most plausible" number of sources (numerically: up to 3, at the moment). Further, a modular and ergonomic platform version of the software is under development.

In connection with these and other brain exploration modalities like electrical impedance tomography (EIT), we are now studying conductivity estimation problems. This is the topic of the PhD research work of C. Papageorgakis (co-advised with the Athena project-team and BESA GmbH). In layered models, it concerns the estimation of the conductivity of the skull (intermediate layer). Indeed, the skull was assumed until now to have a given isotropic constant conductivity, whose value can differ from one individual to another. A preliminary issue in this direction is: can we uniquely recover and estimate a single-valued skull conductivity from one EEG recording? This has been established in the spherical setting when the sources are known, see [17]. Situations where sources are only partially known and the geometry is more realistic than a sphere are currently under study. When the sources are unknown, we should look for more data (additional clinical and/or functional EEG, EIT, ...) that could be incorporated in order to recover both the sources locations and the skull conductivity. Furthermore, while the skull essentially consists of hard bone part that may be assumed to have constant electrical conductivity, it also contains spongy bone compartments. These two distinct parts of the skull possess quite different conductivities. The influence of that second value on the overall model is now being studied [19].

6.1.2. Inverse magnetization issues in the thin-plate framework

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

Localizing magnetic sources from measurements of the magnetic field away from the support of the magnetization has been the fundamental issue under investigation by IMPINGE. The goal was to determine magnetic properties of rock samples (*e.g.* meteorites or stalactites) from fine field measurements close to the sample that can nowadays be obtained using SQUIDs (superconducting quantum interference devices). Currently, rock samples are cut into thin slabs and the magnetization distribution is considered to lie in a plane, which makes for a somewhat less indeterminate framework than EEG as regards inverse problems because "less" magnetizations can produce the same field (for the slab has no inner volume). Note however that EEG data consist of values of the normal current and of the associated potential, while in the present setting only values of the normal magnetic field are measured.

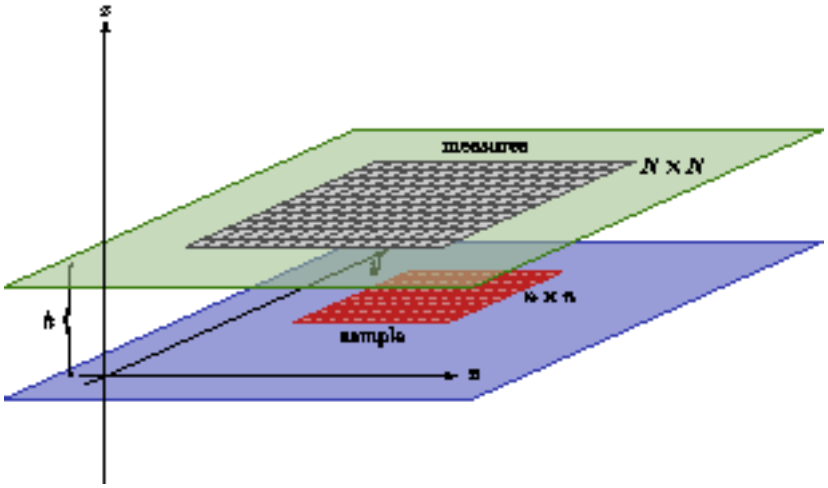


Figure 3. Schematic view of the experimental setup

Figure 3 presents a schematic view of the experimental setup: the sample lie on a horizontal plane at height 0 and its support is included in a rectangle. The vertical component B_3 of the field produced by the sample is measured on points of a horizontal $N \times N$ rectangular grid at height h.

Over the previous years, we mainly focused on developing techniques to recover magnetizations with rather sparse support. To this end, we set up a heuristic procedure to recover sparse magnetizations, based on iterative truncation of the support of the recovered magnetization. In this heuristics, magnetizations were represented by dipoles placed at the points of a regular rectangular $n \times n$, which seemed general enough a model class to correctly approximate the magnetizations commonly encountered in samples.

The procedure turned out to be poor when trying to recover the magnetization itself, due to the severe ill-posedness of the problem and the unexpected existence of magnetizations that produce almost no field at the height where measurements are performed, although the corresponding magnetic distributions strongly differ from truly silent distributions. Nevertheless, whenever the support could be significantly shrunk while keeping the error small (*i.e.*, explaining the data satisfactorily), estimates of the net moment so far, based on the dipolar model obtained by inversion, have been good.

This suggests that recovering the net moment and recovering the magnetization are rather different problems, the first one being less ill-posed than the second. Although the information provided by the net moment of the sample seems to be much weaker than knowing the full magnetic distribution, its importance has been emphasized by the geophysicists at MIT for at least three reasons:

- It yields important geological information on the sample in particular to estimate the magnitude of the ambient magnetic field at the time the rock was formed.
- It can be estimated independently to some extent, using a magnetometer, thereby allowing one to cross-validate the approach.
- From a computation point of view, knowledge of the net moment should lead to numerically stable reconstruction of an equivalent unidirectional magnetization. The support of the latter would provide us with valuable information to test for unidirectionality of the true magnetization, which is an important question to physicists in connection with rocks history and formation.

This year, we addressed the problem of directly recovering the net moment, without recourse to full inversion. Indeed, the latter is rather inefficient as it requires using a cluster and even then, for some samples, days of evaluation in order to obtain only a coarse estimate of the net moment. This research effort led us to investigate three different and complementary approaches.

First, we improved over Fourier based techniques previously designed by reformulating the problem with the help of the Kelvin transform. This gave us an asymptotic expansion of the net moment involving, at the first order, the integrals $\iint B_3(x,y,h)\,\mathrm{d}x\mathrm{d}y$, $\iint x\,B_3(x,y,h)\,\mathrm{d}x\mathrm{d}y$ and $\iint y\,B_3(x,y,h)\,\mathrm{d}x\mathrm{d}y$, computed on a disc with large radius. Although the method is promising, the computations are quite involved and we did not manage yet to obtain higher-order terms. This is a part of D. Ponomarev PhD work.

In parallel, and based on the results obtained with Fourier transform, we investigated a second approach, consisting in directly computing asymptotic expansions of the above integrals, on several domains (namely, the 2-D balls of radius R for the 1, 2 and ∞ norm, that are squares, disks, diamonds). In all cases, we get

$$\iint x\,B_3(x,y,h)\,\mathrm{d}x\mathrm{d}y = \alpha\langle m_1\rangle + \beta(\langle t_1\,m_3\rangle - h\langle m_1\rangle)/R + \mathcal{O}(1/R^3),$$

where $\langle m_1\rangle$ is the moment of the first component m_1 of the magnetization and $\langle t_1\,m_3\rangle$ is the first moment of m_3 with respect to the first variable. The constants α and β depend on the domain where the integral is computed. Therefore, an appropriate linear combination of the integrals computed on the different domains allows us to compute $\langle m_1\rangle$ with an accuracy of $\mathcal{O}(1/R^3)$. Similar results are obtained for $\langle m_2\rangle$ and $\langle m_3\rangle$ with the other integrals. Preliminary numerical experiments confirm the practical usability of these formulas in order to recover the moment of magnetizations. A research report is currently being written to sum up these results.

Finally, a third more ambitious approach has been investigated. As an attempt to generalize the previous expansions, our initial question was: given measurement of B_3, say on a square, find a function $\phi(x,y)$ such that $\iint \phi(x,y)B_3(x,y)\,\mathrm{d}x\mathrm{d}y$ is a the best possible estimate of the net moment components $\langle m_i\rangle$ ($i=1,2,3$). This problem does not admit a solution because, for any $\epsilon>0$, there exists a function ϕ_ϵ allowing to estimate the moment with an error bounded by ϵ. However, when ϵ tends to zero, the function ϕ_ϵ is expected to have strong oscillations, which hinders an accurate computation of $\iint \phi(x,y)B_3(x,y)\,\mathrm{d}x\mathrm{d}y$ since B_3 is only known on a discrete grid of points. We therefore expressed the problem as a bounded extremal problem (see Section 3.3.1): to find the best ϕ_ϵ (with the smallest possible error value ϵ) under the constraint that $\|\nabla\phi_\epsilon\|_2 \le M$. Here, M is a user-defined parameter. We proved theoretical results regarding this bounded extremal problem (existence and uniqueness of a solution, characterization of its solution as a solution of integro-differential equation) and we are currently designing a numerical procedure to compute it. An article on this topic is in preparation.

Still in the course of D. Ponomarev's PhD research, the study of a 2D spectral problem for the truncated Poisson operator in planar geometry has been pursued. It is a simplified formulation of the relation between the magnetization and the magnetic potential (of which the magnetic field is the gradient) and is expected to produce an efficient representation basis (the eigenfunctions of the magnetization-to-field operator). This is a long-standing problem. Noteworthy properties of solutions have been obtained through connections with other spectral problems and asymptotic reductions for large and small values of the main parameters (distance h from the measurement plane to the sample support and sample support size), yielding approximate solutions by means simpler integral equations and ODEs.

The year 2015 was the last of our "équipe associée" IMPINGE with the MIT and Vanderbilt University. The final report is available on the web page of the associate team [0]. This collaboration is currently supported in part by a MIT-France seed funding from the US side, and we applied for a three-years extension of the associate team.

6.1.3. Inverse magnetization issues from sparse spherical data

The team APICS is a partner of the ANR project MagLune concerning Lunar magnetism, associated to the Geophysics and Planetology Department of Cerege, CNRS, Aix-en-Provence (see Section 8.2.2). Measurements of the remanent magnetic field of the Moon let geoscientists think that the Moon used to have a magnetic dynamo for some time, but the exact process that triggered and fed this dynamo is not yet understood, much less why it stopped. In particular, the Moon is too small to have a convecting dynamo like the Earth has. The overall goal of the project is to devise models to explain how this dynamo phenomenon was possible on the Moon.

To this end, the geophysicists from Cerege will go to NASA to perform some measurements on 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 the samples from NASA facilities. Therefore, measurements must be performed with some rudimentary instrument and our colleagues from Cerege designed a specific magnetometer. This device allows them to obtain measurements of the components of the magnetic field produced by the sample, at some discrete set of points located on disks belonging to three cylinders (see Figure 4).

This collaboration started this year and some preparatory work was necessary fix conventions used by our colleagues from Cerege in order to handle their measurements. During his Master 2 internship, Konstantinos Mavreas has developed a method based on rational approximation, using the same ideas as those underlying the FindSources3D tool (see Sections 3.4.2 and 6.1.1), for the case where the field produced by the sample can be well explained by a single magnetic dipole, whose position and moment are unknown. See his report [0]. Konstantinos Mavreas is now engaged in a PhD within APICS and will extend these results to the case of several dipoles.

6.2. Matching problems and their applications

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

This is collaborative work with Stéphane Bila (Xlim, Limoges, France), Yohann Sence (Xlim, Limoges, France), Thierry Monediere (Xlim, Limoges, France), Francois Torrès (Xlim, Limoges, France).

Filter synthesis is usually performed under the hypothesis that both ports of the filter are loaded on a constant resistive load (usually 50 Ohm). In complex systems, filters are however cascaded with other devices, and end up being loaded, at least at one port, on a non purely resistive frequency varying load. This is for example the case when synthesizing a multiplexer: each filter is here loaded at one of its ports on a common junction. Thus, the load varies with frequency by construction, and is not purely resistive either. Likewise, in an emitter-receiver, the antenna is followed by a filter. Whereas the antenna can usually be regarded as a resistive load at some frequencies, this is far from being true on the whole pass-band. A mismatch between the antenna and the

[0] http://www-sop.inria.fr/apics/IMPINGE/
[0] http://www-sop.inria.fr/members/Konstantinos.Mavreas/main.pdf

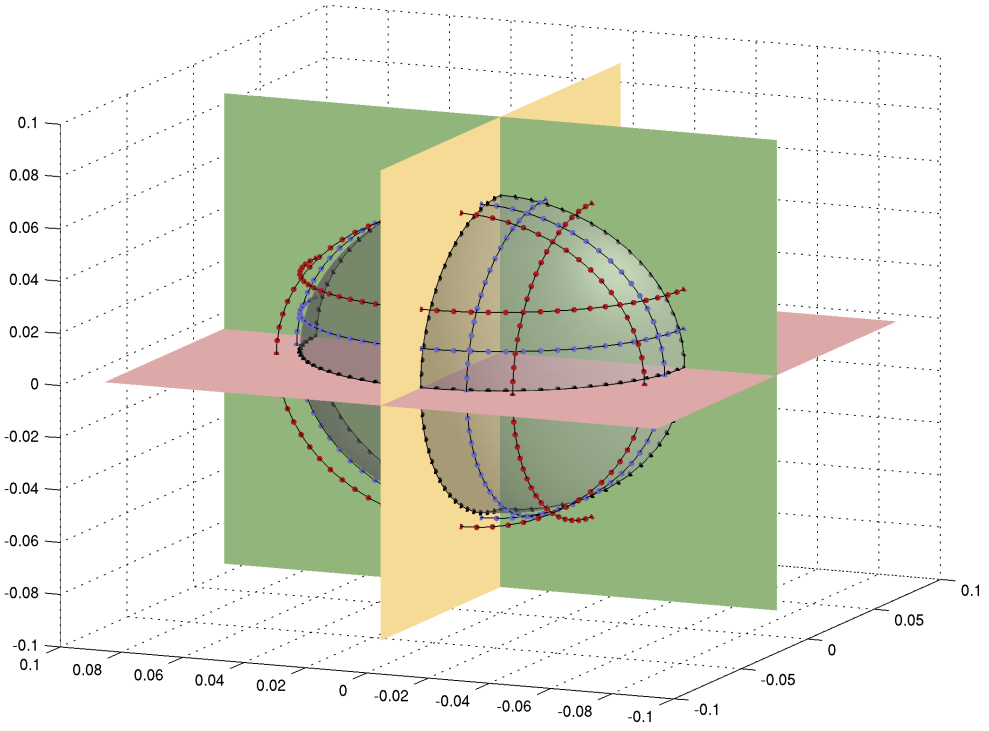


Figure 4. Typical measurements obtained with the instrument of Cerege. Discrete measurements of the field are performed on three cylinders. On each cylinder, the magnetic field $\mathbf{B}$ *is expressed as a component* B_h *co-linear with the axis of the cylinder, and a component* $\mathbf{B_s}$ *parallel to a section of the cylinder.* $\mathbf{B_s}$ *is itself decomposed as a tangential component* B_τ *and a normal component* B_n*, with respect to the circle given by the intersection of the cylinder with the corresponding section. At black points* B_n *is measured, at blue points* B_h *is measured, and at red points* B_τ *is measured.*

filter, however, causes irremediable power losses, both in emission and transmission. Our goal is therefore to develop a method for filter synthesis that allows us to match varying loads on specific frequency bands, while enforcing some rejection properties away from the pass-band.

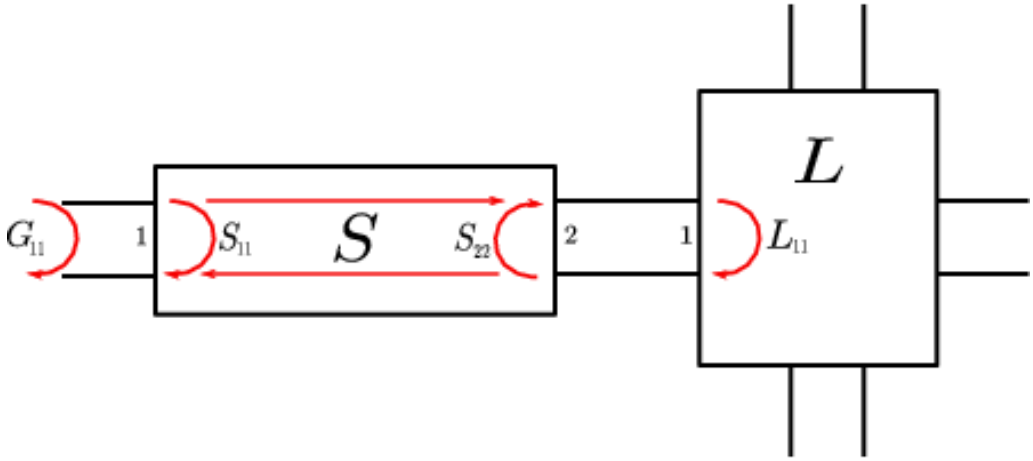


Figure 5. Filter plugged on a system with reflexion coefficient L_{11}

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

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

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

6.2.1. Approach based on interpolation

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

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

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

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

which accounts for the losslessness of the filter. The frequencies (w_k) are perfect matching points, as $\delta(S_{2,2}(w_k), L_{1,1}(w_k)) = 0$ holds, while the real zeros (x_k) of r are perfect rejection points (i.e. $\delta(S_{2,2}(x_k), L_{1,1}(x_k)) = 1$). The interpolation problem is therefore a point-wise version of our original matching-rejection problem. The monic restriction on p and q ensures the realisability of the filter in terms of coupled resonating circuits. If a perfect phase shifter is added in front of the filter, realized for example with a transmission line on a narrow frequency band, these monic restrictions can be dropped and an interpolation point w_{n+1} added, thereby yielding another interpolation problem $\widehat{\mathcal{P}}$. Our main result, states that $\mathcal{P}$ as well as $\widehat{\mathcal{P}}$ admit a unique solution. Moreover the evaluation map defined by $\psi(p) = (p/q(x_1), \cdots, p/q(x_n))$ is a homeomorphism from monic polynomials of degree n onto $\mathbb{D}^n$ ($\mathbb{D}$ the complex open disk), and ψ^{-1} is a diffeomorphism on an open, connected, dense set of $\mathbb{D}^n$. This last property has shown crucial for the design of an effective computational procedure based on continuation techniques. Current implementation of the latter tackles instances of $\mathcal{P}$ or $\widehat{\mathcal{P}}$ for $n = 10$ in less than $0.1\ sec$, and allows for us a recursive use of this interpolation framework in multiplexer synthesis problems. We presented these techniques at the European Microwave Week 2015 in the workshop dedicated to "Recent Advances in the Synthesis of Microwave Filters and Multiplexers". The detailed mathematical proofs can be found in [21] and will be submitted shortly. On a related topic, namely the de-embedding of filters in multiplexers, our work has been published in [13].

6.2.2. *Uniform matching and global optimality considerations*

The previous interpolation procedure provides us with a matching/rejecting filtering characteristics at a discrete set of frequencies. This can serve as a starting point for heavier optimization procedures where the matching and rejection specifications are expressed uniformly over the bandwidth. Although the practical results thus obtained have shown to be quite convincing, we have no proof of their global optimality. This led us to seek alternative approaches able to asses, at least in simple cases, global optimality of the derived response. Following the approach of Fano and Youla, we considered the problem of a designing a 2×2 lossless frequency response, under the condition that a specified load can be "unchained" from one of its port. This classically amounts to set interpolation conditions on the response at the transmission zeros of the Darlington extension of the load. When the load admits a rational representation of degree 1, and if the transmission zeros of the overall system are fixed, then we were able to show that the uniform matching problem over an interval reduces to a convex minimization problem with convex constraints over the set of non-negative polynomials of given degree. In this case, which is already of some practical interest for antenna matching (antenna usually exhibit a single resonance in their matching band which is reasonably approximated at order 1), it is therefore possible to perform filter synthesis with a guarantee on the global optimality of the obtained characteristics. Procedures to derive the solution are currently being investigated, and lie at the heart of our contribution to the ANR-project Cocoram.

6.3. Unambiguous de-embedding of filters

Participants: Matthias Caenepeel, Martine Olivi, Fabien Seyfert.

This work was conducted in collaboration with Yves Rolain (VUB, Brussels, Belgium)

Coupling topologies that admit multiple realizations may lead to ambiguous de-embedding tuning procedures where distinct coupled resonator circuits are identified from the same measurements. This is for example the case of the well-known coupling topologies in triplets, quadruplets and extended boxed. If no additional measurements are performed on the DUT (device under tuning), the different solutions to the coupling matrix synthesis problem are undistinguishable, as they yield similar scattering responses. We therefore studied specific tuning strategies to discriminate among them. The later uses a sequence of measurements of the DUT, obtained after varying some discriminating tuning parameters of the filter and testing for coherence of the extracted circuits. This work was presented by Matthias Caenepeel at IMS 2015 in Phoenix [15] and at the

EuMC 2015 in Paris [16]. In a similar vein Matthias is currently developing techniques taking advantage of the differential information provided by EM solvers in order to compute the Jacobian matrix of the identified coupling matrix(ces) with respect to the geometrical parameters of the filter.

6.4. Orthogonal Polynomials

Participant: Laurent Baratchart.

We studied this year the asymptotic behavior of the orthonormal polynomials P_n with respect to a non-negative weight w on a simply connected planar domain Ω:

$$\int_\Omega P_n \overline{P}_k w \, dm = \delta_{n,k},$$

with $\delta_{n,k}$ the Kronecker symbol. We proved that if Ω has boundary $\partial\Omega$ of class $C^{1,\alpha}$, $\alpha > 0$, and if w converges in some appropriate sense to a boundary function $w_1 \in L^p(\partial\Omega)$ while not vanishing "too much" at the boundary, then

$$P_n(z) = \left(\frac{n+1}{\pi}\right)^{1/2} z^n S^-_{w_1}(\Phi(z))\Phi^n(z)\Phi'(z)\{1+o(1)\}$$

outside the convex hull of Ω, with Φ the conformal map from the complement of Ω onto the complement of the unit disk normalized so that $\Phi'(\infty) = \infty$, and $S^-_{w_1}$ the so-called exterior Szegő function of w_1.

This generalizes considerably known asymptotics on analytic domains with Hölder smooth non vanishing weights [10]. The proof rests on some Hardy space theory, conformal mapping and $\overline{\partial}$ techniques. An exposition of the result was given at the conference *Orthogonal and Multiple Orthogonal Polynomials*, August 9-14 2015, Oaxaca (Mexico). An article is being written to report on this result.

6.5. Asymptotics of Rational Approximants

Participant: Laurent Baratchart.

This is joint work with M. Yattselev (IUPUI).

We studied best rational approximants in the *sup* norm to an analytic function f on compact set K of the analyticity domain Ω with connected complement. We showed that if the function can be continued analytically except over a set of logarithmic capacity zero comprising at most finitely many branchpoints, then the n-th root of the approximation error converges as n goes large to $e^{-2/C}$, with C the minimal Green capacity in $\mathbb{C} \setminus K$ of a compact set E outside of which f is single valued. Moreover, if $C > 0$, the normalized counting measure of the poles converges to the Green equilibrium distribution on E. We are currently considering the case of infinitely many branchpoints so as to get a somewhat final result on weak asymptotics in rational approximation to functions with polar singular set.

The proof rests on a blend of AAK-theory and potential theory.

BIPOP Project-Team

6. New Results

6.1. The contact complementarity problem, and Painlevé paradoxes

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

The contact linear complementarity problem is an set of equalities and complementarity conditions whose unknowns are the acceleration and the contact forces. It has been studied in a frictionless context with possibly singular mass matrix and redundant constraints, using results on well-posedness of variational inequalities obtained earlier by the authors [26]. This is also the topic of the first part of the Ph.D. thesis of Alejandro Blumentals where the frictional case is treated as a perturbation of the frictionless case [37]. The contact LCP is directly related to the so-called Painlevé's paradox of contact mechanics. In collaboration with C. Liu (Beijing university PKU) some results have been obtained from the analysis of a compliant model in the limit [34]. It shows on the classical sliding rod system that the inconsistent mode yield to instantaneous transition to a sticking mode. This is quite coherent with previous results obtained by Le xuan Anh in 1991 on the Painlevé-Klein system (bilateral constraints with Coulomb friction). With R. Kikuuwe from Kyushu University, we have also proposed a new formulation of the Baumgarte's stabilisation method, for unilateral constraints and Coulomb's friction , which sheds new light on Painlevé paradoxes as well [29].

6.2. Analysis of compliant nonlinear contact models

Participants: Bernard Brogliato, Guillaume James, Alexandre Vieira.

The master thesis of A. Vieira consisted of the study of suitable numerical method for compliant contact/impact models like the Simon-Hunt-Crossley and the Kuwabara-Kono models. These two models extend Hertz' contact by adding a dissipative force that takes the form of nonlinear viscous friction (nonlinear spring/dashpot). The fact that the Kuwabara-Kono dissipation is non-Lipschtiz requires particular care.

6.3. Discrete-time sliding mode control

Participants: Vincent Acary, Bernard Brogliato, Olivier Huber.

This topic concerns the study of time-discretized sliding-mode controllers. Inspired by the discretization of nonsmooth mechanical systems, we propose implicit discretizations of discontinuous, set-valued controllers [3]. This is shown to result in preservation of essential properties like simplicity of the parameters tuning, suppression of numerical chattering, reachability of the sliding surface after a finite number of steps, and disturbance attenuation by a factor h or h^2 [22]. This work was part of the ANR project CHASLIM. Within the framework of CHASLIM we have performed many experimental validations on the electropneumatic setup of IRCCyN (Nantes), which nicely confirm our theoretical and numerical predictions: the implicit implementation of sliding mode control, drastically improves the input and output chattering behaviours, both for the classical order-one ECB-SMC and the twisting algorithms [33], [42], [27], [28]. In particular the high frequency bang-bang controllers which are observed with explicit discretizations, are completely suppressed. The implicit discretization has been applied to the classical equivalent-based-control SMC, and also to the twisting sliding-mode controller. The case of a nonlinear controller is studied in [35].

6.4. Lur'e set-valued dynamical systems: State observers

Participants: Bernard Brogliato, Christophe Prieur.

Lur'e systems are quite popular in Automatic Control since the fifties. Set-valued Lur'e systems possess a static feedback nonlinearity that is a multivalued function. We study in [53], [32] state observers for particular Lur'e systems which are Moreau's sweeping processes modelling Lagrange dynamics with frictionless unilateral constraints.

6.5. Measure Driven ODEs

Participants: Bernard Brogliato, Christophe Prieur.

Measure driven Ordinary differential equations are analyzed in [31] from the point of view of input-to-state stability (ISS). This relies on the solution concept introduced by Bressan and Rampazzo. Lyapunov-like functions are used to caracterize the ISS. The link with impulsive ODEs and switching systems is made.

6.6. Numerical analysis of multibody mechanical systems with constraints

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

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

Participants: Vincent Acary, Bernard Brogliato, Mounia Haddouni.

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

6.6.2. Multibody systems with clearances (dynamic backlash)

Participants: Vincent Acary, Bernard Brogliato, Narendra Akadkhar.

The PhD thesis of N. Akadkhar under contract with Schneider Electric concerns the numerical simulation of mechanical systems with unilateral constraints and friction, where the presence of clearances in imperfect joints plays a crucial role. A first work deals with four-bar planar mechanisms with clearances at the joints, which induce unilateral constraints and impacts, rendering the dynamics nonsmooth. The objective is to determine sets of parameters (clearance value, restitution coefficients, friction coefficients) such that the system's trajectories stay in a neighborhood of the ideal mechanism (*i.e.* without clearance) trajectories. The analysis is based on numerical simulations obtained with the projected Moreau-Jean time-stepping scheme. These results have been reported in [47]. It is planned to extend these simulations to frictional cases and to mechanisms of circuit breakers.

6.7. Nonlinear waves in granular chains

Participants: Guillaume James, Bernard Brogliato, Alexandre Vieira.

Granular chains made of aligned beads interacting by contact (e.g. Newton's cradle) are widely studied in the context of impact dynamics and acoustic metamaterials. While much effort has been devoted to the theoretical and experimental analysis of solitary waves in granular chains, there is now an increasing interest in the study of breathers (spatially localized oscillations) in granular systems. Due to their oscillatory nature and associated resonance phenomena, static or traveling breathers exhibit much more complex dynamical properties compared to solitary waves. Such properties have strong potential applications for the design of acoustic metamaterials allowing to efficiently damp or deviate shocks and vibrations. Our contribution to this field is twofold. In the work [52], the existence of static breathers is analyzed in granular metamaterials consisting of hollow beads with internal masses. Using multiple scale analysis and exploiting the unilateral character of Hertzian interactions, we show that long-lived breather solutions exist but time-periodic breathers do not (breather solutions actually disperse on long time scales). Moreover, in a collaboration with Y. Starosvetsky and D. Meimukhin (Technion), we numerically study the persistence of traveling breathers in

granular chains with local potentials under the effect of contact damping. Using a viscoelastic damping model (Hertz-Kuwabara-Kono model), we show that breathers can be generated by simple impacts in granular chains made from various materials (breathers propagate over a significant number of sites before being damped). The design of an experimental setup to test these theoretical predictions is underway. Another series of works concerns more specifically the modeling and numerical analysis of dissipative impacts : introduction of appropriate variables and simplifications for different models of contact damping (James, Brogliato), and comparative tests for various numerical discretizations of the Hunt-Crossley and Kuwabara-Kono models (Vieira, Brogliato, James).

6.8. Traveling pulses in the Burridge-Knopoff model

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

The Burridge-Knopoff model describes the earthquake faulting process through the interaction of two plates modeled as a chain of blocks elastically coupled subject to a friction force. We study the existence of soliton-like solutions for the excitable Burridge-Knopoff model with different friction forces. We report for the first time the propagation of a one-pulse solitary wave where the position of the blocks remains unchanged after the passage of the wave. Extensive numerical simulations are done for different friction laws and a systematic investigation of the influence of the pulling velocity and the coupling constant is done. For a piecewise linear frictional law, we prove the existence of a traveling pulse in the weak coupling limit. A lower bound of the propagation speed is derived together with results on the shape of the traveling wave.

6.9. Propagation in space-discrete excitable systems

Participant: Arnaud Tonnelier.

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

6.10. Inverse modeling with contact and friction

6.10.1. Inverse statics of plates and shells with frictional contact

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

We pursued our work on the static inversion of thin elastic shells, in the presence of contact and friction with an external object. We have shown how to formulate draping as a local constrained minimization problem, and we have generalized the adjoint method to this constrained case. These new results are included in Romain Casati's PhD thesis, defended in June 2015, and will be part of a paper to be submitted in 2016.

6.11. Continnum modeling of granular materials

6.11.1. Continuum modeling of granular materials

Participants: Florence Bertails-Descoubes, Gilles Daviet.

We have proposed a new numerical framework for the continuous simulation of dilatable materials with pressure-dependent (Coulomb) yield stress, such as sand or cement. Relying upon convex optimization tools, we have shown that the continuous equations of motion coupled to the macroscopic nonsmooth Drucker-Prager rheology can be interpreted as the exact analogous of the solid frictional contact problem at the heart of Discrete Element Methods (DEM), extended to the tensorial space. Combined with a carefully chosen finite-element discretization, this new framework allowed us to avoid regularizing the continuum rheology while benefiting from the efficiency of nonsmooth optimization solvers, mainly leveraged by DEM methods so far. Our numerical results were successfully compared to analytic solutions on model problems, such as the silo discharge, and we retrieved qualitative flow features commonly observed in reported experiments of the literature. This work is currently under review at the Journal of Non Newtonian Fluid Mechanics, and a preliminary version is available as a research report [43]. Furthermore, we have recently extended the approach to account for flows with a varying density, leveraging the Material Point Method to discretize the Drucker Prager yield criterion without linearization. This work will be submitted to ACM SIGGRAPH in 2016.

6.12. Nonsmooth optimisation and applications

6.12.1. Semidefinite programming and combinatorial optimization

Participant: Jérôme Malick.

We have worked with Frederic Roupin (Prof. at Paris XIII) and Nathan Krislock (Assistant Prof. at North Illinois University, USA) on the use of semidefinite programming to solve combinatorial optimization problems to optimality. Nathan was the guest of the team during 2 months (June/July).

We have worked on a generic semidefinite-based solver for solve binary quadratic optimization problems. Using the generality of the bounds proposed in [54]. Our article is in revision in ACM Transaction of Mathematical Software. Our solver and our data sets are available online at http://lipn.univ-paris13.fr/BiqCrunch/.

Specializing the method of the k-cluster problem, we have proposed in [51] an algorithm able to solve exactly k-cluster instances of size 160. In practice, our method works particularly fine on the most difficult instances (with a large number of vertices, small density and small k).

6.12.2. Stochastic optimization for electricity production

Participant: Jérôme Malick.

Everyday, electricity generation companies submit a generation schedule to the grid operator for the coming day; computing an optimal schedule is called the unit-commitment problem. In collaboration with W. van Ackooij from EDF, we have proposed in [44] a two-stage formulation of unit-commitment to better include the impact of renewable energies. We present a primal-dual decomposition approach to tackle large-scale instances of these two-stage problems, wherein both the first and second stage problems are full unit-commitment problems. We provide an analysis of the theoretical properties of the algorithm, as well as computational experiments showing the interest of the approach for real-life large-scale unit-commitment instances.

6.13. Robotics

6.13.1. Mobile manipulation by humanoid robots

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

This year's contributions to the field of mobile manipulation by humanoid robots have been three-fold: a lexicographic MPC approach to the decision of using optional contacts when necessary to maintain balance (and only when necessary), a robust MPC approach to online generation of dynamic walking motion on uneven ground such as stairs, and an analysis of the role of viability and capturability in collision prevention, using once again a lexicographic MPC approach.

6.13.2. Reactive trajectory generation

Participants: Pierre-Brice Wieber, Dimitar Dimitrov, Saed Al Homsi.

The goal of the collaboration with Adept Technologies is to generate time optimal trajectories in the presence of moving obstacles in real time. Three approaches with increasing computational complexity have been proposed and validated experimentally. The cheapest approach begins with a standard bang-bang control which is time-optimal in the absence of obstacles, and simply projected on dynamic limits imposed by collision avoidance. This leads to reasonable results where collisions are explicitly avoided, but time-optimality is lost in the process. A more complex approach introduces an MPC scheme minimizing a weighted L1-norm, which is tuned to generate a time-optimal behavior in the absence of obstacles. In the presence of obstacles, time-optimality is once again lost, however, results are much improved with respect to the previous approach. The final, and most complex approach, considers time-optimality as a lexicographic objective: a lexicographic MPC scheme is proposed, which achieves time-optimality in the presence of obstacles, with reasonable online computation time. This work has been submitted to ICRA 2016.

COMMANDS Project-Team

7. New Results

7.1. Optimal control of ordinary differential equations

7.1.1. Periodic optimal controls for the Purcell microswimmer

Participant: Pierre Martinon.

We investigate in [31] some geometric and numerical aspects related to optimal control problems for the so-called Purcell Three-link swimmer, in which the cost to minimize represents the energy consumed by the swimmer. More precisely, we focus on the periodic aspect of optimal trajectories and controls. Linearizing the control system along a reference extremal, we estimate the conjugate points, which play a crucial role for the second order optimality conditions. With techniques imported by the sub-Riemannian geometry, we also show that the nilpotent approximation of the system provides a model which is integrable, obtaining explicit expressions in terms of elliptic functions. This approximation allows to compute optimal periodic controls for small deformations of the body. Numerical simulations are presented using Hampath and Bocop codes. A first paper was submitted in october 2015.

7.1.2. Study of optimal health insurance policies

Participant: Pierre Martinon.

In collaboration with the Economy department of Ecole Polytechnique, we analyze the design of an optimal medical insurance contract under ex post moral hazard, i.e., when illness severity cannot be observed by insurers and policyholders may exaggerate their health expenditures. This problem is reformulated in the optimal control framework, and we study the possible existence of deductibles or bunching phenomenons in optimal contracts. A paper will be submitted in early 2016.

7.2. Optimal control of partial differential equations

7.2.1. Local minimization algorithms for dynamic programming equations

Participant: Axel Kröner.

The numerical realization of the dynamic programming principle for continuous-time optimal control leads to nonlinear Hamilton-Jacobi-Bellman equations which require the minimization of a nonlinear mapping over the set of admissible controls. This minimization is often performed by comparison over a finite number of elements of the control set. In this paper we demonstrate the importance of an accurate realization of these minimization problems and propose algorithms by which this can be achieved effectively. The considered class of equations includes nonsmooth control problems with l1-penalization which lead to sparse controls. See the reprint [28].

7.2.2. Suboptimal feedback control of PDEs by solving HJB equations on adaptive sparse grids

Participant: Axel Kröner.

An approach to solve finite time horizon sub-optimal feedback control problems for partial differential equations is proposed by solving dynamic programming equations on adaptive sparse grids. The approach is illustrated for the wave equation. A semi-discrete optimal control problem is introduced and the feedback control is derived from the corresponding value function. The value function can be characterized as the solution of an evolutionary Hamilton-Jacobi Bellman (HJB) equation which is defined over a state space whose dimension is equal to the dimension of the underlying semi-discrete system. Besides a low dimensional semi-discretization it is important to solve the HJB equation efficiently to address the curse of dimensionality. We propose to apply a semi-Lagrangian scheme using spatially adaptive sparse grids. Sparse grids allow the discretization of the value functions in (higher) space dimensions since the curse of dimensionality of full grid methods arises to a much smaller extent. For additional efficiency an adaptive grid refinement procedure is explored. We present several numerical examples studying the effect the parameters characterizing the sparse grid have on the accuracy of the value function and the optimal trajectory. See the report [27].

7.2.3. Numerical approximation of level set power mean curvature flow

Participant: Axel Kröner.

In this paper we investigate the numerical approximation of a variant of the mean curvature flow. We consider the evolution of hypersurfaces with normal speed given by H^k, $k \geq 1$, where H denotes the mean curvature. We use a level set formulation of this flow and discretize the regularized level set equation with finite elements. In a previous paper we proved an a priori estimate for the approximation error between the finite element solution and the solution of the original level set equation. We obtained an upper bound for this error which is polynomial in the discretization parameter and the reciprocal regularization parameter. The aim of the present paper is the numerical study of the behavior of the evolution and the numerical verification of certain convergence rates. We restrict the consideration to the case that the level set function depends on two variables, i.e. the moving hypersurfaces are curves. Furthermore, we confirm for specific initial curves and different values of k that the flow improves the isoperimetrical deficit. See the report [29].

7.3. Finance and stochastic control

7.3.1. Second order Pontryagin's principle for stochastic control problems

Participant: Frédéric Bonnans.

In this Hal reprint [25], we discuss stochastic optimal control problems whose volatility does not depend on the control, and which have finitely many equality and inequality constraints on the expected value of functions of the final state, as well as control constraints. The main result is a proof of necessity of some second order optimality conditions involving Pontryagin multipliers.

7.3.2. On the convergence of the Sakawa-Shindo algorithm in stochastic control

Participant: Frédéric Bonnans.

In the accepted paper [32], we analyze an algorithm for solving stochastic control problems, based on Pontryagin's maximum principle, due to Sakawa and Shindo in the deterministic case and extended to the stochastic setting by Mazliak. We assume that either the volatility is an affine function of the state, or the dynamics are linear. We obtain a monotone decrease of the cost functions as well as, in the convex case, the fact that the sequence of controls is minimizing, and converges to an optimal solution if it is bounded. In a specific case we interpret the algorithm as the gradient plus projection method and obtain a linear convergence rate to the solution.

7.3.3. Optimal multiple stopping problems

Participant: Frédéric Bonnans.

In the paper [13] we extend some results by Carmona and Touzi [8], who studied an optimal multiple stopping time problem in a market where the price process is continuous. We generalize their results when the price process is allowed to jump. Also, we generalize the problem associated to the valuation of swing options to the context of jump diffusion processes. We relate our problem to a sequence of ordinary stopping time problems. We characterize the value function of each ordinary stopping time problem as the unique viscosity solution of the associated Hamilton–Jacobi–Bellman variational inequality. In the paper [14] we deal with numerical solutions to an optimal multiple stopping problem. The corresponding dynamic programing (DP) equation is a variational inequality satisfied by the value function in the viscosity sense. The convergence of the numerical scheme is shown by viscosity arguments. An optimal quantization method is used for computing the conditional expectations arising in the DP equation. Numerical results are presented for the price of swing option and the behavior of the value function.

7.4. Electricity production

7.4.1. Equilibria over energy markets

Participant: Benjamin Heymann.

Motivated by electricity markets we introduce in this paper a general network market model, in which agents are located on the nodes of a graph, a traded good can travel from one place to another through edges considering quadratic losses. An independent operator has to match locally production and demand at the lowest expense. As argued in our previous paper "Cost-minimizing regulations for a wholesale electricity market" this setting is relevant to describe some real electricity markets, pricing behavior and market power coming from the fact that generators can bid above their true value. In a general setting of many distributed generator agents connected by a transmission network, bidding piece-wise linear cost functions, we propose a pricing optimal mechanism model to reduce market power. Our main results are the expression of the optimal mechanism design, two algorithms for the allocation problem and market power estimations. To deduce these nice properties, we intensively use convex analysis and some monotone behaviors of the set-valued maps involved. Furthermore, these algorithms make it possible to numerically compute a Nash equilibrium for the procurement auction, which is important to compare the optimal mechanism and the standard auction setting. Finally, we also show some interesting examples. In the continuation of this work, we introduce a class of biding games for which we prove the existence of a Nash equilibrium. We give a sufficient condition for uniqueness, propose a numerical scheme to compute the extreme Nash Equilibria and show that the equilibrium strategies are convex for a subclass of games. We apply this framework to electricity auctions.

7.4.2. Energy management for a micro-grid

Participants: Frédéric Bonnans, Benjamin Heymann, Pierre Martinon, Olivier Tissot.

We study in [33] the energy management problem for a microgrid including a diesel generator and a photovoltaic plant with a battery storage system. The objective is to minimize the total operational cost over a certain timeframe, primarily the diesel consumption, while satisfying a prescribed power load. After reformulation, the decision variables can be reduced to the charging /discharging power for the battery system. We take into account the switching cost for the diesel generator, the non-convex objective, and the long-term aging of the batteries. We solve this problem using a continuous optimal control framework, with both a direct transcription method (time discretization) and a Dynamic Programming method (Hamilton Jacobi Bellman). This project is a collaboration between team COMMANDS (Inria Saclay, France) and Centro de Energia (Universidad de Chile, Chile). Ongoing works include more refined battery aging models, and modeling the stochastic nature of the photovoltaic power and power load.

7.5. Energy management in transport

7.5.1. Energy management for an hybrid vehicle

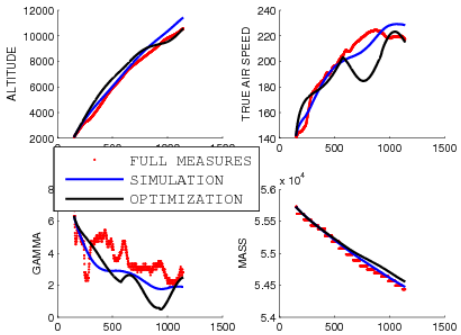
Participants: Florine Bleuse, Frédéric Bonnans, Pierre Martinon.

In the framework of the PhD thesis of F.Bleuse, 'Optimal control and robustness for rechargeable hybrid vehicles'. The study is focused on the so-called parallel architecture, with both the thermal and electric engines able to move the vehicle. The main axis is to optimize the use of the thermal engine. We started to develop a methodology with two time scales for solving the problem of computing a feedback control.

7.5.2. Collaboration with the startup Safety Line

Participants: Frédéric Bonnans, Pierre Martinon, Olivier Tissot.

We pursue our collaboration with Safety Line, using more refined atmospheric models (including for instance predicted wind data). Future works include high performance optimization for the cruise phase as well as analyzing the validity of the parameter estimation performed with the data from the flight recorders.



SAFETY LINE
take control of your safety

bocop

Figure 1. Parameter identification and trajectory optimization

DISCO Project-Team

7. New Results

7.1. Algebraic Analysis Approach to Linear Functional Systems

Participants: Alban Quadrat [Disco], Rosane Ushirobira [Non-A].

7.1.1. Artstein's transformation of linear time-delay systems

Artstein's classical results show that a linear first-order differential time-delay system with delays in the input is equivalent to a linear first-order differential system without delays thanks to an invertible transform which includes integral and delay operators. Within a constructive algebraic approach, we show how Artstein's reduction can be found again and generalized as a particular isomorphism problem between the finitely presented modules defined by the two above linear systems over the ring of integro-differential time-delay operators. Moreover, we show that Artstein's reduction can be obtained in an automatic way by means of symbolic computation, and thus can be implemented in computer algebra systems.

7.1.2. Algebraic analysis for the Ore extension ring of differential time-varying delay operators

No algebraic (polynomial) approach seems to exist for the study of linear differential time-delay systems in the case of a (sufficiently regular) time-varying delay. Based on the concept of skew polynomial rings developed by Ore in the 30s, we construct the ring of differential time-delay operators as an Ore extension and to analyze its properties. A characterization of classical algebraic properties of this ring, such as noetherianity, its homological and Krull dimensions and the existence of Gröbner bases, are given in terms of the time-varying delay function. The algebraic analysis approach to linear systems theory allows us to study linear differential time-varying delay systems (e.g. existence of autonomous elements, controllability, parametrizability, flatness, behavioral approach) through methods coming from module theory, homological algebra and constructive algebra.

7.2. New Techniques for Robust Control of Linear Infinite-Dimensional Systems

Participants: Yacine Bouzidi [Disco], Petteri Laakkonen [Univ. Tampere], Adrien Poteaux [Lille 1], Alban Quadrat [Disco], Arnaud Quadrat [SAGEM], Guillaume Rance [SAGEM], Fabrice Rouillier [Ouragan].

7.2.1. Computer algebra methods for testing the structural stability of multidimensional systems

We present new computer algebra based methods for testing the structural stability of n-D discrete linear systems (with $n \geq 2$). More precisely, starting from the usual stability conditions which resumes to deciding if an hypersurface has points in the unit polydisc, we show that the problem is equivalent to deciding if an algebraic set has real points and use state-of-the-art algorithms for this purpose. Our strategy has been implemented in `Maple` and its relevance demonstrated through numerous experimentations.

Moreover, we also consider the specific case of two-dimensional systems and focus on the practical efficiency aspect. For such systems, the problem of testing the stability is reduced to that of deciding if a bivariate algebraic system with finitely many solutions has real ones. Our first contribution is an algorithm that answers this question while achieving practical efficiency. Our second contribution concerns the stability of two dimensional systems with parameters. More precisely, given a two-dimensional system depending on a set of parameters, we present a new algorithm that computes regions of the parameters space in which the considered system is structurally stable.

7.2.2. Computer algebra methods for the stability analysis of differential systems with commensurate time-delays

Within the frequency-domain approach, the asymptotic stability of of linear differential systems with commensurate delays is ensured by the condition that all the roots of the corresponding quasipolynomial have negative real parts. A classical approach for checking this condition consists in computing the set of critical zeros of the quasipolynomial, i.e., the roots (and the corresponding delays) of the quasipolynomial that lie on the imaginary axis, and then analyzing the variation of these roots with respect to the variation of the delay. Based on solving algebraic systems techniques, we propose a certified and efficient symbolic-numeric algorithm for computing the set of critical roots of a quasipolynomial. Moreover, using recent algorithmic results developed by the computer algebra community, we present an efficient algorithm for the computation of Puiseux series at a critical zero which allows us to finely analyze the stability of the system with respect to the variation of the delay

7.2.3. A fractional ideal approach to the robust regulation problem

We show how fractional ideal techniques developed in [8] can be used to obtain a general formulation of the internal model principle for stabilizable infinite-dimensional SISO plants which do not necessarily admit coprime factorization. This result is then used to obtain necessary and sufficient conditions for the robust regulation problem. In particular, we find again all the standard results obtained in the literature.

7.2.4. Robust control as an application to the homological perturbation lemma:

Within the lattice approach to transfer matrices developed in [8], we have recently shown how standard results on robust control can be obtained in a unified way and generalized when interpreted as a particular case of the so-called Homological Perturbation Lemma. This lemma plays a significant role in algebraic topology, homological algebra, algebraic and differential geometry, computer algebra .... Our results show that it is also central to robust control theory for infinite-dimensional linear systems.

7.2.5. A symbolic-numeric method for the parametric H_∞ loop-shaping design problem

We develop a symbolic-numeric method for solving the H_∞ loop-shaping design problem for a low order single-input single-output system with parameters. Due to the system parameters, no purely numerical algorithm can indeed solve the problem. Using Gröbner basis techniques and the rational univariate representation of zero-dimensional algebraic varieties, we first give a parametrization of all the solutions of the two algebraic Riccati equations associated with the H_∞ control problem. Then, using results on the spectral factorization problem, a certified symbolic-numeric algorithm is obtained for the computations of the positive definite solutions of these two algebraic Riccati equations. Finally, we present a certified symbolic-numeric algorithm which solves the H_∞ loop-shaping design problem for the above class of systems.

7.3. Improved algorithm for computing separating linear forms for bivariate systems

Participants: Yacine Bouzidi [Disco], Sylvain Lazard [Vegas], Guillaume Moroz [Vegas], Marc Pouget [Vegas], Fabrice Rouillier [Ouragan].

We present new algorithms for computing linear separating forms, RUR decompositions and isolating boxes of the solutions. We show that these three algorithms have worst-case bit complexity $\widetilde{O}_B(d^6 + d^5\tau)$, where $\widetilde{O}$ refers to the complexity where polylogarithmic factors are omitted and O_B refers to the bit complexity. We also present probabilistic Las-Vegas variants of our two first algorithms, which have expected bit complecity $\widetilde{O}_B(d^5 + d^4\tau)$. A key ingredient of our proofs of complexity is an amortized analysis of the triangular decomposition algorithm via subresultants, which is of independent interest.

7.4. Stable H_∞ Controller for Infinite-dimensional systems

The controllers, besides the stabilization, are often designed to achieve some performance and robustness objectives by minimizing H_∞ norm of some cost functions. The resulting controller may be stable or unstable. The unstable controllers, however, are more sensitive to sensor/actuator faults, or nonlinearities. It is not an easy task to design a stable controller for systems having infinitely many zeros and poles in the right-half-plane. By using the similar idea in [88], stable H_∞ controller design method will be presented for a certain class of infinite-dimensional plants. The plants may have infinitely many unstable zeros, however, it is assumed that these zeros are *unformly separated*. Under some certain assumptions, first, a sufficient condition will be presented to construct a real unit function, which satisfies certain interpolation conditions at the right-half-plane zeros of the plant and some H_∞ norm constraints. Then, by utilizing this result, stable H_∞ controller design method are presented.

7.5. Multiplicity and Stable Varieties of Time-delay Systems: A Missing Link

Multiple spectral values in dynamical systems are often at the origin of complex behaviors as well as unstable solutions. In this work, an unexpected property of multiple spectral values is emphasized. It has been shown that the variety corresponding to such a multiple root defines a stable variety for the steady state. Under mild assumptions, for the reduced examples we show that such a multiple spectral value is nothing else than the spectral abscissa.

7.6. Delay effect in chemical reactions

Belousov-Zhabotinskii (BZ) reaction, which is a very complicated reaction, has been widely studied in bio-science and chemistry, since its dynamic behaviour is similar to real biological oscillators [89]. For certain type of chemical reactions, the use of the law of mass-action kinetics may lead to some simple models expressed by ordinary differential equations. The main feature of BZ reaction, oscillatory behaviour, has been represented by a simple mechanism and the model of this mechanism can be described by ordinary differential equations. However, delayed mass-actions kinetics lead to more accurate models by conserving the simplicity and a relative reduced number of parameters. In [83], [95], [96], [82], some delay-differential models are proposed for Belousov-Zhabotinskii (BZ) reaction with a fewer of concentrations compared to the models obtained by ordinary differential equations. However, in most of these works, the delay, which occurs due to the required time to provide sufficient energy, has not been taken into account. Recently, we consider a more realistic Belousov-Zhabotinskii model, which includes two independent delays. The novelty of the proposed model with respect to the existing ones in the literature can be summarized as follows; one of these delays is introduced to reproduce qualitatively the behavior of the model proposed by [84] with a less number of concentrations as in [95]. Second, the remaining delay appears naturally since the reactants do not react suddenly in the chemical reactions, i.e. the delay stems from the needed time for the occurence of reaction, called “delayed concentration”.

7.7. H_∞-stability analysis of neutral systems with commensurate delays

Participants: Catherine Bonnet, Le Ha Vy Nguyen.

We have analyzed [32] the H_∞-stability of neutral systems with commensurate delays and multiple chains of poles asymptotic to a same set of points on the imaginary axis. First, by approximation, the location of poles of large modulus is determined. This analysis requires to consider several subclasses of systems where poles of high modulus exhibit various patterns. Second, we derive necessary and sufficient conditions for H_∞-stability which are easy to check as expressed in terms of the degrees of the polynomials involved in the numerator and denominator of the transfer function.

7.8. H_∞-Stabilization of neutral delay systems

Participants: Catherine Bonnet, Yutaka Yamamoto [Kyoto University].

We have considered two particular neutral delay systems with one delay having a chain of poles clustering the imaginary axis from left or right. For these systems the existence of coprime factorizations have been investigated. The extension to more general systems is still in progress.

7.9. Interval Observer of a new type

Participants: Frederic Mazenc [Disco], Emilia Fridman [Tel-Aviv University].

In [19], we addressed the fundamental problem of constructing for nonlinear systems observers that converge in finite time and, at the same time, provided with upper and lower bounds for the solutions when disturbances are present. This new technique of estimation relies on the use of past values of the output, as done to construct some already known observers which converge in finite time, and on a recent technical result pertaining to the theory of the monotone systems The result applies to systems with additive disturbances and disturbances in the output. The nonlinear terms are not supposed to be globally Lipschitz, but it is requested that they depend only on the input and output variables. The fundamental advantage over classical interval observer techniques is that no information on the initial conditions of the solutions of the studied system are needed.

7.10. Trajectory based approach

Participants: Frederic Mazenc [Disco], Silviu Niculescu [Disco], Michael Malisoff [LSU].

In the work [22], we provided a new stability analysis technique, which is based on the study of the behaviors of the solutions over any interval $[t-T, T]$, where t represents the time and T is an appropriately chosen constant. Thus trajectory-based approach is completely new in the sense that it neither reply on Lyapunov functions nor on the small gain theorem. One of its most striking feature is that it applies to a broad number of systems (systems with delay, continuous/discrete systems, ODE coupled with difference equations).

In [30] and [55] we provided several significant applications of the main result of [22]. In [30] in two results, we use a Lyapunov function for a corresponding undelayed system to provide a new method to prove stability of linear continuous-time time-varying systems with bounded time-varying delays. We allow uncertainties in the coefficient matrices of the systems. Our main results use upper bounds on an integral average involving the delay. The results establish input-to-state stability with respect to disturbances. We also provided in [55] a novel reduction model approach that ensures global exponential stabilization of linear systems with a time-varying pointwise delay in the input, which allows the delay to be discontinuous and uncertain. Finally, we provided an alternative to the reduction model method, based on a different dynamic extension.

7.11. Positive Systems Approach

Participants: Frederic Mazenc [Disco], Michael Malisoff [LSU].

We presented new methods to prove stability of time-varying systems with delays by taking advantage of the theory of the positive and cooperative systems [24], [23]. We used linear time-varying Lyapunov functionals, operators with integral terms, and positive systems, and we provided robustness of the stability with respect to multiplicative uncertainty in the vector fields. We allowed cases where the delay may be unknown, and where the vector fields defining the systems are not necessarily bounded. The results apply to neutral time-varying systems but are very distinct from those of the paper [69].

7.12. Attitude dynamics, control and observation

Participants: Frederic Mazenc [Disco], Maruthi Akella [Univ of Texas], Divya Thakur [Univ of Texas], Sunpil Yang [Univ of Texas].

We addressed several problems pertaining to the control of fully actuated rigid-body attitude dynamics. The fundamental tool we used is the adaptation of the so called strictification approach to the features of the attitude dynamics (see [3] for an introduction to the 'strictifiation' paradigm). In particular

1) The contribution [31] output feedback stabilization of fully actuated rigid-body attitude dynamics in the presence of unknown point-wise time-delay in the input torque. Specifically, rate-gyros are unavailable here and only the attitude state represented by the unit quaternion is assumed to be measured. It is worth mentioning that the presence of unknown time-delay in the measured variables, imposes formidable technical challenges for the output-feedback attitude stabilization problem on hand. One of the central difficulties stems from the availability of only a weak Lyapunov-like function for the passivity based dynamic output feedback controller in the absence of delay. This obstacle is circumvented in this contribution by a novel process of partially strictifying the underlying weak Lyapunov-like function.

2) In [57], we considered stabilization of fully actuated rigid-body attitude dynamics in the absence of angular velocity measurements and presents new robustness results to bounded unknown external disturbance torques. In particular, it is assumed that only body orientation is measured in the form of a unit-quaternion signal. It is well known that the passivity properties of the dynamics allows design of velocity-free controllers using a first-order stable filter driven by measured states. When external disturbance torques are taken into account, however, the robustness properties of these passivity-based output feedback controllers cannot be readily analyzed because the Lyapunov-like function from which the controller is derived has a time-derivative that is only negative semidefinite, and therefore non-strict. This obstacle is circumvented through a new partial-strictification approach which ultimately allows the characterization of robustness properties for this closed-loop system.

3) In [18], we proposed a smooth angular velocity observer for the attitude tracking control of a rigid body in the absence of angular velocity measurements. The observer design ensures asymptotic convergence of angular velocity state estimation errors irrespective of the control torque or the initial attitude state of the spacecraft. Unlike existing rate observer formulations that attain estimation error convergence by imposing certain switching conditions or hybrid-logic, the proposed observer has a smooth structure that ensures continuity of all estimated states.Lyaounov strictification is again the key technical result making us to establish the results.

7.13. Introduction of artificial delays for control and observation

Participants: Frederic Mazenc [Disco], Silviu Niculescu [Disco], Michael Malisoff [LSU], Nikolaos Bekiaris-Liberis [Tech. Univ. of Crete].

It is well-known that, in some cases, control or observation problems for systems with or without inherent delay can be solved by artificially introducing delays. We obtained in this field of reseach two distinct new results.

1) In [56] and [54], we have considered a family of linear time-varying systems with an input, an output and delays in the input. We have shown that, under classical stabilizability and detectability assumptions, all the systems of this family can be exponentially stabilized through a time-varying feedback depending on past values of the output and the input and this without the use of observers or dynamic extensions. Hence, the simplicity of the design and the determination of the value of the solutions in finite time are the main features of the new approach.

2) In [54], we provided a new backstepping result for time-varying systems with input delays. The novelty of the contribution is in the bounds on the controls, and the facts that (i) one does not need to compute any Lie derivatives to apply our controls, (ii) the controls have no distributed terms, and (iii) no differentiability conditions on the available controls for the subsystems are needed. The result is obtained by the introduction of constant pointwise delay in the input. Thus this result is significantly different for backstepping results for systems with delay in the input as presented for instance in [70].

7.14. Continuous-discrete observers

Participants: Frederic Mazenc [Disco], Emilia Fridman [Tel-Aviv University], Michael Malisoff [LSU], Vincent Andrieu [LAGEP].

We solved several problems of observer design pertaining to the fundamental and difficult case where the measurements are available at discrete instants only.

1) We considered the problem of stabilizing a linear continuous-time system with discrete-time measurements and a sampled input with a pointwise constant delay [20]. In a first part, we designed a continuous-discrete observer which converges when the maximum time interval between two consecutive measurements is sufficiently small. In a second part, we constructed a dynamic output feedback by using a technique which is strongly reminiscent of the reduction model approach. It stabilizes the system when the maximal time between two consecutive sampling instants is sufficiently small. No limitation on the size of the delay is imposed and an ISS property with respect to additive disturbances is established.

2) The problem of designing continuous-discrete observers for a large class of continuous time nonlinear time-varying systems with discrete time measurements has been addressed in several contributions: [12], [17] and [53]. Some technical obstacle encountered in [12] were overcome in [17] by using the notion of cooperative systems, which led to results consisting in explicit expressions of the largest sampling interval under which the observers converge to the solutions of the original system

7.15. Sensor faults: detectability and distributed Fault Diagnosis. A positive invariance based approach.

Participants: Sorin Olaru [correspondent], Vasso Reppa [L2S], Abid Kodakkadan [L2S], Marios Polycarpou [University of Cyprus].

The paper [62] introduces the performance analysis of local monitoring modules of a distributed diagnosis scheme tailored to detect multiple sensor faults in a class of nonlinear systems. The local modules monitor the healthy operation of subsets of sensors (local sensor sets). Every module is designed to detect the occurrence of faults in the local sensor sets when some analytical redundancy relations (ARRs) are violated. The set of ARRs is formulated using structured residuals and adaptive thresholds based on a nonlinear observer. In order to characterize the sensitivity of every monitoring module to local sensor faults, we obtain structural fault detectability conditions based on adaptive thresholds, and strong fault detectability conditions based on ultimate robust positively invariant sets. These conditions correspond to explicit relationships between the local sensor faults, the worst-case bounds on modeling uncertainties and the design parameters of the local monitoring module.

In a recent paper [44], we considered the abnormal functioning of sensors (measurement channels) deployed for monitoring and control of discrete linear time invariant systems affected by additive uncertainties. The main objective was to analyze the sensor fault detectability via a robust positive invariance based technique. The analysis relies on the categorization of detectable faults and leads to certain conditions for guaranteed nondetectability, guaranteed detectability and implicit detectability.

As a support to this line of research, in the paper [73] we presented a methodology for computing robust positively invariant sets for linear, discrete time-invariant systems that are affected by additive disturbances, with the particularity that these disturbances are subject to state-dependent bounds. The proposed methodology requires less restrictive assumptions compared to similar established techniques, while it provides the framework for determining the state-dependent (parameterized) ultimate bounds for several classes of disturbances. The added value of the proposed approach is illustrated by an optimization-based problem for detecting the mode of functioning of a switching system.

7.16. Fault tolerant control design for multi-sensor networked control systems

Participants: Sorin Olaru [correspondent], Nikola Stankovic [L2S], Silviu Niculescu [L2S], Florin Stoican [Univ. Politehnica, Bucharest].

In the paper [27], we consider a multi-sensor networked control configuration with linear plant which is affected by a bounded additive disturbance. Shared network is used for the communication between sensors and controller. It is assumed that the sensors are prone to abrupt faults, while the controller's input may be updated with a varying time-delay. In order to identify and isolate the sensor(s) providing faulty information, we equip the controller with a set-based detection and isolation routine. Furthermore, in the case when the network induces time-delays, control is performed based on the knowledge we have on the mathematical model of the plant. In the presence of model inaccuracies or disturbance, such a control action may not guarantee satisfying performance of the system. Therefore, a stabilising controller with delay compensation has been designed.

7.17. Constrained Control of Uncertain, Time-varying Linear Discrete-Time Systems Subject to Bounded Disturbances

Participants: Sorin Olaru [correspondent], Nam Nguyen [Technion, Israel], Per-Olof Gutman [Technion, Israel], Morten Hovd [NTNU, Trondheim, Norway].

In the paper [26], robust invariance for ellipsoidal sets with respect to uncertain and/or time-varying linear discrete-time systems with bounded additive disturbances is revisited. We provide an extension of an existing invariance condition and propose a novel robust interpolation based control design involving several local unconstrained robust optimal controls. It is shown that at each time instant a quadratic programming problem is solved on-line for the implementation. Proofs of recursive feasibility and input-to-state stability are provided to support the theoretical foundation.

7.18. Explicit robust constrained control for linear systems : analysis, implementation and design based on optimization

Participants: Sorin Olaru [correspondent], Ngoc Anh Nguyen [L2S], Pedro Rodriguez Ayerbe [L2S], Martin Gulan [STUBA, Bratislava].

Piecewise affine (PWA) feedback control laws is relevant for the control of constrained systems, hybrid systems; equally for the approximation of nonlinear control. However, they are associated with serious implementation issues. Motivated from the interest in this class of particular controllers, the thesis of Ngoc Anh Nguyen is mostly related to their analysis and design. The first part of this thesis aims to compute the robustness and fragility margins for a given PWA control law and a linear discrete-time system. More precisely, the robustness margin was defined as the set of linear time-varying systems such that the given PWA control law keeps the trajectories inside a given feasible set. On a different perspective, the fragility margin contains all the admissible variations of the control law coefficients such that the positive invariance of the given feasible set is still guaranteed. The second part of this thesis focuses on inverse optimality problem for the class of PWA controllers. Namely, the goal is to construct an optimization problem whose optimal solution is equivalent to the given PWA function. The methodologyis based on convex lifting [33]: an auxiliary 1-dimensional variable which enhances the convexity characterization into recovered optimization problem. Accordingly, if the given PWA function is continuous [35], the optimal solution to this reconstructed optimization problem will be shown to be unique. Otherwise, if the continuity of this given PWA function is not fulfilled, this function will be shown to be one optimal solution to the recovered problem [36]. In view of applications in linear model predictive control (MPC), it was shown that any continuous PWA control law can be obtained by a linear MPC problem with the prediction horizon at most equal to 2 prediction steps [65]. Aside from the theoretical meaning, this result can also be of help to facilitate implementation of PWA control laws by avoiding storing state space partition [66]. Another utility of convex liftings [34] will be shown in the last part of this thesis to be a control Lyapunov function. Accordingly, this convex lifting will be deployed in the so-called robust control design based on convex liftings for linear system affected by bounded additive disturbances and polytopic uncertainties [60]. Both implicit and explicit controllers can be obtained. This method can also guarantee the recursive feasibility and robust stability. However, this control Lyapunov function is only defined over the maximal λ-contractive set for a given subunitary λ which is known to be smaller than the maximal controllable

set. Therefore, an extension of the above method to the N-steps controllable set will be presented. This method is based on a cascade of convex liftings where an auxiliary variable will be used to emulate a Lyapunov function. Namely, this variable will be shown to be non-negative, to strictly decrease for N first steps and to stay at 0 afterwards. Accordingly, robust stability is sought.

7.19. Predictive Control for multi-agent (multi-vehicle) systems

Participants: Sorin Olaru [correspondent], Ionela Prodan [LCIS], Minh Tri Nguyen [L2S], Cristina Stoica [L2S], Silviu Niculescu [L2S], Fernando Fontes [FEUP U. Porto], Joao Sousa [FEUP U. Porto], Fernando Lobo Pereira [FEUP U. Porto], Alexandra Grancharova [U. Sofia, Bulgaria].

We continued a mature line of research on the tracking problems for multi-agent systems. In [75] we presented a series of developments on predictive control for path following via a priori generated trajectory for autonomous aerial vehicles. The strategy partitions itself into offline and runtime procedures with the assumed goal of moving the computationally expensive part into the offline phase and of leaving only tracking decisions to the runtime. First, it will be recalled that differential flatness represents a well-suited tool for generating feasible reference trajectory. Next, an optimization-based control problem which minimizes the tracking error for the nonholonomic system is formulated and further enhanced via path following mechanisms. Finally, possible changes of the selection of sampling times along the path and their impact on the predictive control formulation will be discussed in detail.

On a relatively different frameowrk, in [71] we investigate multiple agents evolving in the same environment with the objective of preservation of a predefined formation. This formation aims to reinforce the safety of the global system and further lighten the supervision task. One of the major issues for this objective is the task assignment problem, which can be formulated in terms of an optimization problem by employing set-theoretic methods. In real time the agents will be steered into the defined formation via task (re)allocation and classical feedback mechanisms. The task assignment calculation is often performed in an offline design stage, without considering the possible variation of the number of agents in the global system. These changes (i.e., including/excluding an agent from a formation) can be regarded as a typical fault, due to some serious damages on the components or due to the operator decision. In this context, our work proposes a new algorithm for the dynamical task assignment formulation of multi-agent systems in view of real-time optimization by including fault detection and isolation capabilities. This algorithm allows to detect whether there is a fault in the global multi-agent system, to isolate the faulty agent and to integrate a recovered/healthy agent. The proposed methods will be illustrated by means of a numerical example with connections to multi-vehicle systems.

7.20. Invariant sets for time-delay systems

Participants: Sorin Olaru [correspondent], Mohammed Laraba [L2S], Silviu Niculescu [L2S].

The characterization of invaraint sets for dynamical systems affected by time-delays is a long standing research topic in our group and this year new results have been obtained [52], [51] towards construction of invariant sets in the original state space (also called D-invariant sets) by exploiting the forward mappings. As novelties, the present paper contains a sufficient condition for the existence of ellipsoidal D-contractive sets for dDDEs, and a necessary and sufficient condition for the existence of D-invariant sets in relation to time-varying dDDE stability. Another contribution is the clarification of the relationship between convexity (convex hull operation) and D-invariance. In short, this shown that the convex hull of two D-invariant sets is not D-invariant but the convex hull of a non-convex D-invariant set is D-invariant.

7.21. Biochemical system modelized through a PDE

Participants: Frédéric Mazenc, Abdou Dramé [City Univ. of New York], Peter Wolenski [LSU].

We studied a model of chemostat relying on a Partial Differential Equation. More precisely, we studied in [13] the stability of periodic solutions of distributed parameters biochemical system with periodic input $S_{in}(t)$ (which respresent the substrate input concentration). We established that if the function $S_{in}(t)$ is periodic then the system has a periodic solution that possess the robust stability property called input to state stability and this when sufficiently small perturbations are acting on $S_{in}(t)$.

7.22. Modelling of cell dynamics in Acute Myeloid Leukemia

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

Modelling of Acute Myeloid Leukemia strated a few years ago. Starting from a PDE model of hematopoiesis given in [77], we have derived several models of healthy or cancer cell dynamics in hematopoiesis which according to some conditions admit one or two equilibrium points. Often taking profit of the positivity of the system we have derived this year several sufficient (or necessary and sufficient) conditions which ensure stability properties ranging from local symptotic stability to global exponential stability and obtained, when appropriate, an estimation of a subset of the bassin of attraction [14], [40].

7.23. Observability analysis of AC electric machines

Participants: Mohamad Koteich [CentraleSupelec, L2S, Renault], Guillaume Sandou [correspondent], Gilles Duc [CentraleSupelec, L2S], Abdelmalek Maloum [Renault].

High-performance control of electric drives requires an accurate knowledge of the rotor position and/or speed. These mechanical variables are traditionally measured using sensors, which increases the cost and reduces both the robustness and the reliability of the system. This emphasizes the importance of electric drives control without shaft sensors, often referred to as sensorless control : it consists of replacing sensors with a state observer algorithm, that estimates the desired mechanical variables from currents and voltages sensing and based on the system's model. Nevertheless, before designing a state observer, the observability of the system should be examined, that is, it should be checked whether the states to be estimated can be reconstructed, unambiguously, from the input/output signals of the system.

This work addresses the modeling and the observability analysis of electric drives in the view of mechanical sensors removal. Firstly, electrical machines models are elaborated, and it is shown that a unified modeling of alternating current machines is feasible, for the purpose of designing unified control and estimation strategies. The observability of the machines' models is next studied in the view of sensorless control. The local instantaneous observability theory is applied, which enables us to formulate physically insightful analytic conditions that can be easily interpreted and tested in real time. The validity of the observability conditions is confirmed by numerical simulations and experimental data, using an extended Kalman observer. This work contributes to novel outlooks on the sensorless alternating current drives and to a deeper understanding of its properties, in order to develop higher performance estimation techniques in the critical operating conditions (mainly at standstill and/or zerostator-frequency). The concepts introduced throughout this work, such as the equivalent flux and the observability vector, with the obtained results, open new horizons in a domain that seems to become mature enough [48], [76], [46], [49], [45], [15], [16], [91], [92], [47].

7.24. Optimization of Line of Sight controller based on high-level optronic criterion

Participants: Sophie Frasnedo [CentraleSupelec, L2S, Sagem], Guillaume Sandou [correspondent], Gilles Duc [CentraleSupelec, L2S], Philippe Feyel [Sagem], Cédric Chapuis [Sagem].

A method to tune the parameters of the controller of an inertially stabilized platform is proposed. This platform carries an electro-optical system. The image quality is obviously influenced by the movements of the platform: the Line of Sight (LoS) of the imager has to remain fixed in an inertial frame. The more the LoS controller manages to counter the movement of the platform, the better the image quality will be. The motion Modulation Transfer Function (motion MTF) measures the amount of blur brought into the image by the motion of the platform. It represents the contrast over spatial frequencies. Up to now, it has mostly been used as a validation tool for controllers already tuned from derived low level and conservative considerations. The proposed methodology aims to tune LoS controllers using directly the motion MTF as a criterion in the design procedure [42].

7.25. Optimization of controller using bayesian optimization

Participants: Sophie Frasnedo [CentraleSupelec, L2S, Sagem], Julien Bect [CentraleSupelec, L2S], Gilles Duc [CentraleSupelec, L2S], Guillaume Sandou [correspondent], Philippe Feyel [Sagem], Cédric Chapuis [Sagem].

A method to globally optimize the parameters of the controller of an inertially stabilized platform is presented. This platform carries an electro-optical system. The quality of the produced image is obviously influenced by the capacity of the controller to compensate for the unwanted motion of the platform. The motion Modulation Transfer Function (motion MTF) measures the amount of blur brought into the image by those parasite movements. The controller is tuned by minimizing a criterion which includes the motion MTF. However, evaluating this criterion is time-consuming. Using an optimization method that needs numerous evaluations of the criterion is not compatible with industrial constraints. Bayesian optimization methods consist in combining prior information about the criterion and previous evaluation results in order to choose efficiently new evaluation points and reach the global minimizer within a reasonable time. In this paper, a Bayesian approach is used to optimize the motion MTF-based criterion. The results are compared with a local optimization of the same MTF-based criterion, initialized with an acceptable initial point. Similar performances are achieved by the proposed methodology, without requiring an initialization point [41].

7.26. Particle Swarm Optimization based Approach for Model Predictive Control Tuning

Participants: Mohamed Lotfi Derouiche [CentraleSupelec, L2S, Ecole Nationale d'Ingénieur de Tunis], Guillaume Sandou [correspondent], Soufiene Bouallegue [Ecole Nationale d'Ingénieur de Tunis], Joseph Haggège [Ecole Nationale d'Ingénieur de Tunis].

In this work, a new Model Predictive Controller (MPC) parameters tuning strategy is proposed using a perturbed Particle Swarm Optimization (pPSO) approach. This original LabVIEW implementation of this metaheuristic algorithm is firstly validated on some test functions in order to show its efficiency and validity. The optimization results are compared with the standard PSO as well as a LabVIEW implemented Genetic Algorithm (GA) approaches. The parameters tuning problem, i.e. the weighting factors on the output error and input increments of the MPC algorithm, is after that formulated and systematically resolved, using the proposed LabVIEW pPSO algorithm. The case of a Magnetic Levitation (MAGLEV) system is investigated to illustrate the robustness and superiority of the proposed pPSO-based tuning MPC approach. All obtained simulation results, as well as the statistical analysis tests, are compared and discussed in order to improve the effectiveness of the proposed pPSO-based MPC tuning methodology.

7.27. Traffic rescheduling for CBTC train system running in a mixed traffic

Participants: Juliette Pochet [CentraleSupelec, L2S, SNCF], Guillaume Sandou [correspondent], Sylvain Baro [SNCF].

Railway companies need to achieve higher capacities on existing infrastructures such as high density suburban mainlines. Communication based train control (CBTC) systems have been widely deployed on dedicated subway lines. However, deployment on shared rail infrastructure, where CBTC and non CBTC trains run, leads to a mixed positioning and controlling system with different precision levels and restrictions. New performance and complexity issues are to arise. In this work, a method for traffic rescheduling, adapted to a CBTC system running in a mixed traffic, is introduced. A genetic algorithm solves the problem to optimize the cost function. It determines the dwell times and running times of CBTC-equipped trains, taking into account the non-equipped trains planning and fixed-block localization. In addition, reordering can be allowed by modifying the problem constraints. The work is supported by a new simulation tool developed by SNCF and adapted to mixed traffic study. The approach is illustrated with a case study based on a part of an East/West line in Paris region network, proving the ability of the method to find good feasible solutions when delays occur in the traffic.

7.28. Combined Feedback Linearization and MPC for Wind Turbine Power Tracking

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

The problem of controlling a variable-speed-variable-pitch wind turbine in non conventional operating points is addressed.We aim to provide a control architecture for a general active power tracking problem for the turbine's entire operating envelope. The presented control enables to cope with system non linearities while handling state and input constraints, and avoiding singular points. Simulations are carried out based on the CART turbine parameters. Comparatives results show that the proposed controller outperforms the classic PI regulator.

GECO Project-Team

6. New Results

6.1. New results: geometric control

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

- In [12] and [20] we study the sub-Finsler geometry as a time-optimal control problem. In particular, we consider non-smooth and non-strictly convex sub-Finsler structures associated with the Heisenberg, Grushin, and Martinet distributions. Motivated by problems in geometric group theory, we characterize extremal curves, discuss their optimality, and calculate the metric spheres, proving their Euclidean rectifiability.
- In [18] we compare different notions of curvature on contact sub-Riemannian manifolds. In particular we introduce canonical curvatures as the coefficients of the sub-Riemannian Jacobi equation. The main result is that all these coefficients are encoded in the asymptotic expansion of the horizontal derivatives of the sub-Riemannian distance. We explicitly compute their expressions in terms of the standard tensors of contact geometry. As an application of these results, we obtain a sub-Riemannian version of the Bonnet-Myers theorem that applies to any contact manifold.
- In sub-Riemannian geometry the coefficients of the Jacobi equation define curvature-like invariants. We show in [21] that these coefficients can be interpreted as the curvature of a canonical Ehresmann connection associated to the metric, first introduced by Zelenko and Li. We show why this connection is naturally nonlinear, and we discuss some of its properties.
- On a sub-Riemannian manifold we define in [22] two type of Laplacians. The macroscopic Laplacian, as the divergence of the horizontal gradient, once a volume is fixed, and the microscopic Laplacian, as the operator associated with a geodesic random walk. We consider a general class of random walks, where all sub-Riemannian geodesics are taken in account. This operator depends only on the choice of a complement to the sub-Riemannian distribution. We address the problem of equivalence of the two operators. This problem is interesting since, on equiregular sub-Riemannian manifolds, there is always an intrinsic volume (e.g. Popp's one) but not a canonical choice of complement. The result depends heavily on the type of structure under investigation: we describe the relationship between the two approaches in the case of contact structures, Carnot groups, quasi-contact structures.
- In [2] we study 3D almost-Riemannian manifolds, that is, generalized Riemannian manifolds defined locally by 3 vector fields that play the role of an orthonormal frame, but could become collinear on some singular set. Almost-Riemannian manifolds were deeply studied in dimension 2. In this paper we start the study of the 3D case which appear to be reacher with respect to the 2D case, due to the presence of abnormal extremals which define a field of directions on the singular set. We study the type of singularities of the metric that could appear generically, we construct local normal forms and we study abnormal extremals. We then study the nilpotent approximation and the structure of the corresponding small spheres. We finally give some preliminary results about heat diffusion on such manifolds.

New results on motion planning are the following.

- In [7] (written while D. Prandi was PhD student in the team) we study the complexity of the motion planning problem for control-affine systems. Such complexities are already defined and rather well-understood in the particular case of nonholonomic (or sub-Riemannian) systems. Our aim is to generalize these notions and results to systems with a drift. Accordingly, we present various definitions of complexity, as functions of the curve that is approximated, and of the precision of the approximation. Due to the lack of time-rescaling invariance of these systems, we consider geometric

and parametrized curves separately. Then, we give some asymptotic estimates for these quantities. As a byproduct, we are able to treat the long-time local controllability problem, giving quantitative estimates on the cost of stabilizing the system near a non-equilibrium point of the drift.

- In [11] and [1] we propose new conditions guaranteeing that the trajectories of a mechanical control system can track any curve on the configuration manifold. We focus on systems that can be represented as forced affine connection control systems and we generalize the sufficient conditions for tracking known in the literature. The new results are proved by a combination of averaging procedures by highly oscillating controls and the notion of kinematic reduction.
- In
- [17] we introduce the concept of Developmental Partial Differential Equation (DPDE), which consists of a Partial Differential Equation (PDE) on a time-varying manifold with complete coupling between the PDE and the manifold's evolution. In other words, the manifold's evolution depends on the solution to the PDE, and vice versa the differential operator of the PDE depends on the manifold's geometry. DPDE is used to study a diffusion equation with source on a growing surface whose growth depends on the intensity of the diffused quantity. The surface may, for instance, represent the membrane of an egg chamber and the diffused quantity a protein activating a signaling pathway leading to growth. Our main objective is to show controllability of the surface shape using a fixed source with variable intensity for the diffusion. More specifically, we look for a control driving a symmetric manifold shape to any other symmetric shape in a given time interval. For the diffusion we take directly the Laplace-Beltrami operator of the surface, while the surface growth is assumed to be equal to the value of the diffused quantity. We introduce a theoretical framework, provide approximate controllability and show numerical results. Future applications include a specific model for the oogenesis of Drosophila melanogaster.

6.2. New results: quantum control

New results have been obtained for the control of the bilinear Schrödinger equation.

- In [4] we study the so-called spin-boson system, namely a two-level system in interaction with a distinguished mode of a quantized bosonic field. We give a brief description of the controlled Rabi and Jaynes–Cummings models and we discuss their appearance in the mathematics and physics literature. We then study the controllability of the Rabi model when the control is an external field acting on the bosonic part. Applying geometric control techniques to the Galerkin approximation and using perturbation theory to guarantee non-resonance of the spectrum of the drift operator, we prove approximate controllability of the system, for almost every value of the interaction parameter.
- The main result in [9] is the approximate controllability of a bilinear Schrödinger equation modeling a system of two ions trapped in a cavity. A new spectral decoupling technique is introduced, which allows to analyze the controllability of the infinite-dimensional system through finite-dimensional considerations. The controllability of a simplified version of the model has been obtained in [16].
- In [13] and [3] we study the controllability of a closed control-affine quantum system driven by two or more external fields. We provide a sufficient condition for controllability in terms of existence of conical intersections between eigenvalues of the Hamiltonian in dependence of the controls seen as parameters. Such spectral condition is structurally stable in the case of three controls or in the case of two controls when the Hamiltonian is real. The spectral condition appears naturally in the adiabatic control framework and yields approximate controllability in the infinite-dimensional case. In the finite-dimensional case it implies that the system is Lie-bracket generating when lifted to the group of unitary transformations, and in particular that it is exactly controllable. Hence, Lie algebraic conditions are deduced from purely spectral properties. We conclude the analysis by proving that approximate and exact controllability are equivalent properties for general finite-dimensional quantum systems.

In [26], written with the members of the European project QUAINT, state-of-the-art quantum control techniques are reviewed and put into perspective by a consortium uniting expertise in optimal control theory and applications to spectroscopy, imaging, quantum dynamics of closed and open systems. Key challenges are addressed and a roadmap to future developments is sketched.

6.3. New results: neurophysiology

In [27] we present a new version of the image inpainting algorithm that GECO developed in the recent years. This new version is called the Averaging and Hypoelliptic Evolution (AHE) algorithm, and is based upon a semi-discrete variation of the Citti–Petitot–Sarti model of the primary visual cortex V1. In particular, we focus on reconstructing highly corrupted images (i.e. where more than the 80% of the image is missing).

6.4. New results: switched systems

- In [5] we consider a continuous-time linear switched system on $\mathbb{R}^n$ associated with a compact convex set of matrices. When it is irreducible and its largest Lyapunov exponent is zero there always exists a Barabanov norm associated with the system. We look at two types of issues: (a) properties of Barabanov norms such as uniqueness up to homogeneity and strict convexity; (b) asymptotic behaviour of the extremal solutions of the linear switched system. Regarding Issue (a), we provide partial answers and propose four related open problems. As for Issue (b), we establish, when $n = 3$, a Poincaré–Bendixson theorem under a regularity assumption on the set of matrices. We then revisit a noteworthy result of N.E. Barabanov describing the asymptotic behaviour of linear switched system on $\mathbb{R}^3$ associated with a pair of Hurwitz matrices $\{A, A + bc^T\}$.
- Motivated by an open problem posed by J.P. Hespanha, in [23] we extend the notion of Barabanov norm and extremal trajectory to classes of switching signals that are not closed under concatenation. We use these tools to prove that the finiteness of the L2-gain is equivalent, for a large set of switched linear control systems, to the condition that the generalized spectral radius associated with any minimal realization of the original switched system is smaller than one.
- In [14] in the totally observed case and in [23] in the general case, we answer an open problem posed by J.P. Hespanha in 2003. We first extend the notion of Barabanov norm and extremal trajectory to classes of switching signals that are not closed under concatenation. We use these tools to prove that the finiteness of the L_2-gain is equivalent, for a large set of switched linear control systems, to the condition that the generalized spectral radius associated with any minimal realization of the original switched system is smaller than one.
- In [24] we address the stability of non-autonomous difference equations by providing a suitable representation of the solution at time t in terms of the initial condition and time-dependent matrix coefficients. This enables us to characterize the asymptotic behavior of solutions in terms of that of such coefficients. As a consequence, we obtain necessary and sufficient stability criteria for non-autonomous linear difference equations. In the case of difference equations with arbitrary switching, we obtain a generalization of the well-known criterion for autonomous systems due to Hale and Silkowski, which, as the latter, is delay-independent. These results are applied to transport and wave propagation on networks. In particular, we show that the wave equation on a network with arbitrarily switching damping at external vertices is exponentially stable if and only if the network is a tree and the damping is bounded away from zero at all external vertices but one.
- For linear systems in continuous time with random switching, we characterize in [25] the Lyapunov exponents using the Multiplicative Ergodic Theorem for an associated system in discrete time. An application to control systems shows that here a controllability condition implies that arbitrary exponential decay rates for almost sure stabilization can be obtained.

A result related to switched system is the one obtained in [6] and [15]: we study the stability of linear time-varying delay differential equations where the delay enters as a switching parameter. In [6] we give a collection of converse Lyapunov–Krasovskii theorems for uncertain retarded differential equations. We show that the

existence of a weakly-degenerate Lyapunov–Krasovskii functional is a necessary and sufficient condition for the global exponential stability of linear retarded functional differential equations. In [15] the fundamental question that we consider is the following: assuming that every individual (constant-delay) subsystem is exponentially stable, can we characterize the cases when the system is not exponentially stable? This is nothing else than the so-called Markus-Yamabe instability and we give new conditions ensuring it.

I4S Project-Team

7. New Results

7.1. Reflectometry

7.1.1. Experimental validation of the inverse scattering method for distributed characteristic impedance estimation

Participant: Qinghua Zhang.

This work has been carried out in collaboration with Florent Loete (GEEPS-SUPELEC) and with Michel Sorine, formerly member of the Inria SISYPHE EPI.

Recently published theoretic results and numerical simulations have shown the ability of inverse scattering-based methods to diagnose soft faults in electric cables, in particular, faults implying smooth spatial variations of cable characteristic parameters. The purpose of the present work is to realize laboratory experiments confirming the ability of the inverse scattering method for retrieving spatially distributed characteristic impedance from reflectometry measurements. Various smooth or stepped spatial variations of characteristic impedance profiles are tested. This study has been accomplished in the framework of the ANR SODDA project and the results have been published in IEEE Transactions on Antennas and Propagation [16].

7.2. Automatic control

7.2.1. Observability conservation by output feedback and observability Gramian bounds

Participants: Qinghua Zhang, Liangquan Zhang.

Though it is a trivial fact that the observability of a linear state space system is conserved by output feedback, it requires a rigorous proof to generalize this result to uniform complete observability, which is defined with the observability Gramian. The purpose of this work is to complete such a proof. Some issues in existing results are also discussed. The uniform complete observability of closed loop systems is useful for the analysis of some adaptive systems and of the Kalman filter. This study has been accomplished in the framework of the ITEA MODRIO project and the results have been published in Automatica [20].

7.2.2. Weighted principal component analysis for Wiener system Identification: regularization and non-Gaussian excitations

Participant: Qinghua Zhang.

This work has been carried out in collaboration with Vincent Laurain (CRAN/CNRS/Université de Lorraine) and with Jiandong Wang (Peking University).

Finite impulse response (FIR) Wiener systems driven by Gaussian inputs can be efficiently identified by a well-known correlation-based method, except those involving even static nonlinearities. To overcome this deficiency, another method based on weighted principal component analysis (wPCA) has been recently proposed. Like the correlation-based method, the wPCA is designed to estimate the linear dynamic subsystem of a Wiener system without assuming any parametric form of the nonlinearity. To enlarge the applicability of this method, it is shown in this work that high order FIR approximation of IIR Wiener systems can be efficiently estimated by controlling the variance of parameter estimates with regularization techniques. The case of non-Gaussian inputs is also studied by means of importance sampling. The results of this study have been presented in [22].

7.2.3. LPV system common state basis estimation from independent local LTI models

Participant: Qinghua Zhang.

This work has been carried out in collaboration with Lennart Ljung (Linköping University).

For the identification of a linear parameter varying (LPV) system steered by a scheduling variable evolving within a finite set, the local approach consists in separately estimating local linear time invariant (LTI) models corresponding to fixed values of the scheduling variable. It is shown in this work that, without any global structural assumption of the considered LPV system, the local state-space LTI models do not contain the necessary information about the similarity transformations making them coherent. Nevertheless, it is possible to estimate these similarity transformations from input-output data under appropriate input excitation conditions. These estimations result in a common state basis of the transformed local LTI models, so that they form a coherent global LPV model, suitable for numerical simulations in the case of fast scheduling variable evolutions. This study has been accomplished in the framework of the ITEA MODRIO project and the results have been presented in [39].

7.3. Damage detection and linear state analysis

7.3.1. Vibration monitoring by eigenstructure change detection based on perturbation analysis

Participants: Michael Doehler, Qinghua Zhang, Laurent Mevel.

Vibration monitoring, notably in the fields of civil, mechanical and aeronautical engineering, aims at detecting damages at an early stage, in general by using output-only vibration measurements under ambient excitation. In this work, a new method is developed for the detection of small changes in the eigenstructure of such systems. The main idea is to transform the multiplicative eigenstructure change detection problem to an additive one, by means of perturbation analysis based on the assumption of small eigenstructure changes. Another transformation then further simplifies the detection problem into the framework of a linear regression subject to additive white Gaussian noises, leading to a numerically efficient solution of the considered problem. Compared to existing methods, it has the advantages of focusing on chosen system parameters and efficiently addressing random uncertainties. The results of this study have been presented in [31].

7.3.2. Stochastic hybrid system actuator fault diagnosis by adaptive estimation

Participant: Qinghua Zhang.

Based on the interacting multiple model (IMM) estimator for hybrid system state estimation and on the adaptive Kalman filter for time varying system joint state-parameter estimation, a new algorithm, the adaptive IMM estimator, is developed in this work for actuator fault diagnosis in stochastic hybrid systems. The working modes of the considered hybrid systems are described by stochastic state-space models, and the mode transitions are characterized by a Markov model. Actuator faults are modeled as parameter changes, and the related fault diagnosis problem is solved by the proposed adaptive IMM estimator through joint state-parameter estimation. This study has been accomplished in the framework of the ITEA MODRIO project and the results have been presented in [40].

7.3.3. Damage detection on real structures

Participants: Dominique Siegert, Laurent Mevel.

This article presents the feasibility study of a new structure for a 10-m-span bridge deck, taking into account the possibilities offered by new and high-strength materials and the advantages of a traditional environmental-friendly material. Small localized damages are hardly detected by global monitoring methods. The effectiveness of vibration-based detection depends on the accuracy of the modal parameter estimates and is limited by the low sensitivity of the modal parameters to a local stiffness reduction. This paper presents the application of SSDD to detect the change of the modal parameters of the investigated structure. Further analysis with a finite element model was conducted for assessing the consistency of the expected location and extent of the damaged elements. [15].

7.3.4. Damage detection and simulated validation

Participants: Michael Doehler, Laurent Mevel, Saeid Allahdadian.

This section is devoted to the numerical and theoretical validation of stochastic subspace damage detection. Sample length and sensor noise robustness were investigated. [24], [23], [25].

7.3.5. Damage quantification

Participants: Michael Doehler, Laurent Mevel.

Fault detection for structural health monitoring has been a topic of much research during the last decade. Localization and quantification of damages, which are linked to fault isolation, have proven to be more challenging, and at the same time of higher practical impact. While damage detection can be essentially handled as a data-driven approach, localization and quantification require a strong connection between data analysis and physical models. This paper builds upon a hypothesis test that checks if the mean of a Gaussian residual vector whose parameterization is linked to possible damage locations has become non-zero in the faulty state. It is shown how the damage location and extent can be inferred and robust numerical schemes for their estimation are derived based on QR decompositions and minmax approaches. Finally, the relevance of the approach is assessed in numerical simulations of two structures.[30].

7.3.6. Optical fiber for damage detection

Participant: Dominique Siegert.

A technique has been developed to detect and quantify structural damages. It consists of updating the model parameters associated to the damage, i.e. Young modulus, from strain sensor outputs obtained by optical fiber. Early damage detection can be expected using the local information given by the strain measurement. The method has been applied to a 8 meter post-tensioned concrete beam under a static loading. The model updating problem can be formulated as a minimization problem, i.e minimize a data misfit functional. To solve this problem, we use a gradient-based method. The gradient of the functional is computed at a low computational cost by means of the adjoint state. The technique is able to detect the damaged area in a post-tensioned concrete beam and to estimate its level of damage. [38]

7.4. Smarts roads and R5G

7.4.1. Positive surface temperature pavement

Participants: Jean Dumoulin, Nicolas Le Touz.

The mobility during winter season in France mainly relies on the use of de-icers, with an amount ranging from two hundreds thousands tons up to two millions tons for the roads only. Besides the economic impact, there are many concerns on their environmental and infrastructure, both on roads and on airports. In such context and in the framework of the R5G (5th Generation Road) project driven by IFSTTAR, investigations were carried out on the way to modify the infrastructure to maintain pavement surface at a temperature above water freezing point. Two distinct approaches, that can could be combined, were selected. The first one consisted in having a heated fluid circulating in a porous layer within an asphalt concrete pavement sample. The second one specifically relied on the use of paraffin phase change materials (PCM) in cement concrete pavement ones. Experiments on enhanced pavement samples were conducted in a climatic chamber to simulate winter conditions for several continuous days, including wind and precipitations, and monitored by infrared thermography. [45], [34]

7.4.2. Road structure design with energy harvesting capabilities

Participants: Nicolas Le Touz, Jean Dumoulin.

Facing the heavy organisational, financial and environmental constraints imposed by usual winter maintenance salting operations, pavement engineers have been led to look for alternative solutions to avoid ice or snow deposit at pavements surface. Among the solutions, one is self-de-icing heating pavements, for which two technologies have been developed so far: one is based on embedded coils circulating a heated calorific fluid under the pavement surface; the other one relies on the use of embedded resistant electric wires. The use and operation of such systems in the world is still limited and was only confined to small road stretches or specific applications, such as bridges which are particularly sensitive to frost. One of the most significant coil technology example in Europe is the SERSO-System (Solar Energy recovery from road surfaces) built in 1994, on a Switzerland bridge. Many of these experiences are referenced in the technical literature, which provides state-of-the art papers (see for instance Eugster) and useful detailed information dealing with the construction and operational management of such installation. The present study is taking part of the Forever Open Road Concept addressed by the R5G: 5th Generation Road , one of the major project supported by IFSTTAR. It considers a different design of self-de-icing road that simplify its mode of construction and maintenance, compared to the two technologies mentioned above. It should also be noted that similar to pavements instrumented with coils, such structure could be used in the reversible way to capture the solar energy at the pavement surface during sunny days and store it, to either warm the pavement at a later stage or for exogenous needs (e.g. contribution to domestic hot water). To complete our study we also considered the use of semi-transparent pavement course wearing in place of the traditional opaque one. In the present study, a 2D model was developed using FEM approach. It combines 2 numerical models. One is dedicated to the calculation of the heat transfer inside the porous layer between the fluid and the structure according to the geometry studied and the physical properties of the components of the system. The second one addresses the heat transfer inside the different layer of the pavement and was adapted to allow the insertion of a semi-transparent surface layer (for sun radiation). The temperature spatial distribution within the structure and its surface is calculated at different time step according to the evolution of boundary conditions at its surface. Various location in France were selected and calculation of the temperature field was carried-out over a year. Discussion on the performances of such system versus its location is proposed. Influence of a semi-transparent layer is also discussed. Future works will compared numerical simulations with experiments thank to a dedicated test bench under development and that will allow to test various structure in parallel. [32]

7.5. Non Destructive Testing using Infrared Thermography

7.5.1. Optimal designs of experience for thermal NDT

Participants: Antoine Crinière, Jean Dumoulin.

During previous works, square pulsed thermography was used to carry out non destructive testing of bonding quality of CFRP glued on civil engineering structures during reinforcement operations. The use of such wave form excitation was motivated by “on-site” requirements, but also by measurements duration, number of composite layers to test, depth of possible faulting areas versus temperature elevation allowed at composite level according to inner heat diffusion. Nevertheless, square pulsed excitation implies to choose an adapted heat duration. This duration is directly linked to the reliability of the parameter estimator. According to these observations, an indicator able to predict the sufficient heating time when the reliability of the parameter estimator reached an asymptotic evolution behaviour was studied. Based on the absolute thermal contrast, the proposed indicator Iph is defined with the maximum thermal contrast and the time delay between the heating time and the appearance of the maximum contrast. This indicator allows to take into account the detectability as well as the induced flaw temporal effect on the thermal contrast shape evolution. This paper will present the establishment of this indicator for optimal square heating time and present an analysis of results obtained with numerical simulations and laboratory experiments. [28]

7.5.2. Thermal NDT and signal processing

Participant: Jean Dumoulin.

This work deals with the detection of non-emergent small structures like mosaic, hidden under a plaster layer, with various spatial layout and nature. Three post processing approach by PPT, SVD and Polynomial analysis were conducted on this experimental and simulated data set. Results obtained are analysed and discussed. Finally, influence of IR camera used will be also addressed and discussed in the dissertation. [35]

7.6. Outdoor InfraRed Thermography

7.6.1. Vision enhancement through Infrared imaging for transport infrastructures

Participant: Jean Dumoulin.

Fog conditions are the cause of severe car accidents in European western countries because of the poor induced visibility. Its occurrence and intensity are still very difficult to forecast for weather services. Furthermore, visibility determination relies on expensive instruments and does not ease their dissemination. Lately, it has been demonstrated the benefit of infrared cameras to detect and to identify objects in fog while visibility is too low for eye detection. Over the past years, such cameras have become more cost effective. A research program between IFSTTAR and Cerema studied the possibility to retrieve visibility distance in a fog tunnel during its natural dissipation. The purpose of this work is to retrieve atmospheric visibility with a technique based on the combined use of infrared thermography, Principal Components Analysis (PCA) and Partial Least-Square (PLS) regression applied to infrared images.[44] and [17]

7.6.2. Outdoor thermal monitoring of large scale structures by infrared thermography

Participants: Jean Dumoulin, Antoine Crinière.

With the constant increase of the road traffic coupled with the ageing of transport infrastructure, studying and developing robust system which allows to monitor and assess those structures is of growing interest. Among the techniques used [1], thermal monitoring with infrared thermography appears to be a good compromise between a non-intrusive method and possible added value after post-processing of acquired data. Through the past decade studies have shown the ability to monitor concrete and asphalt structure by active IR thermography. On site measurement using passive thermography have also been studied, by applying qualitative methods and quantitative one. These methods have been used to perform punctual control of various duration (few hours to few days). However, infrared thermography, when it is used in a quantitative mode (not in laboratory conditions) and not in a qualitative mode (vision applied to survey), needs to process thermal radiative corrections on the raw data acquired in real time, to take into account the influences of the natural environment's evolution with time. The ICT system called "IrLaW" is based on a multi sensing approach. It connects and synchronizes information acquired by a weather station, a GPS and an infrared camera. To fulfill ICT objectives (OGCcompliant), a specific hardware architecture was also designed and studied to allow the whole system integration in a TCP/IP network. [29]

Maxplus Team

7. New Results

7.1. Théorie spectrale max-plus et géométrie métrique/Max-plus spectral theory and metric geometry

7.1.1. Introduction

Participants: Marianne Akian, Stéphane Gaubert, Cormac Walsh.

Étant donné un noyau $a : S \times S \to \mathbb{R} \cup \{-\infty\}$, on peut lui associer le problème spectral max-plus

$$\sup_{y \in S} a(x,y) + u(y) = \lambda + u(x), \quad \forall x \in S, \tag{3}$$

dans lequel on cherche le vecteur propre $u : S \to \mathbb{R} \cup \{-\infty\}$ et la valeur propre correspondante $\lambda \in \mathbb{R} \cup \{-\infty\}$. Comme nous l'avons rappelé dans les §3.2 et 3.3 , le problème spectral (9) intervient en contrôle ergodique: l'ensemble S est l'espace des états, et l'application $a(x,y)$ fournit le gain associé à la transition $x \to y$. Le cas où S est fini est classique, l'on a alors un résultat précis de représentation de l'espace propre, à l'aide d'un certain graphe, dit graphe critique. Des résultats existent également lorsque S est compact et que le noyau vérifie certaines propriétés de régularité.

Dans [51], nous avons considéré le cas où S est non compact. Lorsque $\lambda = 0$, l'espace propre est analogue à l'espace des fonctions harmoniques défini en théorie (classique ou probabiliste) du potentiel. En introduisant l'analogue max-plus de la frontière de Martin, nous avons obtenu un analogue de la formule de représentation de Poisson des fonctions harmoniques : toute solution u de (9) peut être représentée sous la forme :

$$u = \sup_{w \in \mathcal{M}_m} w + \mu_u(w) \ , \tag{4}$$

où $\mathcal{M}_m \subset (\mathbb{R} \cup \{-\infty\})^S$ est l'analogue max-plus de la frontière de Martin minimale (l'ensemble des fonctions harmoniques extrémales normalisées), et où μ_u joue le rôle de la mesure spectrale. Nous avons montré aussi que les éléments de l'espace de Martin minimal peuvent être caractérisés comme les limites de "quasi-géodésiques". La frontière de Martin max-plus généralise dans une certaine mesure la frontière d'un espace métrique construite à partir des horo-fonctions (fonctions de Busemann généralisées), ou horo-frontière. Ces résultats inspirent les travaux des sections suivantes, qui portent sur des cas remarquables d'espaces métriques (§7.1.2) ou sur des applications en théorie des jeux (§7.2.2).

English version

Let the kernel $a : S \times S \to \mathbb{R} \cup \{-\infty\}$ be given. One may associate the max-plus spectral equation (9), where the eigenvector $u : S \to \mathbb{R} \cup \{-\infty\}$ and the eigenvalue $\lambda \in \mathbb{R} \cup \{-\infty\}$ are unknown. As we recalled in §3.2 and refmonotone, this spectral problem arises in ergodic optimal control: the set S is the *state space*, and the map $a(x,y)$ is the *transition reward*. The case when S is finite is classical, a precise spectral theorem is known, with a characterisation of the eigenspace in terms of a critical graph. Some results have been shown when S is compact, assuming that the kernel a satisfies some regularity properties.

In [51], we considered the case where S is non-compact. When $\lambda = 0$, the eigenspace is analoguous to the set of harmonic functions defined in classical or probabilistic potential theory. By introducing a max-plus analogue of the classical Martin boundary, we obtained an analogue of the Poisson representation of harmonic functions, showing that any solution u of (9) may be represented as in (10) where $\mathcal{M}_m \subset (\mathbb{R} \cup \{-\infty\})^S$ is a max-plus analogue of the minimal Martin boundary (the set of normalised extremal harmonic functions), and μ_u plays the role of the spectral measure. We also showed that the elements of the minimal Martin boundary can be characterised as limits of certain "almost-geodesics". The max-plus Martin boundary generalises to some extent the boundary of metric spaces defined in terms of horofunctions (generalised Busemann functions), or horoboundary. These results have inspired the work of the next sections, which deal either with interesting examples of metric spaces (§7.1.2) or with applications to zero-sum games (§7.2.2).

7.1.2. Isométries de la géométrie de Hilbert/Isometries of the Hilbert geometry

Participants: Cormac Walsh, Bas Lemmens [Kent University, UK].

Dans nos travaux précédents, nous avons étudié la géométrie de Hilbert (d'un ensemble convexe) en dimension finie, en particulier son horo-frontière et son groupe des isométries. Le chapitre de livre [167] donne une vue d'ensemble de ces travaux. Le cas de la dimension infinie est aussi intéressant, et a été utilisé depuis de nombreuses années en analyse non linéaire. Malgré cela, la géométrie de ces espaces est très peu connue en dimension infinie.

On s'interesse par exemple au problème suivant. En dimension finie, il est connu que la géométrie de Hilbert est isométrique à un espace normé si et seulement si le convexe est un simplexe. On a montré [38] plus généralement que la géométrie de Hilbert est isométrique à un espace de Banach si et seulement si le convexe est le cône des fonctions positives continues sur un espace topologique compact. Pour cela, on a étudié l'horo-frontière en dimension infinie.

On continue à travailler sur ce sujet avec Bas Lemmens de l'Université de Kent.

English version

Previously, we have been studying the Hilbert geometry in finite dimensions, especially its horofunction boundary and isometry group. The book chapter [167] contains a survey of this work. However, the infinite dimensional case is also interesting, and has been used as a tool for many years in non-linear analysis. Despite this, very little is known about the geometry of these spaces when the dimension is infinite.

An example of a problem in which we are interessed is the following. In finite dimension it is known that a Hilbert geometry is isometric to a normed space if and only if it is a simplex. We have shown [38] that, more generally, a Hilbert geometry is isometric to a Banach space if and only if it is the cross-section of a positive cone, that is, the cone of positive continuous functions on some compact topological space. To solve this problem we found it useful to study the horofunction boundary in the infinite-dimensional case.

We are continuing to study similar problems in relation to this topic in collaboration with Bas Lemmens of the University of Kent.

7.1.3. Croissance des boules dans la géométrie de Hilbert/Volume growth in the Hilbert geometry

Participants: Cormac Walsh, Constantin Vernicos [Université Montpellier 2].

Avec Constantin Vernicos de l'Université Montpellier 2, nous étudions la croissance du volume de la boule d'une géométrie de Hilbert (d'un ensemble convexe) en fonction du rayon. En particulier, nous étudions l'entropie volumique:

$$\lim_{r\to\infty} \frac{\log \operatorname{Vol} B(x,r)}{r}, \tag{5}$$

où $B(x,r)$ désigne la boule de centre x et de rayon r, et Vol est une notion de volume particulière, telle que celle définie par Holmes–Thompson ou celle de Busemann. L'entropie ne dépend pas du choix particulier de x, ni de celui du volume. Il est connu que pour l'espace hyperbolique, ou toute géométrie de Hilbert dont la frontière est C^2 et de courbure strictement positive, l'entropie est égale à $n-1$ lorsque la dimension de l'espace est n, et il a été prouvé recemment que ceci correspond aussi à l'entropie maximale d'une géométrie de Hilbert en dimension n.

Constantin Vernicos a montré que, en dimension 2 et 3, l'entropie volumique d'une géométrie d'Hilbert sur une convexe est égale à l'*approximabilité* de la convexe, ce qui est le taux de croissance exponentielle du nombre de sommets nécessaire pour approximer la convexe par un polytope à ϵ près, quand ϵ diminue.

Ceci motive l'étude de la croissance du volume dans le cas de polytopes. Dans ce cas, la croissance est polynomiale de degré n, plutôt qu'exponentielle, et il est important de comprendre le lien entre le coefficient dominant du polynôme exprimant le volume et la complexité du polytope. Nous avons obtenu une formule pour ce coefficient, laquelle dépend de la structure combinatoire du polytope. Cette formule suggère de définir une nouvelle notion de approximabilité en utilisant une quantité combinatoire different que le nombre de sommets, et d'étudier la relation entre cette approximabilité et l'entropie volumique. On pourrait supposer que les deux quantités sont égales, ce qui impliquerait en particulier que l'entropie volumique d'une convexe est égale à celle de son dual.

English version

In a collaboration with Constantin Vernicos of Université Montpellier 2, we are investigating how the volume of a ball in a Hilbert geometry grows as its radius increases. Specifically, we are studing the volume entropy (11) where $B(x,r)$ is the ball with center x and radius r, and Vol denotes some notion of volume, for example, the Holmes–Thompson or Busemann definitions. Note that the entropy does not depend on the particular choice of x, nor on the choice of the volume. It is known that the hyperbolic space, or indeed any Hilbert geometry with a C^2-smooth boundary of stricty positive curvature, has entropy $n-1$, where n is the dimension, and it has recently been proved that this is the maximal entropy possible for Hilbert geometries of the given dimension.

Constantin Vernicos has shown that, in dimension 2 and 3, the volume entropy of a Hilbert geometry on a convex body is equal to the *approximability* of the body, that is, the exponential rate of growth of the number of vertices needed to approximate the body by a polytope within ϵ, as ϵ decreases.

This motivates studying the volume growth in the polytopal case. Here the growth is polynomial rather than exponential, of degree n, and it is important to know how the constant on front of the highest term depends on the complexity of the polytope. We have a formula for this constant in terms of the combinatorial structure of the polytope. This formula suggests defining a new notion of approximability using a different combinatorial quantity from the number of vertices, and studying the relationship between this approximability and the volume entropy. One might conjecture that the two quantities are equal, which would imply in particular that the volume entropy of a convex body is equal to that of its dual.

7.1.4. Consensus non-commutatif et contraction d'opérateurs de Kraus/Noncommutative consensus and contraction of Kraus maps

Participants: Stéphane Gaubert, Zheng Qu.

Dans le travail [16], on s'est intéressé à la vitesse de convergence vers l'équilibre d'une itération de la forme $x^{k+1} = T(x^k)$, $x^k \in X$, où T est une application linéaire préservant un cône dans un espace de Banach X, telle que $T(e) = e$, pour un certain vecteur e dans l'interieur du cône. On s'intéresse aussi à l'itération dans l'espace dual, $y^{k+1} = T^*(y^k)$, $y^k \in X^*$, lorsque $\langle y^0, e\rangle = 1$.

Le cas classique est celui où $T(x) = Px$ est un opérateur de Markov. L'itération primale traduit alors la convergence vers le "consensus", et l'itération duale traduit la convergence de la distribution de probabilité en temps k vers l'état stationnaire. Dans ce cas, le taux de contraction (en un coup) $\kappa(P)$ d'une itération primale, pour la semi-norme de Hilbert $\|z\|_H := \max_i z_i - \min_j z_j$, ainsi que le taux de contraction d'une itération duale, pour la métrique en variation totale, coïncident et sont caractérisés par une formule dûe à Doeblin et Dobrushin (coefficient d'ergodicité),

$$\kappa(P) := 1 - \min_{i,j} \sum_{s=1}^{n} \min\left(P_{is}, P_{js}\right).$$

On a donné ici une généralisation de cette formule au cas d'opérateurs abstraits, qui s'applique en particulier aux opérateurs de Kraus qui interviennent en information quantique. Ces derniers opérent sur l'espace des matrices symmétriques, et sont de la forme

$$T(x) = \sum_k a_k x a_k^* \qquad \text{avec} \qquad \sum_k a_k a_k^* = I \ .$$

Dans [114], nous avons étudié des questions de complexité pour les applications de Kraus, montrant en particulier qu'il est NP-dur de vérifier qu'une application de Kraus envoie le cone dans son interieur.

English version

In [16], we studied the speed of convergence to equilibrium of an iteration of the form $x^{k+1} = T(x^k)$, $x^k \in X$, where T is a linear map preserving a cone in a Banach space X, such that $T(e) = e$, for some vector e in the interior of the cone. We also considered the iteration in the dual space X^*, $y^{k+1} = T^*(y^k)$, $y^k \in X^*$, where $\langle y^0, e\rangle = 1$.

The classical application arises when $T(x) = Px$ is a Markov operator. Then, the primal iteration represents the dynamics of consensus, whereas the dual iteration represents the evolution of the probability distribution as a function of time. Then, the (one-shot) contraction rate $\kappa(P)$ of the primal iteration, with respect to Hilbert's seminorm $\|z\|_H := \max_i z_i - \min_j z_j$, and the contraction rate of the dual iteration, with respect to the total variation metric, coincide, and are characterized by a formula of Doeblin and Dobrushin (ergodicity coefficient),

$$\kappa(P) := 1 - \min_{i,j} \sum_{s=1}^{n} \min\left(P_{is}, P_{js}\right).$$

We gave here a generalization of this formula to an abstract operators on a cone. This covers in particular the Kraus maps arising in quantum information theory. The latter maps act on the space of symmetric matrices. They can be written as

$$T(x) = \sum_k a_k x a_k^* \qquad \text{with} \qquad \sum_k a_k a_k^* = I \ .$$

In [114], we studied complexity issues related to Kraus maps, and showed in particular that checking whether a Kraus map sends the cone to its interior is NP-hard.

7.2. Algèbre linéaire max-plus, convexité tropicale et jeux à somme nulle/Max-plus linear algebra, tropical convity and zero-sum games

7.2.1. Polyèdres tropicaux/Tropical polyhedra

Participants: Xavier Allamigeon, Stéphane Gaubert, Eric Goubault [CEA], Ricardo Katz [Conicet, Argentine].

On étudie les analogues max-plus ou tropicaux des ensembles convexes. Ceux-ci sont utiles en particulier pour représenter de manière effective les ensembles d'états accessibles de systèmes à événements discrets [9], ils sont aussi apparus récemment en géométrie tropicale, dans toute une série de travaux à la suite de Sturmfels et Develin [97]. Les polyèdres max-plus peuvent aussi être vus comme des limites de déformations de polyèdres classiques, sur lesquels ils donnent un éclairage de nature combinatoire. Toutes ces motivations ont inspiré la recherche d'analogues des résultats fondamentaux d'analyse convexe classique: séparation, projection, points extrémaux, à la suite en particulier de [8].

Dans un travail de X. Allamigeon, S. Gaubert, et E. Goubault [62], [63], on a mis en évidence un critère combinatoire pour la caractérisation des sommets des polyèdres tropicalement convexes. Celui-ci s'exprime à l'aide d'hypergraphes orientés, et de leurs composantes fortement connexes. Ce critère possède la propriété d'être vérifiable en un temps presque linéaire en la taille de l'hypergraphe.

On en déduit un analogue tropical de la méthode de la double description [63] (méthode très utilisée sur les polyèdres classiques, et dûe à Motzkin *et al.* [148]). Cet algorithme permet de calculer les sommets d'un polyèdre défini de façon externe (intersection de demi-espaces ou d'hyperplans tropicaux). Grâce au critère combinatoire précédent, l'algorithme améliore de plusieurs ordres de grandeur les techniques connues jusqu'alors. Ceci est confirmé par de nombreuses expérimentations. Ce travail est motivé par des applications à l'analyse statique [61] et aux systèmes à événements discrets [102], dans lesquelles la manipulation de tels polyèdres est le goulot d'étranglement.

Il est connu qu'un polyèdre tropical peut être représenté comme l'enveloppe convexe d'un ensemble minimal de points et rayons, donnés par ses sommets et ses rayons extrêmes [112]. Dans un travail réalisé par X. Allamigeon et R. Katz [64], et effectué en partie lors de visites de R. Katz à Inria, on étudie la question duale de la caractérisation des représentations minimales par demi-espaces. On montre qu'un polyèdre tropical possède *essentiellement* une unique représentation minimale par demi-espaces, lorsque leurs apex appartiennent au polyèdre. On montre que les apex de ces demi-espaces non-redondants correspondent à certains sommets du complexe tropical introduit par Develin et Sturmfels [97]. On introduit également un critère combinatoire pour l'élimination de demi-espaces redondants à l'aide d'hypergraphes orientés.

Dans un travail de X. Allamigeon et R. Katz [65], nous étudions la tropicalisation des représentations par demi-espaces des polyèdres convexes sur le corps des séries de Puiseux. Nous démontrons ainsi une conjecture de Develin et Yu [98]. Celle-ci assure qu'étant donné un polytope tropical pur, il existe un polytope *relevé* sur les séries de Puiseux, dont les demi-espaces associés aux faces se "tropicalisent" en une représentation par demi-espaces du polytope tropical initial.

Des applications de ces travaux à l'algorithmique, concernant en particulier les jeux répétés, sont discutées dans la Section 7.4.1 .

English version

We study the max-plus or tropical analogues of convex sets. These have been used in particular to represent effectively the accessible sets of certain discrete event systems [9]. They also appeared in tropical geometry, following the work of Sturmfels and Develin [97]. Max-plus polyhedra can be thought of as limits of deformations of classical polyhedra, on which they give a combinatorial insight. These motivations have inspired the investigation of analogues of basic results of classical convex analysis: separation, projection, representation by extreme points, following [8].

In a work of X. Allamigeon, S. Gaubert, and E. Goubault [63], we introduce a combinatorial criterion for the characterization of the vertices of tropically convex polyhedra. It is expressed in terms of directed hypergraphs and their strongly connected components. This criterion can be verified in almost linear time in the size of the hypergraph.

This allows to develop a tropical analogue of the double description method [63] (this method is widely used for classical convex polyhedra, and is due to Motzkin *et al.* [148]). This algorithm is able to determine all the vertices of a polyhedron defined externally (intersection of tropical half-spaces of hyperplanes). Thanks to the combinatorial criterion mentioned above, the algorithm improves the existing methods by several orders of magnitude. This is confirmed by several experiments. This is motivated by applications to static analysis [61] and discrete event systems [102], in which computing such polyhedra turns out to be the bottleneck.

It is well-known that a tropical polyhedron can be represented as the convex hull of a minimal set of points and rays, provided by its vertices and extreme rays [112]. In a work of X. Allamigeon and R. Katz [64], partly done during visits of R. Katz at Inria, the dual problem of characterizing the minimal representations by half-spaces is studied. We show that a tropical polyhedron admits *essentially* a unique minimal external representation by half-spaces, provided that their apices belong to the polyhedron. We prove that the apices of

these half-spaces correspond to certain vertices of the tropical complex introduced by Develin and Sturmfels [97]. We also establish a combinatorial criterion allowing to eliminate redundant half-spaces using directed hypergraphs.

In a work of X. Allamigeon and R. Katz [35], we study the tropicalization of the representation by half-spaces of convex polyhedra over the field of Puiseux series. In particular, we prove a conjecture of Develin and Yu [98]. It states that, given a pure tropical polytope, there exists a lifting polytope over Puiseux series, such that the facet-defining half-spaces are "tropicalized" into a representation by half-spaces of the initial polytope.

Some algorithmic applications of this work concerning in particular mean payoff games, will be discussed in Section 7.4.1 .

7.2.2. *Points fixes d'applications monotones homogènes et jeux à somme nulle/Fixed points of order preserving homogeneous maps and zero-sum games*

Participants: Marianne Akian, Stéphane Gaubert, Antoine Hochart.

Pour les jeux répétés à somme nulle, un problème de base est de savoir si le paiement moyen par unité de temps est indépendant de l'état initial. Ici, on définit le paiement moyen directement au moyen de l'opérateur de Shapley (ou de la programmation dynamique) du jeu, lequel préserve l'ordre et commute avec l'addition d'une constante. Dans le cas particulier des jeux à zero joueur, i.e. de chaînes de Markov avec fonctionnelle additive, la solution du problème ci-dessus est fournie par le théorème ergodique. Dans [11], [21], on généralise ce résultat au cas des jeux répétés à espace d'états fini. Cette généralisation est basée sur l'étude de la sous-classe d'opérateurs de Shapley *sans-paiement* (le paiement a lieu seulement le dernier jour), lesquels commutent avec la multiplication par une constante positive. L'intérêt de cette sous-classe est qu'elle inclue la fonction de récession d'un opérateur de Shapley, lorsqu'elle existe. Nous montrons que le paiement moyen est indépendant de l'état initial pour toutes les perturbations des paiements instantannés dépendantes de l'état si, et seulement si, une condition d'ergodicité est vérifiée. Cette dernière est caractérisée par l'unicité, à constante additive près, du point fixe de la fonction de récession de l'opérateur de Shapley, ou, dans le cas particulier des jeux stochastiques à nombre fini d'actions et information parfaite, par une condition d'accessibilité dans un hypergraphe orienté, entre deux sous-ensembles conjugués d'états. On montre aussi que l'ergodicité d'un jeu ne dépend que de la probabilité de transition et qu'elle peut être vérifiée en temps polynomial lorsque le nombre d'états est fixé. Dans [26], on généralise la condition d'accessibilité dans un hypergraphe orienté au cas de jeux avec espaces d'actions arbitraires.

English version

A basic question for zero-sum repeated games consists in determining whether the mean payoff per time unit is independent of the initial state. Here the mean payoff is defined in terms of the Shapley operator (dynamic programming operator) of the game, which is an order preserving map commuting with the addition of a constant. In the special case of "zero-player" games, i.e., of Markov chains equipped with additive functionals, the answer to the above question is provided by the mean ergodic theorem. In [11], [21], we generalize this result to repeated games with a finite state space. This generalization is based on the study of the subclass of *payment-free* Shapley operators (the payment only occurs when the game stops), which are commuting with the multiplication by a positive constant, and which include the recession function of any Shapley operator, when it exists. We show that the mean payoff is independent of the initial state for all state-dependent perturbations of the rewards if and only if an ergodicity condition is satisfied. The latter is characterized by the uniqueness modulo additive constants of the fixed point of the recession function of the Shapley operator, or, in the special case of stochastic games with finite action spaces and perfect information, by a reachability condition involving conjugate subsets of states in directed hypergraphs. We show that the ergodicity condition for games only depends on the support of the transition probability and that it can be checked in polynomial time when the number of states is fixed. In [26], we generalize the above reachability condition to the case of games with arbitrary actions spaces,

7.2.3. *Puissances exterieures tropicales de matrices/Tropical compound matrix identities*

Participants: Marianne Akian, Stéphane Gaubert, Adi Niv.

English version

In [43], [45], we proved some identities on matrices using a weak and strong transfer principles. In the present work, we prove identities on compound matrices in extended tropical semirings. Such identities include analogues to properties of conjugate matrices, powers of matrices and $\operatorname{adj}(A)\det(A)^{-1}$, all of which have implications on the eigenvalues of the corresponding matrices. A tropical Sylvester-Franke identity is provided as well. Even though part of these identities hold over any commutative ring, they cannot be adjusted to semirings with symmetry using the existing weak and strong transfer principles. By reducing these identities to definite matrices, we introduce a transfer principle for formal series, allowing us to infer tropical identities from classical ones. We provide the proofs both via this wider principle and by means of graph theory arguments.

7.2.4. Matrices totalement positives tropicales/Tropical totally positive matrices

Participants: Stéphane Gaubert, Adi Niv.

English version

We investigate totally positive and totally non-negative matrices over the tropical symmetrized semiring. We show these matrices are diagonally dominant, and are determined by their 2×2 minors. We provide the role of the classical double echelon forms in the tropical setting, and find a so called “staircase" form to finite matrices. We establish the connection to the classical sets of totally positive and totally non-negative matrices through the valuation on the field of Puiseux series. In particular, we find the connection to elementary matrix factorization, positivity of eigenvalues and planar networks.

7.2.5. Algèbre supertropicale/Supertropical algebra

Participant: Adi Niv.

English version

Several properties of matrices over the tropical algebra are studied using the supertropical algebra introduced in [126].

The only invertible matrices in tropical algebra are diagonal matrices, permutation matrices and their products. However, the pseudo-inverse A^{∇}, defined as $\frac{1}{det(A)}adj(A)$, with $det(A)$ being the tropical permanent, inherits some classical algebraic properties and has some surprising new ones. In [19], defining B and B' to be tropically similar if $B' = A^{\nabla}BA$, we examine the characteristic (max-)polynomials of tropically similar matrices as well as those of pseudo-inverses. Other miscellaneous results include a new proof of the identity for $det(AB)$ and a connection to stabilization of the powers of definite matrices.

In a joint work with Louis Rowen (Bar Ilan Univ.) [37], we study the pathology that causes tropical eigenspaces of distinct supertropical eigenvalues of a non-singular matrix A, to be dependent. We show that in lower dimensions the eigenvectors of distinct eigenvalues are independent, as desired. The index set that differentiates between subsequent essential monomials of the characteristic polynomial, yields an eigenvalue λ, and corresponds to the columns of the eigenmatrix $A + \lambda I$ from which the eigenvectors are taken. We ascertain the cause for failure in higher dimensions, and prove that independence of the eigenvectors is recovered in case the “difference criterion” holds, defined in terms of disjoint differences between index sets of subsequent coefficients. We conclude by considering the eigenvectors of the matrix $A^{\nabla} := \frac{1}{detA)}adj(A)$ and the connection of the independence question to generalized eigenvectors.

In a joint work with Zur Izhakian (University of Aberdeen) and Louis Rowen (Bar Ilan Univ.) [36], extending earlier work on supertropical adjoints and applying symmetrization, we provide a symmetrized supertropical version SL_n of the special linear group, which we partition into submonoids, based on “quasi-identity” matrices, and we display maximal sub-semigroups of SL_n. We also study the monoid generated by SL_n. Several illustrative examples are given of unexpected behavior. We describe the action of elementary matrices on SL_n, which enables one to connect different matrices in SL_n, but in a weaker sense than the classical situation.

7.3. Algèbre max-plus, déformations et asymptotiques /Max-plus algebra, deformations and asymptotic analysis

7.3.1. Introduction

Comme indiqué dans le §3.7 , l'algèbre max-plus est la limite d'une déformation de l'algèbre classique, ou plutôt du semi-corps des réels positifs. Elle peut aussi fournir des estimations de ces déformations, puisque

$$\max(a,b) \leq \epsilon \log\left(e^{a/\epsilon} + e^{b/\epsilon}\right) \leq \epsilon \log(2) + \max(a,b) \ . \tag{6}$$

L'utilisation de ces propriétés a déjà conduit dans le passé aux travaux sur les perturbations de valeurs propres [42], [41], [40], ou sur les grandes déviations [1], [47]. Dans les travaux qui suivent, nous exploitons ces propriétés dans des contextes reliés ou similaires à ceux de nos travaux précédents.

English version

As detailled in §3.7 , max-plus algebra is the limit of a deformation of classical algebra, or more precisely of the semi-field of usual real positive numbers. It can also give estimations for these deformations using for instance (12). By using these properties, we already obtained some works on singular perturbations of matrix eigenvalues [42], [41], [40], or on large deviations [1], [47]. In the works described below, we are exploiting again these properties in contexts that are related or similar to those of our earlier works.

7.3.2. Méthodes tropicales de localisation de valeurs propres de matrices/Tropical methods for the localisation of matrix eigenvalues

Participants: Marianne Akian, Stéphane Gaubert, Andrea Marchesini.

Dans un travail avec Meisam Sharify [50], on a comparé les modules des valeurs propres d'un polynôme matriciel au moyen des racines tropicales du polynôme obtenu en appliquant une norme donnée aux coefficients. En particulier, on a obtenu des inégalités de type majorisation qui généralisent les bornes obtenues par Polya et Ostrowski dans le cas de polynômes scalaires.

Une partie de la thèse d'Andrea Marchesini, présentée dans [49], montre des inégalités de type majorisation entre les modules des valeurs propres d'une matrice et les valeurs propres tropicales de la matrice de ses modules. En particulier, les majorations généralisent l'inégalité de Friedland [108] concernant le rayon spectral.

Nous avons aussi amélioré et généralisé ces inégalités [27], en appliquant différents changements de variables diagonaux à la matrice complexe initiale, lesquels sont construits à partir des variables duales du problème d'affectation optimale paramètrique construit à partir d'une matrice tropicale associée à la matrice complexe. En particulier, lorsqu'on les applique à une matrice companion par blocs, ces inégalités sont similaires à celles de [50].

English version

In a work with Meisam Sharify [50], we compared the moduli of the eigenvalues of a matrix polynomial to the tropical roots of a polynomial obtained by applying a norm to the coefficients of the original matrix polynomial. In particular, we obtained majorization type inequalities which generalize the bounds of Polya and Ostrowski available for scalar polynomials.

One part of the thesis of Andrea Marchesini, presented in [49], shows majorization type inequalities between the moduli of the eigenvalues of a complex matrix and the tropical eigenvalues of the matrix obtained by applying the modulus entrywise. In particular, the upper bounds generalize the inequality of Friedland [108] concerning the spectral radius. The above inequalities were obtained by using the permanental and tropical analogues of the exterior power of a matrix and by showing (combinatorially) properties of their eigenvalues similar to the ones of usual exterior powers.

We also improved and generalized these inequalities, see [27], by applying to the original complex matrix, different diagonal scalings constructed from the dual variables of the parametric optimal assignment constructed from an associated tropical matrix. In particular, when applied to a block companion matrix, our inequalities are similar to the ones in [50].

7.3.3. Méthodes tropicales pour le calcul numérique de valeurs propres de matrices/Tropical methods for the numerical computation of matrix eigenvalues

Participants: Marianne Akian, Stéphane Gaubert, Andrea Marchesini.

Un des buts de la thèse d'Andrea Marchesini était d'utiliser les résultats de localisation de valeurs propres tels que ceux obtenus ci-dessus pour améliorer la précision des algorithmes de calcul numérique de valeurs propres de matrices ou de polynômes matriciels, en particulier en construisant des changements d'échelle exploitant les calculs tropicaux, à effectuer préalablement à l'appel d'algorithmes classiques comme QZ. Le "changement d'échelle tropical" introduit par Stéphane Gaubert et Meisam Sharify [115] dans le cas de polynôme matriciels quadratiques consiste en un changement de variable multiplicatif de la variable scalaire du polynôme matriciel. Dans la deuxième partie de la thèse d'Andrea Marchesini, en collaboration avec Françoise Tisseur de l'Université de Manchester [22], on considère un changement de variables diagonal du polynôme matriciel construit à partir des variables duales du problème d'affectation optimale paramètrique construit dans l'esprit de [40], [34]. On montre l'intérêt de ces changements d'échelle en terme de conditionnement des valeurs propres, et la supériorité du changement de variables diagonal par rapport au changement d'échelle tropical.

English version

One of goals of the PhD thesis of Andrea Marchesini was to use results on the localisation of eigenvalues like the above ones, to improve the accuracy of the numerical compution of the eigenvalues of a complex matrix or matrix polynomial, in particular by applying scaling methods using tropical techniques, which may be used before calling usual algorithms as QZ. The "tropical scaling" introduced by Stéphane Gaubert and Meisam Sharify [115] in the case of quadratic matrix polynomials consists in a multiplicative scaling of the scalar variable of the matrix polynomial. In the second part of the PhD thesis of Andrea Marchesini, corresponding to a work with Françoise Tisseur from Manchester University [22], we consider a diagonal scaling of the matrix polynomial constructed from the dual variables of the parametric optimal assignment constructed in the same spirit as in [40], [34]. We show the interest of these scaling methods on the eigenvalue conditioning, and the superiority of the diagonal scaling with respect to the tropical scaling.

7.3.4. Tropicalisation du chemin central, et application à la courbure/Tropicalization of the central path and application to the curvature

Participants: Xavier Allamigeon, Pascal Benchimol, Stéphane Gaubert, Michael Joswig [TU Berlin].

En optimisation, une classe importante d'algorithmes, dits *de points intérieurs*, consiste à suivre une courbe appelée *chemin central* jusqu'à atteindre la solution optimale. Le chemin central d'un programme linéaire $\mathrm{LP}(A,b,c) \equiv \min\{c\cdot x \mid Ax \leq b,\ x \geq 0\}$ est défini comme l'ensemble des solutions optimales (x^μ, w^μ) des problèmes à barrière logarithmique:

$$\begin{aligned} \text{minimiser} \quad & c\cdot x - \mu(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i) \\ \text{sous les contraintes} \quad & Ax + w = b,\ x > 0,\ w > 0 \end{aligned}$$

Les performances d'un algorithme de point intérieur sont intimement liées à la forme du chemin central. En particulier, la courbure mesure de combien un chemin diffère d'une ligne droite. Intuitivement, un chemin central à forte courbure devrait être plus difficile à approximer par des segments de droites, ce qui suggère davantage d'itérations des algorithmes de points intérieurs. La courbure totale du chemin central a été étudiée par Dedieu, Malajovich et Shub [94] à travers le théorème de Bezout dans le cas multihomogène, et par De

Loera, Sturmfels and Vinzant [93] à l'aide de la théorie des matroïdes. Ces deux travaux fournissent une borne supérieure en $O(n)$ sur la courbure totale moyenne sur l'ensemble des régions formées par l'arrangement d'hyperplans en dimension n. Le cube de Klee-Minty redondant de [100] et le "serpent" de [99] sont des instances qui montrent que la courbure totale peut être de l'ordre de $\Omega(m)$ pour un polytope défini par m inégalités.

Dans un travail de X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig, nous avons étudié la tropicalisation du chemin central. Le *chemin central tropical* est défini comme la limite logarithmique des chemins centraux d'une famille paramétrique de programmes linéaires LP$(A(t), b(t), c(t))$, où les entrées $A_{ij}(t)$, $b_i(t)$ and $c_j(t)$ sont des fonctions définissables dans une structure o-minimale appelée *corps de Hardy*.

Une première contribution a été de fournir une caractérisation entièrement géométrique du chemin central tropical. Nous avons montré que le centre analytique est donné par le plus grand élément de l'ensemble des points tropicaux admissibles. De plus, tout point du chemin central tropical coincide avec le plus grand élément de l'ensemble admissible tropical intersecté avec un ensemble de sous-niveau de la fonction de coût tropicale.

Grâce à cette caractérisation, nous avons réfuté l'analogue continu de la conjecture de Hirsch proposé par Deza, Terlaky et Zinchenko. Ainsi, nous avons construit une famille de programmes linéaires définis par $3r + 4$ inequalities in dimension $2r + 2$, où le chemin central a une courbure totale en $\Omega(2^r)$. Cette famille est obtenue en relevant des programmes linéaires tropicaux qui proviennent d'une construction de Bezem, Nieuwenhuis et Rodríguez-Carbonell [73]. Afin d'estimer la courbure dans ce contre-exemple, nous introduisons une notion d'angle combinatoire, qui est de nature tropicale. Cela nous permet de définir un analogue combinatoire de la courbure totale qui fournit un minorant de la courbure totale classique.

Ces résultats sont rassemblés dans le document [60].

English version

In optimization, path-following interior point methods are driven to an optimal solution along a trajectory called the central path. The *central path* of a linear program LP$(A, b, c) \equiv \min\{c \cdot x \mid Ax \leq b,\ x \geq 0\}$ is defined as the set of the optimal solutions (x^μ, w^μ) of the barrier problems:

$$\begin{aligned} \text{minimize} \quad & c \cdot x - \mu(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i) \\ \text{subject to} \quad & Ax + w = b,\ x > 0,\ w > 0 \end{aligned}$$

The performance of an interior point method is tightly linked to the shape of its central path. In particular, the curvature measures how far a path differs from a straight line. Intuitively, a central path with high curvature should be harder to approximate with line segments, and thus this suggests more iterations of the interior point methods. The total curvature of the central path has been studied by Dedieu, Malajovich and Shub [94] via the multihomogeneous Bézout Theorem and by De Loera, Sturmfels and Vinzant [93] using matroid theory. These two papers provide an upper bound of $O(n)$ on the total curvature averaged over all regions of an arrangement of hyperplanes in dimension n. The redundant Klee-Minty cube of [100] and the "snake" in [99] are instances which show that that the total curvature can be in $\Omega(m)$ for a polytope described by m inequalities. By analogy with the classical Hirsch conjecture, Deza, Terlaky and Zichencko [99] conjectured that $O(m)$ is also an upper bound for the total curvature.

In a work of X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig, we have studied the tropicalization of the central path. The *tropical central path* is defined as the logarithmic limit of the central paths of a parametric family of linear programs LP$(A(t), b(t), c(t))$, where the entries $A_{ij}(t)$, $b_i(t)$ and $c_j(t)$ are definable functions in an o-minimal structure called the *Hardy field*.

A first contribution is to provide a purely geometric characterization of the tropical central path. We have shown that the tropical analytic center is the greatest element of the tropical feasible set. Moreover, any point of the tropical central path is the greatest element of the tropical feasible set intersected with a sublevel set of the tropical objective function.

Thanks to this characterization, we disprove the continuous analog of the Hirsch conjecture proposed by Deza, Terlaky and Zinchenko, by constructing a family of linear programs with $3r+4$ inequalities in dimension $2r+2$ where the central path has a total curvature in $\Omega(2^r)$. This family is gotten by lifting tropical linear programs which come from a construction of Bezem, Nieuwenhuis and Rodríguez-Carbonell [73]. In order to estimate the curvature in this counter example, we introduce a notion of a combinatorial angle, which is tropical in nature. This allows us to define a combinatorial analogue of the total curvature which provides a lower bound for the classical total curvature.

These results are gathered in the preprint [60].

7.3.5. Etude des ensembles semi-algébriques tropicaux/Tropicalization of semi-algebraic sets

Participants: Xavier Allamigeon, Stéphane Gaubert, Mateusz Skomra.

Suite à son stage de M2, Mateusz Skomra a débuté en octobre 2015 une thèse sous la direction de Xavier Allamigeon et Stéphane Gaubert portant sur la tropicalisation des ensembles semi-algébriques. Cette thèse est financée par une bourse de la région Ile-de-France. La thèse de Mateusz vise en particulier à étudier l'analogue tropical de la programmation sur le cône des matrices positives, dans le but d'obtenir de nouveaux algorithmes ou résultats de complexité pour des sous-classes de problèmes.

English version

Following his M2 internship, Mateusz Skomra has started in October 2015 a PhD thesis under the supervision of Xavier Allamigeon and Stéphane Gaubert, on the tropicalization of semi-algebraic sets. This thesis is funded by a grant from Ile-de-France. One goal is to study the tropical analogue of semidefinite programming, in order to define new algorithms or to establish new complexity results for some subclasses of problems.

7.4. Algorithmes/Algorithms

7.4.1. Algorithmique des polyèdres tropicaux/Algorithmics of tropical polyhedra

Participants: Xavier Allamigeon, Pascal Benchimol, Stéphane Gaubert, Michael Joswig [TU Berlin].

Dans un travail de X. Allamigeon, P. Benchimol, S. Gaubert et M. Joswig [13], nous avons défini un analogue tropical de l'algorithme du simplexe qui permet de résoudre les problèmes de *programmation linéaire tropicale*, *i.e.*

$$\begin{aligned} \text{minimiser} \quad & \max_{1\le j\le n} c_j + x_j \\ \text{sous les contraintes} \quad & \max\big(\max_{1\le j\le n}(a^+_{ij}+x_j), b^+_i\big) \ge \max\big(\max_{1\le j\le n}(a^-_{ij}+x_j), b^-_i\big), \quad i=1,\cdots,m \\ & x \in (\mathbb{R}\cup\{-\infty\})^n \end{aligned} \tag{7}$$

où les entrées du programme $a^{\pm}_{ij}$, $b^{\pm}_i$, c_j sont à valeur dans $\mathbb{R}\cup\{-\infty\}$. Ces problèmes sont intimement liés à la résolution de jeux répétés à somme nulle, puisque résoudre un jeux à paiement moyen déterministe est équivalent à déterminer si un problème de programmation linéaire admet un point réalisable [44].

Comme son homologue usuel, le simplexe tropical pivote entre des points de base (tropicaux), jusqu'à atteindre l'optimum du programme linéaire. La différence fondamentale avec l'algorithme du simplexe classique est que le pivotage est réalisé de manière purement combinatoire, en s'appuyant sur des descriptions locales du polyèdre tropical défini par les contraintes à l'aide d'(hyper)graphes orientés. Ceci nous a permis de prouver que *l'étape de pivotage (incluant le calcul des coûts réduits) a la même complexité en temps que dans l'algorithme classique, i.e.* $O(n(m+n))$. Ceci est d'autant plus inattendu que la structure des arêtes tropicales entre deux points de base sont géométriquement plus complexes (elles sont constituées de plusieurs segments de droite, jusqu'à n).

Le simplexe tropical a la propriété d'être fortement corrélé avec l'algorithme du simplexe classique. Grâce au principe de Tarski, le simplexe usuel peut être transposé tel quel sur des programmes linéaires dont les coefficients en entrée sont non plus des réels, mais sur le corps $\mathbb{R}\{\{t\}\}$ des séries de Puiseux généralisées en une certaine indéterminée t, *i.e.* des objets de la forme :

$$c_{\alpha_1} t^{\alpha_1} + c_{\alpha_2} t^{\alpha_2} + \cdots \tag{8}$$

où les α_i sont des réels, les coefficients c_{α_i} sont des réels non-nuls, et où la séquence des $\alpha_1, \alpha_2, \cdots$ est strictement croissante et soit finie, soit non-bornée. L'opposé du plus petit exposant de la série, $-\alpha_1$, est appelé *valuation* de la série. Un programme linéaire tropical est dit *relevé* en un problème linéaire sur $\mathbb{R}\{\{t\}\}$, si la valuation des coefficients en entrée de ce dernier sont égaux aux coefficients du problème tropical. Dans nos travaux, nous avons établi la correspondance suivante entre le simplexe usuel et le simplexe tropical : *pour tout programme linéaire tropical générique, l'algorithme du simplexe tropical trace l'image par la valuation du chemin sur l'algorithme du simplexe usuel sur n'importe quel relèvement du programme tropical dans* $\mathbb{R}\{\{t\}\}$.

Les résultats présentés ci-dessus sont rassemblés dans l'article [13]. Ils ont fait l'objet de plusieurs présentations en conférence [54], [55] [59].

Ces résultats ouvrent la possibilité de relier la complexité du l'algorithme du simplexe usuel avec celles des jeux déterministes. Pour ces derniers, on sait seulement que leur résolution est dans la classe de complexité $\mathsf{NP} \cap \mathsf{coNP}$, et on ignore s'il existe un algorithme de complexité polynomiale. De façon similaire, on ne sait pas caractériser de façon précise la complexité de l'algorithme du simplexe usuel. Celle-ci dépend fortement de la règle de pivotage utilisée, et il existe des problèmes sur lesquelles de nombreuses règles de pivotage ont une complexité exponentielle. L'existence d'une règle de pivotage qui permettrait au simplexe de terminer en temps polynomial sur n'importe quelle instance est encore aujourd'hui une question ouverte.

Dans un deuxième travail, nous avons relié les deux problèmes ouverts précédents, grâce à l'algorithme du simplexe tropical. Nous avons en effet exhibé une classe de règles de pivotage, dites *combinatoires*, et avons montré qu'elles satisfont la propriété suivante : *s'il existe une règle de pivotage combinatoire qui permet de résoudre tout problème de programmation linéaire usuel en temps polynomial, alors on peut résoudre les jeux à paiement moyen en temps (fortement) polynomial.* Le terme *combinatoire* fait référence au fait que la règle est définie en fonction du signe des mineurs de la matrice des coefficients du problème linéaire. Ce résultat est décrit dans l'article [56], et a été présenté dans plusieurs conférences [57], [58].

Enfin, dans un travail de X. Allamigeon, P. Benchimol et S. Gaubert [53], nous avons étendu les résultats aux règles de pivotage *semi-algébriques*, classe incluant la règle dite du *shadow-vertex*. Celle-ci est connue pour avoir fourni plusieurs bornes de complexité moyenne et lisse sur l'algorithme du simplexe. Nous avons donc tropicalisé l'algorithme du simplexe shadow-vertex, et nous avons montré que cet algorithme permet de résoudre les jeux à paiement moyen en temps polynomial en moyenne.

English version

In an ongoing work of X. Allamigeon, P. Benchimol, S. Gaubert and M. Joswig, we introduced a tropical analogue of the simplex algorithm, allowing one to solve problems of *tropical linear programming*, which are of the form (13), where the coefficients of the program, $a_{ij}^{\pm}$, $b_i^{\pm}$, c_j take their values in the max-plus semiring $\mathbb{R} \cup \{-\infty\}$. These problems are closely related to mean payoff games, as solving a game of this kind is equivalent to determine whether a tropical linear program admits a feasible point [44].

Like the classical simplex algorithm, the tropical simplex algorithm performs pivoting operations between basis points, until it reaches the optimum. The main discrepancy with the classical algorithm is that the pivoting is now a purely combinatorial operation, which is performed by using a local description of the polyhedron by a directed hypergraph. This allowed us to show that *a tropical pivoting step (including computing reduced costs) has the same complexity as in the classical simplex algorithm, i.e.* $O(n(m+n))$. This is all the more

surprising as the tropical edge between two given points has a geometrically more complex structure in the tropical case (it is constituted of up to n ordinary line segments).

The tropical simplex algorithm turns out to be closely related to the classical one. Thanks to Tarski's principle, the latter is also valid for linear programs over the field $\mathbb{R}\{\{t\}\}$ of generalized Puiseux series in an indeterminate t. These series are of the form (14), where the α_i are real numbers, the coefficients c_{α_i} are non-zero reals, and the sequence $\alpha_1, \alpha_2, \cdots$ is strictly increasing and either finite or unbounded. The opposite of the smallest exponent of the series, $-\alpha_1$, is called *valuation*. A tropical linear program is said to be *lifted* to a linear program over $\mathbb{R}\{\{t\}\}$ if the valuation of the coefficients of the latter are sent to the coefficients of the former by the valuation. We showed the following relation between the classical simplex algorithm and its tropical analogue: *for all generic tropical linear program, the tropical simplex algorithm computes the image by the valuation of the path of the classical simplex algorithm, applied to any lift in* $\mathbb{R}\{\{t\}\}$ *of the original program*.

These results are gathered in the article [13]. They have been presented in several conferences [54], [55] [59].

They allow one to relate the complexity of the classical simplex algorithm with the complexity of mean payoff games. The latter is unsettled, these games are known to be in the class $\mathsf{NP} \cap \mathsf{coNP}$ but it is not known whether they can be solved in polynomial time. Basic complexity issues regarding the classical simplex algorithm are also unsettled: its execution time depends on the pivoting rule, and many pivoting rules have been shown to have exponential worst case behaviors. The existence of a pivoting rule leading the simplex to terminate in polynomial time is still an open question. . In a second work, we related these two open questions, via the tropical simplex algorithm. We identified a class of pivoting rules, which are said to be *combinatorial*, and show that they have the following property: *if there is a combinatorial pivoting rule allowing one to solve every classical linear programming problem in polynomial time, then, mean payoff games can be solved in (strongly) polynomial time.* By *combinatorial*, we mean that the rule depends only of the coefficients of the system through the signs of minors of the coefficients matrix. This result is given in the article [56]. It has been presented to the conferences [57], [58].

Finally, in a work of X. Allamigeon, P. Benchimol and S. Gaubert [53], we extended the latter results to *semi-algebraic* pivoting rules, which include the so-called *shadow-vertex* rule. This rule has been exploited in the literature to establish several average-case and smooth complexity bounds on the simplex algorithm. We tropicalized the shadow-vertex simplex algorithm, and showed that it solves mean payoff games in polynomial time on average.

7.4.2. Approximation max-plus de fonctions valeurs et équations de Riccati généralisées/Max-plus approximation of value functions and generalized Riccati equations

Participants: Stéphane Gaubert, Zheng Qu, Srinivas Sridharan.

Le travail de thèse de Zheng Qu, supervisée par S. Gaubert et S. Tang, a porté sur le développement de méthodes tropicales en programmation dynamique approchée [154]. Celle-ci permettent d'attenuer la malédiction de la dimension, pour certaines classes de problèmes de contrôle optimal.

Un développement de ce travail est paru dans [17], où il est montré qu'une classe de relaxations convexes introduites par Sridharan et al. pour traiter numériquement un problème de contrôle quantique sont en fait exactes (pas de saut de relaxation).

English version

The PhD work of Zheng Qu, supervised by S. Gaubert and S. Tang, dealt with the développement of tropical methods in approximate dynamic programming [154]. These allow one to attenuate the curse of dimensionality for certain optimal control problems.

A development of this work appeared in [17]. It is shown there that a class of convex relaxations introduced Sridharan et al. to solve numerically some quantum control problem is exact.

7.4.3. Approximation probabiliste d'équations d'Hamilton-Jacobi-Bellman et itération sur les politiques

Participants: Marianne Akian, Eric Fodjo.

La thèse d'Eric Fodjo traite de problèmes de contrôle stochastique (de diffusions) issus en particulier de problèmes de gestion de portefeuille avec coûts de transaction. La programmation dynamique conduit à une équation aux dérivées partielles d'Hamilton-Jacobi-Bellman, sur un espace de dimension au moins égale au nombre d'actifs risqués. La malédiction de la dimension ne permet pas de traiter numériquement ces équations en dimension grande (supérieure à 5). On se propose d'aborder ces problèmes avec des méthodes numériques associant itération sur les politiques, discrétisations probabilistes, et discrétisations max-plus, afin d'essayer de monter plus en dimension. Une autre piste est de remplacer l'itération sur les politiques par une approximation par des problèmes avec commutations optimales.

Nous considérons actuellement des équations d'Hamilton-Jacobi-Bellman fortement non-linéaires associées à des problèmes de contrôle de diffusions faisant intervenir un contrôle discret (prenant un nombre fini de valeurs) et éventuellement un contrôle continu. On construit un algorithme numérique probabiliste de faible complexité, en combinant les propriétés de distributivité idempotente obtenues par McEneaney, Kaise et Han [128], [145] pour le même type d'équations et la méthode numérique probabiliste proposée par Fahim, Touzi et Warin [104] pour résoudre des équations d'Hamilton-Jacobi-Bellman fortement non-linéaires, lorsque la volatilité ne varie pas trop.

English version

The PhD thesis of Eric Fodjo concerns stochastic control problems obtained in particular in the modelisation of portfolio selection with transaction costs. The dynamic programming method leads to a Hamilton-Jacobi-Bellman partial differential equation, on a space with a dimension at least equal to the number of risky assets. Curse of dimensionality does not allow one to solve numerically these equations for a large dimension (greater to 5). We propose to tackle these problems with numerical methods combining policy iterations, probabilistic discretisations, max-plus discretisations, in order to increase the possible dimension. Another solution is to replace policy iterations by an approximation with optimal switching problems.

Our current work concerns fully nonlinear Hamilton-Jacobi-Bellman equations associated to diffusion control problems with finite horizon involving a finite set-valued (or switching) control and possibly a continuum-valued control. We construct a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [128], [145] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [104] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much.

7.5. Applications

7.5.1. Introduction

Nous présentons maintenant plusieurs travaux de nature appliquée, touchant à des domaines variés, dans lesquels nous exploitons certaines des techniques mathématiques présentées précédemment, et particulièrement celles qui relèvent de la théorie de Perron-Frobenius non-linéaire et de la convexité tropicale. Ces applications utilisent aussi des techniques d'algèbre linéaire ou d'optimisation convexe.

English version

In this section, we describe several applied works in which we use some of the theoretical tools developed by the team, including non-linear Perron-Frobenius theory and tropical convexity. Some of these applications also make an intensive use of linear algebraic and convex programming methods.

7.5.2. Preuve formelle d'inégalités non-linéaires/Formal proofs of non-linear inequalities

Participants: Xavier Allamigeon, Stéphane Gaubert, Victor Magron, Benjamin Werner [LIX].

La thèse de Victor Magron [140], dirigée par Benjamin Werner, codirigée par Stéphane Gaubert et Xavier Allamigeon, a porté sur la certification de bornes inférieures de fonctions multivariées à valeurs réelles, définies par des expressions semi-algébriques ou transcendantes, et sur la preuve de validité de celles-ci au moyen de certificats dans l'assistant de preuves Coq.

L'un des développements de ce travail est paru dans [18],

English version

The PhD work of Victor Magron [140], supervised by Benjamin Werner, and cosupervised by Stéphane Gaubert and Xavier Allamigeon, dealt with the certification of lower bounds for multivariate functions, defined by semi-algebraic or transcendental expressions, and their correctness proof through certificates checked in the Coq proof assistant. A development of this work appeared in [18]

7.5.3. Géométrie de l'ordre de Loewner et application au calcul d'invariants quadratiques en analyse statique de programme/Geometry of the Loewner order and application to the synthesis of quadratic invariants in static analysis of program

Participants: Xavier Allamigeon, Stéphane Gaubert, Éric Goubault [LIX], Sylvie Putot [LIX], Nikolas Stott.

Nous introduisons un nouveau domaine abstrait numérique reposant sur les ellipsoïdes pour la vérification formelle de systèmes linéaires switchés. La nouveauté de ce domain ne réside pas dans l'utilisation des ellipsoïdes en tant qu'abstraction, mais dans le fait que nous dépassons deux difficultés clés qui ont jusqu'à maintenant limiter l'utilisation des ellipsoïdes en interprétation abstraite. La première difficulté est que l'ensemble des ellipsoïdes ne constitue par un treillis. Par conséquent, il n'y a pas a priori de choix canonique pour l'abstraction de l'union de deux ensembles, ce qui rend l'analyse moins prévisible (elle dépend du choix de "bonnes" bornes supérieures). La seconde difficulté est que les travaux récents utilisant les ellipsoïdes reposent sur des méthodes à base d'inégalités linéaires matricielles (LMI). Ces dernières sont efficaces sur des exemples de taille modérée, mais elles sont limités par la complexité des algorithmes de points intérieurs. Ceux-ci ne passent pas aussi bien à l'échelle dans le cas des LMI que dans le cas de la programmation linéaire ou du second-ordre.

Plus précisément, nous réduisons la question de l'abstraction de l'union de deux ensembles par une ellipsoïde à la selection d'une borne inférieure de deux matrices positives pour l'ordre de Löwner. Nous montrons qu'il existe une unique procédure de sélection ayant la propriété d'être invariante par transformation linéaire des variables de programmes. Nous montrons que la borne inférieure ainsi sélectionnée peut être calculée en $O(n^3)$ opérations arithmétiques. Nous établissons aussi que cette borne inférieur coïncide avec l'ellipsoïde de volume minimal, si bien que, de façon surprenante, deux approches distinctes et naturelles mènent à la même sélection. Par ailleurs, nous montrons qu'un invariant ellipsoïdal peut être calculé de manière efficace. Notre algorithme est fondé sur une généralisation non-linéaire de l'algorithme power, utilisé habituellement pour calculer la plus grande valeur propre d'une matrice. Nous illustrons notre approche en l'appliquant à des exemples de systèmes linéaires switchés. Nous montrons que l'algorithme power conduit à des gains en temps de calcul très importants par rapport aux méthodes de type LMI, au pr!x d'une perte de précision limitée.

Ce travail est décrit dans l'article [29], qui a reçu le prix du meilleur article à la conférence EMSOFT 2015.

English version

We introduce a new numerical abstract domain based on ellipsoids designed for the formal verification of switched linear systems. The novelty of this domain does not consist in the use of ellipsoids as abstractions, but rather in the fact that we overcome two key difficulties which so far have limited the use of ellipsoids in abstract interpretation. The first issue is that the ordered set of ellipsoids does not constitute a lattice. This implies that there is a priori no canonical choice of the abstraction of the union of two sets, making the analysis less predictable as it relies on the selection of good upper bounds. The second issue is that most recent works using on ellipsoids rely on LMI methods. The latter are efficient on moderate size examples but they are inherently limited by the complexity of interior point algorithms, which, in the case of matrix inequality problems, do not scale as well as for linear programming or second order cone programming problems.

In more details, we reduce the question of abstracting by an ellipsoid the union of two sets to the selection of a minimal upper bound of two positive semidefinite matrices with respect to the Löwner order. We show that there is a unique selection procedure which has the property of being invariant with respect to linear transformations of the program variables. We show that the minimal upper bound can be computed with the same cost as performing a Cholesky decomposition, i.e., in $O(n^3)$ arithmetic operations. We also establish that it coincides with the minimal volume ellipsoid, so that, surprisingly, two distinct natural approaches lead to the same choice of selection. Moreover, we show that an an invariant ellipsoid can be computed by a scalable algorithm. This is based on a non-linear generalization of the power algorithm which is classically used to compute the dominant eigenvalue of a matrix. We illustrate our approach by applying it to examples of switched linear systems. We show that the power iteration leads to important speedups by comparison with LMI based methods, at the price of a limited loss of precision.

This work is described in the article [29], and won the best paper award at the conference EMSOFT 2015.

7.5.4. Optimisation de l'affectation temps réel des moyens de secours des pompiers/Optimization of the real time assignment of firemen vehicles

Participants: Marianne Akian, Xavier Allamigeon, Vianney Boeuf, Stéphane Gaubert, Stéphane Raclot [BSPP].

La thèse de Vianney Boeuf est effectuée en partenariat avec la Brigade de sapeurs pompiers de Paris (BSPP). Elle est motivée par l'optimisation des moyens de secours, en incluant les questions de dimensionnement et d'affectation temps réel des moyens. On s'intéresse en particulier à l'affectation des engins et véhicules de secours, éventuellement empruntés à différentes casernes. Ce travail intervient en complément du travail de l'équipe au sein du projet ANR Democrite, qui porte sur l'évaluation du risque en milieu urbain.

English version

The PhD work of Vianney is carried out with the Brigade of Paris Firemen (BSPP). It is motivated by the issue of optimization of emergency resources, including the real time dynamic assignment of engines or emergency vehicles. This work is carried out in complement to the ANR project Democrite, dealing with risk evaluation in urban environment.

7.5.5. Analyse de performance d'un centre de reception des appels d'urgence fondée sur les systèmes polynomiaux tropicaux/Performance evaluation of an emergency call center based on tropical polynomial systems

Participants: Xavier Allamigeon, Vianney Boeuf, Stéphane Gaubert, Stéphane Raclot [BSPP], Régis Reboul [PP].

Ce travail a pris sa source dans un problème d'évaluation de performance et de dimensionnement, posé par Régis Reboul (Préfecture de Police), portant sur l'analyse de l'évolution projetée de la procédure de traitement des appels d'urgence (17-18-112). Ce travail a aussi bénéficié de l'appui du LtL Stéphane Raclot (BSPP).

Il a amené à la contribution suivante. Nous introduisons une méthode algébrique qui permet d'analyser les performances de systèmes mettant en jeu des priorité et modélisés par des réseaux de Petri. Cette méthode s'applique à la classe de réseaux de Petri dans lesquels les places peuvent être partitionnées en deux catégories : le routage dans certaines places est sujet à des règles de priorité, tandis que le routage dans les autres places est à choix libre.

Nous montrons que les variables compteurs, qui déterminent le nombre de tirage des transitions comme une fonction du temps, sont les solutions d'un système dynamique linéaire par morceaux. Par ailleurs, nous établissons que dans le modèle fluide, les régimes stationnaires sont précisément les solutions d'un ensemble d'équations linéaires par morceaux et lexicographiques, qui constituent un système polynomial sur un semi-corps tropical (min-plus) de germes.

En substance, ce résultat montre que calculer les régimes stationnaires se réduit à la résolution d'un système polynomial tropical. Ceci est l'un des problèmes de base en géométrie tropicale. Cette interprétation fournit des informations sur la nature des solutions ainsi que des algorithmes. En particulier, l'approche tropicale permet de déterminer les différentes phases de congestion du système.

Nous appliquons ensuite cette approche à un cas d'étude relié au projet actuel de la Préfecture de Police de Paris et la Brigade de sapeurs-pompiers de Paris sur la mise en place d'une nouvelle organisation de réception des appels 17/18/112 sur Paris et sa petite couronne. Nous introduisons pour cela un modèle simplifié d'organisation de réception des appels, et nous nous concentrons sur l'analyse d'une fonctionnalité clé de cette organisation : la procédure de réception des appels à deux niveaux. Les opérateurs de niveau 1 reçoivent les appels, les qualifient en fonction de leur urgence, gèrent les appels non-urgents, et transfèrent les appels urgents à des opérateurs de niveau 2 spécialisés et qui complètent l'instruction. Nous résolvons le système d'équations polynomiales tropicales correspondant, et obtenons un calcul explicite des différents phases de congestion en fonction du rapport entre les nombres d'opérateurs de niveau 2 et 1. Nos résultats analytiques sont obtenus pour le modèle fluide. Cependant, ils sont confirmés par des simulations dans lesquelles la sémantique initiale du réseau de Petri est utilisée.

Ce travail a fait l'objet de la publication [28] à la conférence FORMATS 2015.

English version

This work arose from a question raised by Régis Reboul (Préfecture de Police), regarding the analysis of the projected evolution of the treatment of emergency calls (17-18-112). This work also benefited from the help of LtL Stéphane Raclot (BSPP).

It led to the following contribution. We introduce an algebraic approach which allows to analyze the performance of systems involving priorities and modeled by timed Petri nets. Our results apply to the class of Petri nets in which the places can be partitioned in two categories: the routing in certain places is subject to priority rules, whereas the routing at the other places is free choice.

We show that the counter variables, which determine the number of firings of the different transitions as a function of time, are the solutions of a piecewise linear dynamical system. Moreover, we establish that in the fluid model, the stationary regimes are precisely the solutions of a set of lexicographic piecewise linear equations, which constitutes a polynomial system over a tropical (min-plus) semifield of germs.

In essence, this result shows that computing stationary regimes reduces to solving tropical polynomial systems. Solving tropical polynomial systems is one of the most basic problems of tropical geometry. The latter provides insights on the nature of solutions, as well as algorithmic tools. In particular, the tropical approach allows one to determine the different congestion phases of the system.

We apply this approach to a case study relative to the current project led by Préfecture de Police de Paris (PP), involving the Brigade de sapeurs-pompiers de Paris (BSPP), of a new organization to handle emergency calls to Police (number 17), Firemen (number 18), and untyped emergency calls (number 112), in the Paris area. To this purpose, we introduce a simplified model of emergency call center, and we concentrate on the analysis of an essential feature of the organization: the two level emergency procedure. Operators at level 1 initially receive the calls, qualify their urgency, handle the non urgent ones, and transfer the urgent cases to specialized level 2 operators who complete the instruction. We solve the associated system of tropical polynomial equations and arrive at an explicit computation of the different congestion phases, depending on the ratio of the numbers of operators of level 2 and 1. Our analytical results are obtained only for the approximate fluid model. However, they are confirmed by simulations in which the original semantics of the Petri nets (with integer firings) is respected.

This work has been published in the proceedings of the conference FORMATS 2015 [28].

7.5.6. Tarification du tarif des données dans les réseaux mobiles/Smart Data Pricing

Participants: Marianne Akian, Mustapha Bouhtou [Orange Labs], Jean-Bernard Eytard.

Le travail de PhD de Jean-Bernard Eytard, qui a démarré en Octobre, concerne l'optimisation de la tarification des données dans les réseaux mobiles.

English version

The PhD work of Jean-Bernard Eytard, which started in October, concerns the optimal pricing of data trafic in mobile networks.

MCTAO Project-Team

6. New Results

6.1. Optimal control for quantum systems and applications to MRI

Participants: Bernard Bonnard, Thierry Combot [Université de Bourgogne, IMB], Alain Jacquemard [Université de Bourgogne, IMB], Dominique Sugny [Université de Bourgogne, LIC].

Important results have been obtained in this aera that we detail next :

- A complete solution to the time minimal control of a chain of three spins with Ising coupling which is a toy example applicable to quantum computing [42], [3].
- Optimal control of an ensemble of spins systems with application to MRI : this work is performed in the framework of the ANR project Explosys , based on our previous results in the contrast problem in Nuclear Magnetic Imaging. In relation with the laboratory Creatis (Insa Lyon) and TUM (S. Glaser) the objective is to design robust pulses control, with respect to the relaxation parameters and the B0 and B1 inhomogneities. The computations are intricated from both the numerical point of view and exact computaions. From this second point a systematic study of the controlled Bloch equation has been initiated using exact computer algebraic method in relation with the Inria project-team POLSYS .

6.2. Controllability and Optimal control at Low Reynolds number

Participants: Piernicola Bettiol [Université de Bretagne Occidentale (Brest)], Bernard Bonnard, Laetitia Giraldi, Pierre Martinon [project-team COMMANDS], Jean-Baptiste Pomet, Jérémy Rouot.

This new aera is somehow connected to the recent recruitment of L. Giraldi (CR2) in the Mc Tao team. The problem under study is to design strokes for swimmers at low Reynolds numbers, e .g. the Copepod swimmer (an abundant variety od zooplankton) or the Purcell swimmer. The problem was studied from the point of view of geometric optimal control [17], [18] combining theoretical and numerical computations or controllability techniques [19].

6.3. Averaging in control and application to space mechanics

Participants: Bernard Bonnard, Jean-Baptiste Caillau, Helen-Clare Henninger, Jana Němcová [Institute of Chemical Tech, Prague, CZ], Jean-Baptiste Pomet, Jeremy Rouot.

We have obtained results on the structure of the average system for the planar minimum time problem without perturbation in [4], and the “double average” that takes the lunar perturbation into account in [13]. This is also the topic of Helen Henninger’s PhD [1].

The structure of the problem where the consumption (i.e. the L^1 norm of the control) is minimized is studied in [5].

The book [16] is a general reference opus edited by members of the team.

NECS Project-Team

7. New Results

7.1. Network systems and graph analysis

7.1.1. Distributed estimation of graph Laplacian eigenvalues

Participants: A. Kibangou [Contact person], T.-M. D. Tran.

Linear average-consensus is a well-known iterative protocol allowing agents to converge to the average of initial values by taking suitable convex combinations of the messages received from neighbors. From the recent literature, it is known that, after a finite time, some consecutive measurements of a state of the consensus dynamical system can be used to compute the exact average of the initial condition. In [23], we have shown that these measurements can also be used for estimating the Laplacian eigenvalues of the graph representing the network. As recently shown in the literature, by solving the factorization of the averaging matrix, the Laplacian eigenvalues can be inferred. In our paper, the problem is posed as a constrained consensus problem. A first formulation (direct approach) yields a non-convex optimization problem, which we solve in a distributed way using Lagrange multipliers. A second formulation (indirect approach) is obtained after a suitable re-parameterization. The problem is then convex and is solved by using the distributed subgradient algorithm and the alternating direction method of multipliers (ADMM). The proposed algorithms allow estimating the actual Laplacian eigenvalues with high accuracy. However, they face numerical instability when considering very large graphs.

7.1.2. Distributed solution to the network reconstruction problem

Participants: A. Kibangou [Contact person], T.-M. D. Tran.

We address the problem of reconstructing the network topology from data propagated through the network by means of a linear average-consensus protocol. In [34], we propose a new method based on the distributed estimation of graph Laplacian spectral properties. Precisely, the identification of the network topology is implemented by estimating both eigenvalues and eigenvectors of the consensus matrix, which is related to the graph Laplacian matrix. Having already solved in [23] the problem of estimating the eigenvalues (see paragraph above), in this paper we focus on the eigenvectors. We show how the topology can be reconstructed in presence of anonymous nodes, i.e., nodes that do not disclose their ID. Actually, in presence of anonymous nodes, eigenvectors are estimated up to a permutation of rows; the obtained graph is then isomorphic to the original one. Moreoved, under some observability assumption on the consensus dynamical system (if the graph is node-observable or neighborhood-observable from the node of interest) and if all the entries of the initial condition of the network state are distinct, then the node can exactly reconstruct the network topology. If the entries of the initial condition of the network state are independently generated from a continuous probability distribution, then the node can reconstruct the network topology almost surely. The main assumption in this work is: all eigenvalues are distinct, that is the case of most random graphs. Future works encompass the design of the network reconstruction protocol that deals with spectrums in which the multiplicities of the eigenvalues can be higher than 1 and also directed graphs. In addition, numerical issues for large graphs are to be considered for making the proposed method scalable.

7.2. Sensor networks: estimation and data fusion

7.2.1. Multisensor data fusion for attitude estimation

Participants: H. Fourati [Contact person], A. Kibangou, A. Makni, T. Michel, P. Geneves [Tyrex, Inria], N. Layaida [Tyrex, Inria].

Multisensor data fusion has gained in importance over the last decades and found applications in an impressive variety of areas within diverse disciplines: navigation, sensor networks, intelligent transportation systems, security, medical diagnosis, biometrics, environmental monitoring, remote sensing, measurements, robotics, and so forth. Different concepts, techniques, and architectures have been developed to optimize the overall system output in applications for which sensor fusion might be useful and enables development of concrete solutions. These concepts and ideas are treated in the book [35], as a response to the great interest and strong activities in the field of multisensor data fusion during the last few years, both in theoretical and practical aspects.

In the team, we have carried out works related to attitude estimation for pedestrian navigation purpose.

In [32], we investigated a new modeling and filtering approach for rigid body attitude estimation. In contrast to the current state-of-the-art. where the process model is driven by gyroscope measurements, we propose an alternative modeling formulation where the process model is fed by the magnetometer measurements. The resulting dynamic model takes the form of a descriptor system, also known as singular system. Based on this model and using the quaternion formalism we derive a recursive filter whose performance is validated through numerical and experimental tests.

In [20], we focused on two main challenges. The first one concerns the attitude estimation during dynamic cases, in which external acceleration occurs. In order to compensate for such external acceleration, we design a quaternion-based adaptive Kalman filter q-AKF. Precisely, a smart detector is designed to decide whether the body is in static or dynamic case. Then, the covariance matrix of the external acceleration is estimated to tune the filter gain. The second challenge is related to the energy consumption issue of gyroscope. In order to ensure a longer battery life for the Inertial Measurement Units, we study the way to reduce the gyro measurements acquisition by switching on/off the sensor while maintaining an acceptable attitude estimation. The switching policy is based on the designed detector. The efficiency of the proposed scheme is evaluated by means of numerical simulations and experimental tests.

In [33], we investigated the precision of attitude estimation solutions in the context of Pedestrian Dead-Reckoning (PDR) with commodity smartphones and inertial/magnetic sensors by carrying out a concise comparison of various methods. We conducted an experimental study with a precise ground truth obtained with a motion capture system. We precisely quantified the error in attitude estimation obtained with each filter which combines a 3-axis accelerometer, a 3-axis magnetometer and a 3-axis gyroscope measurements.

7.2.2. Sensor placement of unreliable sensors

Participants: F. Garin [Contact person], P. Frasca [U. Twente], B. Gerencsér [U. Catholique de Louvain], J. Hendrickx [U. Catholique de Louvain].

We consider problems in which sensors have to be deployed in a given environment in such a way to provide good coverage of it. It is clear that sensor failures may deteriorate the performance of the resulting sensor network. Then, it is also natural to ask if taking into account such uncertainties changes the coverage optimization problem and leads to a different optimal solution. For simplicity, we start considering a one-dimensional problem, where sensors are to be placed on a line in such a way to optimize the disk-coverage cost. The optimal solution for reliable sensors is simply an equally-spaced configuration of the sensors. If we allow that the sensors may fail to take or communicate their measurements, this solution may instead not be optimal. In our work, we assume that sensor can fail, independently and with a same failure probability, and we aim to minimize, in expectation, the largest distance between a point in the environment and an active sensor. Our first result states that the problem at hand is equivalent to a linear program, albeit with a number of variables growing exponentially with the number of sensors. This fact allows for a computational solution that is tractable if the number of sensors is not large. Secondly, we show that for large number of sensors n, the cost of the equispaced placement is asymptotically optimal, i.e., the ratio between its cost and the optimal cost tends to 1 when n grows. By contrast, we show in that a random sensor placement has an expected cost which is larger. This work is described in the paper [18].

7.3. Control design and networked control

7.3.1. Control design for hydro-electric power-plants

Participants: C. Canudas de Wit [Contact person], S. Gerwig, F. Garin, B. Sari [Alstom].

We have a collaboration with Alstom on collaborative and resilient control of hydro-electric power-plants, with the CIFRE PhD thesis of Simon Gerwig. The first goal of this research is to improve performance of a hydro-electric power-plant outside its design operation conditions, by cancellation of oscillations that occur in such an operation range. Indeed, current operation of power-plants often requires to operate on a variety of conditions, often different from the ones initially considered when designing the plant. At off-design operation pressure, the hydraulic turbine exhibits a vortex rope below the runner. This vortex generates pressure fluctuations after the turbine and can excite the hydraulic pipes. Indeed the water is compressible and the pipe walls elastic, so the system can oscillate. The goal is to damp these pressure oscillations as they create vibrations in the system and can lead to damages. Our first contribution has been to model the effect of the vortex rope on the hydraulic system as an external perturbation source acting on pipes. The pipes themselves are described with equations taking into account water compressibility and pipe-wall elasticity. The resulting model is nonlinear with hyperbolic functions in the equations (analogous to high-frequency transmission lines), from which we obtain a suitably linearized model.

7.3.2. Collaborative source seeking

Participants: C. Canudas de Wit [Contact person], R. Fabbiano, F. Garin.

The problem of source localization consists in finding, with one or several agents possibly cooperating with each other, the point or the spatial region from which a quantity of interest is being emitted. Source-seeking agents can be fixed sensors, that collect and exchange some information about the signal field and try to identify the position of the source (or the smallest region in which it is included), or moving devices equipped with one or more sensors, that physically reach the source in an individual or cooperative way. This is particularly difficult when the agents have limited or no position information and GPS navigation is not available, as in underwater navigation or in cave exploration: for instance, source localization is relevant to many applications of vapor emitting sources such as explosive detection, drug detection, sensing leakage or hazardous chemicals, pollution sensing and environmental studies. Other fields of interest are sound source localization, heat source localization and vent sources in underwater field. Techniques present in literature either are based on a specific knowledge of the solution of the diffusion process, or make use of an extremum-seeking approach, exciting the system with a periodic signal so as to explore the field and collect enough information to reconstruct the gradient of the quantity of interest. Our approach lies in the computation of derivatives (potentially of any order) from Poisson integrals that, for isotropic diffusive source in steady-state, whose solution satisfies the Laplace equation, allows for a gradient search with a small computation load (derivatives are computed by integrals) and without requiring any knowledge of the closed-form solution, avoiding in the same time extremum-seeking oscillations; this has the additional advantage of an intrinsic high-frequency filtering, that makes the method robust to measurement noise. We also propose a distributed version of this algorithm, where agents communicate in order to reconstruct gradient information from local pointwise measurements, and a control law combines the two objectives of formation control (to have a circular formation, so that measurements are taken around circle) and gradient ascent (so as to move towards the source); differently from previous literature, the moving agents do not need to know their absolute position, but only relative bearing angle of their neighbours. This work is the topic of the Ph.D. thesis of Ruggero Fabbiano [12].

7.3.3. Synchronization of heterogenous networks

Participants: E. Lovisari [Contact person], C.-Y. Kao [National Sun Yat-Sen University, Taiwan].

Syncronization of agents in large-scale networks is studied in [19]. Each agent is modeled as a Single Input Single Output operator composed of the series of a common Linear Time-Invariant system and a possibly nonlinear perturbation. Interconnection is represented via a graph whose edges model communication channels between agents, in turn modeled as a nominal component and a possibly nonlinear perturbation. Two agents are synchronized if their outputs are the same, possibly time-varying signal. The main result provides synchronization certificates based on the Robust Control Technique of Integral Quadratic Constraints. Exploitation of graph structures allows then to reduce the computational burden of the certificate in a way that scales with the dimension of the network. This provides framework which unifies and extendes several results already presented in the literature.

7.3.4. Observer-based FDI scheme for switched systems with sensor faults

Participants: H. Fourati [Contact person], D. E. C. Belkhiat [U. Setif], D. Jabri [U. Setif].

The Fault Detection and Isolation (FDI) problem for a class of Switched Linear Systems (SLS) subject to sensor faults and unknown bounded Disturbances is proposed in [24]. The main work is based on the design of a generalized switched observer scheme. The FDI problems have been solved by using a robust control techniques. A suitable trade-off between the robustness to disturbances and the sensitivity to sensor faults was obtained. The main results are reformulated by using Linear Matrix Inequality (LMI) formulation. An example is included to illustrate the efficiency of the proposed approach.

7.4. Transportation networks and vehicular systems

7.4.1. Traffic estimation: sensors placement and data fusion

Participants: C. Canudas de Wit [Contact person], E. Lovisari, A. Kibangou.

Ability to reconstruct the state of a transportation network is of paramount importance. Indeed, such an information is used to forecast traffic evolution, to inform drivers in real-time through navigation systems, to provide statistical information to public authorities to detect in a timely fashion accidents and predict hazardous scenarios, and finally to compute controls and to actuate the network through traffic lights, ramp metering, or adaptive speed limits.

A primary source of information on the state of the network are fixed traffic detectors, namely, devices able to measure density, flow and average speed of vehicles crossing the section of the road where they are placed. We have addressed the Optimal Sensor Placement problem [31], namely, the problem of finding the best physical location for sensors. This is based on a trade-off of two contrasting objectives: the first, to maximize the performance of state reconstruction; the second, to minimize the total economic cost of the network. To simplify the setting, we consider the related problem of reconstruction in a static setting, by considering as performance metric the error covariance of an estimator of the cumulative flows in the network over a long period of time. Since the resulting trade-off problem remains a combinatorial problem, we relax it using a method that we call Virtual Variance algorithm, based on the idea to associate to each sensor a virtual variance, which is large when the sensor is not needed for good reconstruction of the flow vector. The only input that the algorithm needs is an estimate of the matrix of splitting ratios and the nominal variance of each sensor. Since in real application a pre-existing sensor network is often unavailable, possible alternatives are field surveys with operators visually counting vehicles, as commonly done for calibration of traffic software, or temporary non-invasive equipment such as radar traffic detectors.

In addition to fixed traffic detectors, the spread of wireless devices allows new sensing and communication capabilities. In particular, for the traffic application, any vehicle equipped with a GPS device can act as a probe in the traffic and provide Floating Car Data (FCD). If a non negligible fraction of vehicles acts as probe, the collected data provides an estimate of the evolution of speed in the network. Due to privacy reasons, single vehicles traces are usually not directly used, but rather aggregated as average speed of vehicles in segments of road. Advanced methodologies, such as the one used by INRIX, ensure a very fine spatial partition of the network, with segments as short as 250 meters (see the INRIX official website http://www.inrix.com/xd-traffic). Compared to fixed sensors, this technology is less precise, but since it exploits existing communication

systems it is relatively less expensive and already covers all major traffic networks. In our work [30], [29], we propose an algorithm that aims at reconstructing the traffic density by fusing fixed sensors measurements and Floating Car Data. We employ a macroscopic model, partitioning the network in cells and assigning to each cell a density of vehicles. The latter evolves dynamically according to a first order mass-conservation law. Our approach inherits from the CTM the cell-based topology, but we do not directly employ the resulting dynamical model. Instead, inflows and outflows are estimated on the basis of the available flow measurements only, and speed measurements are employed to compute a pseudo-measurement of the density. These quantities are the inputs for the density observer. In addition, we propose a gradient descent method to calibrate the Fundamental Diagram, and we implement the proposed solution using real fixed sensor measurements from the Grenoble Traffic Lab [14] and speed FCD measurements provided by INRIX, one of the most well known traffic solutions companies.

7.4.2. Traffic forecasting

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

Traffic forecasting is one of the most desired tools for traffic management, requested by operators and commuters. In the era of data deluge in which we are, measurements collected by sensors are important sources of information that require analysis, classification and processing in order to detect patterns and behaviours that can be exploited for traffic prediction ([30], [37]). The collected information can be classified by clustering algorithms such as K-means; each cluster collects traffic patterns, which in some cases characterize typical regimes such as congestion. Based on clustered data, we have first developed forecasting schemes based on adaptive Kalman filtering [14]. These schemes were designed for specific origin-destination (OD) pairs, assuming availability of meaurements whatever the time instants. Recently, within the PhD thesis in progress of Andres Ladino Lopez, we considered a network-oriented forecasting scheme, where travel time measurements are assumed to be available only for a few sets of OD pairs and sporadically (missing data), but forecasting is to be achieved for all the OD pairs of the network. To reduce the dimensionality of the problem, we actually predicted the travel time for the internal state of the network. In addition, since travel time measurements for all the OD pairs cannot be available all the time, we faced a missing data problem. To overcome this issue, we resorted to a data imputation based on a dictionary learning approach. From the imputed data, a clusterization was achieved, defining different clusters characterized by a centroid containing the mean of the data and a given dispersion around it. The evolution of the centroid can be used as future observation, herein called pseudo-observation, that can feed a Kalman filter. Therefore the prediction problem was solved as a filtering one. However, the main question was, how to associate the current day data to a specific cluster, since we didn't know its future? To solve this issue, we run Kalman filters for each cluster and then made the fusion of the obtained forecasts.

7.4.3. Traffic control

Participants: C. Canudas de Wit [Contact person], F. Garin, D. Pisarski, P. Grandinetti, E. Lovisari, G. Como [U. Lund], K. Savla [U. of Southern California].

The activities of the team on traffic control can be organized in three parts: freeway traffic control, urban control, and analysis and control of monotone flows.

First,we have studied optimal balancing of vehicle density in the freeway traffic. The optimization is performed in a distributed manner by utilizing the controllability properties of the freeway network represented by the Cell Transmission Model. By using these properties, we identify the subsystems to be controlled by local ramp meters. The optimization problem is then formulated as a non-cooperative Nash game that is solved by decomposing it into a set of two-players hierarchical and competitive games. The process of optimization employs the communication channels matching the switching structure of system interconnectivity. By defining the internal model for the boundary flows, local optimal control problems are efficiently solved by utilizing the method of Linear Quadratic Regulator. The developed control strategy is tested via numerical simulations in two scenarios for uniformly congested and transient traffic. This work is described in the paper [21].

Second, we have considered optimal or near-optimal operation of traffic lights in an urban area. The goal is on-line optimization of traffic light schedule in real time, so as to take into account variable traffic demands, with the objective of obtaining a better use of the road infrastructure. More precisely, we aim at maximizing total travel distance within the network, while also ensuring good servicing of demands of incoming cars in the network from other areas. One way to address the complexity of the resulting optimization problem is to use a simplified averaged model for the traffic variables, and to optimize only the duty-cyles of traffic lights, i.e., the fractions of green time. This, together with a one-step optimization horizon, allows us to turn the problem into a simple linear program [27]. Another approach is to include as optimization variables both duty-cycles and phases of the traffic lights. We show how to turn the resulting problem into a mixed-integer linear program (MILP). Then, to overcome its complexity, we propose a sub-optimal distributed solution, while the global MILP can be used off-line for performance comparison [28].

Third, stability and throughput properties of monotone dynamical flow networks are studied in [15]. Vehicular density on the cells of the networks evolves according to laws that deterministically split the traffic flow at each intersection as a function of the density of other cells around the intersection. By exploiting the theory of monotone operators it is proven that under certain condition the system achieves an equilibrium that maximizes the throughput of the network, namely, if the inflow is smaller than the network capacity, then asymptotically the total outflow matches the total inflow, otherwise the total outflow matches the network capacity. In [25] a different traffic model is employed which uses demand and supply functions to relate density and flows of the network. The Social Optimum Dynamic Traffic Assignment, which is an optimal control problem with cost corresponding to the total travel time of vehicles in the network, is solved making use of ramp metering and speed limits. The optimization is shown to be a convex optimization problem, making its numerical solution feasible by employing well known tools.

7.4.4. Energy-aware control of communicating vehicles

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

The research in this domain focuses mainly on efficient traffic energy consumption and has been carried out at two levels. Strategies for both the vehicles-side and the infrastructure-side eco-management have been proposed or extended. As for the vehicle-side control of communicating vehicles, assuming I2V communication, and therefore full knowledge of the traffic lights timings, the goal is to analyze the driving horizon and compute an energy-efficient speed advisory for the driver. As in previous works, stops at a red traffic light are to be avoided. The novelty of our approach is summarized as follows. Given a set of green traffic light phases, there exist different driving profiles to reach a given destination at a given final time in compliance with traffic lights constraints (i.e. always catching the green light) and city speed limits. The presented strategy is capable of an a priori identification of the most energy-efficient velocity trajectory, by approximating the available paths and their energy cost with an oriented weighted graph. The computational complexity of the graph creation has been reduced in this work from exponential [26] to polynomial, thanks to the introduction of the line graph. The computation time has been consequently significantly reduced. Only after this preliminary stage of path selection, a formal optimization problem is solved in order to calculate the optimal arrival times at each intersection, by explicitly minimizing the energy consumption of the vehicle. This approach qualifies as a pre-trip eco-driving ADAS, since the speed advisory is provided to the driver at the beginning of the driver horizon. However, given the very little computation time required by the algorithm, it may be employed online thus enabling in-trip assistance features. This allows to respond dynamically to traffic perturbations and/or deviations from the speed advisory, and to increase the robustness and the applicability of the strategy in a realistic environment. Simulations in a microscopic traffic simulator demonstrate that the proposed strategy is able to deal online with perturbations coming from traffic and to reduce the overall energy consumption without affecting travel time [16].

At a lower level, the eco-driving from the vehicle perspective has been also addressed in a comprehensive analysis of the optimal driving strategy for different types of powertrains [22].

As for the infrastructure-side eco-management, this year's research focused on extending the results published in [26]. The two-way arterial bandwidth maximization problem is addressed with a particular focus on the

benefits induced by the speed advisory, and on reducing energy consumption. The problem with internal offsets constraints presents difficulties that make necessary the formulation of the problem as an MILP. The first contribution of our work lies in the addition of terms representing traffic energy consumption and network travel time to the objective function of the two-way arterial bandwidth maximization. The segment speeds, as additional control action, allow to reach higher theoretical bandwidths but might induce driving discomfort and higher energy consumption if the variability of the recommended speeds is too high. Furthermore, optimal solutions with low speeds and high travel time are to be avoided, in trade-off with the energy consumption. The second contribution is given by the extensive evaluation of the benefits of bandwidth maximization via a microscopic traffic simulator. Bandwidth is a theoretical quantity and a correlation with known traffic performance metrics needs to be established in order to justify its use. The combined control of offsets and speed advisory is shown to have a large impact on energy consumption without affecting the travel time. Lastly, an analysis of the traffic performance at different levels of traffic demands has been conducted, testing both under-saturated traffic conditions with the existence of a green wave, and saturated conditions. The goal of this analysis is to identify the best operation conditions of the presented approach, assess the performance degradation with traffic load, and, most importantly, propose a demand-dependent optimization. Several strategies were compared to the presented one in order to assess its performance. This work has been submitted for review to the IEEE Transactions on Control Systems Technology.

Finally, a detailed description of the proposed strategies and the achieved results in the domain of the energy-aware traffic management in urban networks can be found in the dissertation [11].

NON-A Project-Team

6. New Results

6.1. Homogeneity Theory

Homogeneity is one of the tools we develop for finite-time convergence anasysis. In 2015 this concept has received various improvements:

- The concept of homogeneous evolution equation in a Banach space has been introduced in [67]. It provides the background for the extencion of all homogeneity-based tools for control design and analysis to distributed parameters systems.
- Scalability is a property describing the change of the trajectory of a dynamical system under a scaling of the input stimulus and of the initial conditions. Particular cases of scalability include the scale invariance and fold change detection (when the scaling of the input does not influence the system output). In the paper [19] is shown that homogeneous systems have this scalability property while locally homogeneous systems approximately possess this property.
- In the paper [25] the notion of homogeneity in the bi-limit is extended to local homogeneity and then to homogeneity in the multi-limit. The converse Lyapunov/Chetaev theorems on (homogeneous) system instability are obtained. The problem of oscillation detection for nonlinear systems is addressed. The sufficient conditions of oscillation existence for systems homogeneous in the multi-limit are formulated.
- The notion of weighted homogeneity is extended in [81] to the time-delay systems. It is shown that the stability/instability of homogeneous functional systems on a sphere implies the global stability/instability of the system. The notion of local homogeneity is introduced, a relation between stability/instability of the locally approximating dynamics and the original time-delay system is established using Lyapunov-Razumikhin approach
- In [27] global delay independent stability is analyzed for nonlinear time-delay systems by applying homogeneity theory. It is shown that finite-time stability can be encountered in this class of systems under uniformity of the convergence time with respect to delay. Some additional tools for stability analysis of time-delay systems using homogeneity are also presented: in particular, it is shown that if a time-delay system is homogeneous with nonzero degree and it is globally asymptotically stable for some delay, then this property is preserved for any delay value, which is known as the independent of delay (IOD) stability.
- Theorems on Implicit Lyapunov Functions for finite-time and fixed-time stability analysis of nonlinear systems are presented in [37]. Based on these resutls, new homogenenous nonlinear control laws are designed for robust stabilization of a chain of integrators. The presented results are extended to Multi-Input Multi-Output in [38]. A time-suboptimal control design algorithm based Implicit Lyapunov Function Method is developed in [40]. A robustness-oriented comparison of the optimal and suboptimal solutions in practical implementations of the proposed controller is performed via the numerical example of double integrator. A novel scheme of practical implimentation of the implicit Lypunov function-based control is developed in [79]. It replaces the implicitely defined Lyapunov function (in the feedback law) with the homogenenous norm of the state. Such a modification simplifies the practical application of the finite-time stabiliting feedback control.
- The uniform stability notion for a class of nonlinear time-varying systems is studied in [42] using the homogeneity framework. It is assumed that the system is weighted homogeneous considering the time variable as a constant parameter, then several conditions of uniform stability for such a class of systems are formulated. The results are applied to the problem of adaptive estimation for a linear system. The detailed report on time-varying homogenety is given in [83].

- In the paper [52] we consider the continuous homogeneous observer defined in the case of the triple integrator. Originally, convergence of the algorithm was only proved when the degree of homogeneity was sufficiently close to 0 without more tractable information. We show here that, in the case of the triple integrator, the observer presents global finite-time stability for any negative degree under constructive conditions on the gains. This is achieved with a homogeneous Lyapunov function design.
- The work [61] addresses the stabilization of dynamical systems in presence of uncertain bounded perturbations using theory. Under some assumptions, the problem is reduced to the stabilization of a chain of integrators subject to a perturbation and is treated in two steps. The evaluation of the disturbance and its compensation. Homogeneous observer and control are the tools utilized to achieve a global asymptotic stability and robustness. The result is formally proven and, to validate the theory, it is applied to the control of the telescopic link of a hydraulic actuated industrial crane used in forestry.
- A geometric homogeneity of evolution equation in a Banach space is introduced in [67]. Scalability property of solutions of homogeneous evolution equations is proven. Some qualitative characteristics of stability of trivial solution are also provided. In particular, finite-time stability of homogeneous evolution equations is studied. Theoretical results are supported by examples from mathematical physics.
- The second order planar nonlinear affine control problem is studied [69]. A homogeneous robust finite-time stabilizing control is developed for the most general case of matched and, the more challenging, mismatched nonlinear perturbations. A homogeneous observer is designed for the planar system. Explicit restrictions on the observer gains and nonlinearities are presented. The main contribution lies in the proposed combination of the explicit and implicit Lyapunov function methods as well as weighted homogeneity while providing finite-time stability analysis.

6.2. Algebraic Technique For Estimation, Differentiation And Its Applications

Algebraic technique is the other tool we develop for providing finite-time convergence.

- The integer order differentiation by integration method based on the Jacobi orthogonal polynomials for noisy signals was originally introduced by Mboup, Join and Fliess. The paper [35] proposes an extention of this method from the integer order to the fractional order to estimate the fractional order derivatives of noisy signals. Two fractional order differentiators are deduced from the Jacobi orthogonal polynomial filter, using the Riemann-Liouville and the Caputo fractional order derivative definitions respectively. Exact and simple formulas for these differentiators are given by integral expressions. Some error bounds are provided for the corresponding estimation errors. The noise error contribution due to a large class of stochastic processes is studied in discrete case.
- Armed with structures, group sparsity can be exploited to improve the performance of adaptive estimation. In the paper [45], the adaptive estimation algorithm for cluster structured sparse signals, called A-CluSS, is proposed. In particular, a hierarchical Bayesian model is built, where both sparse prior and cluster structured prior are exploited simultaneously. The adaptive updating formulas for statistical variables are obtained via the variational Bayesian inference and the resulted algorithms can adaptively estimate the cluster structured sparse signals without knowledge of block size, block numbers and block locations. In [75], a group sparse regularized least-mean-square (LMS) algorithm is proposed to cope with the identification problems for multiple/multi-channel systems. An iterative online algorithm is proposed via proximal splitting method.

6.3. Set-Theoretic Methods of Control And Estimation

Interval and ellipsoidal estimations can be regarded as particular finite-time algorithms, since they provide guaranteed estimates of the values from the intial time. We develop these tools for some years now.

- An approach to interval observer design for Linear Parameter-Varying (LPV) systems is proposed in [20]. Stability conditions are expressed in terms of matrix inequalities. Applying L1/L2 framework the robustness and estimation accuracy with respect to model uncertainty are analyzed.
- New delay-dependent conditions of positivity for linear systems with time-varying delays are introduced in [56]. These conditions are applied to interval observer design for systems with time-varying delays in the state equations and in the measurements. In [28] the problem of interval observer design is addressed for a class of descriptor linear systems with time delays. An interval observation for any input in the system is provided. The control input is designed together with the observer gains in order to guarantee interval estimation and stabilization simultaneously. Efficiency of the proposed approach is illustrated by numerical experiments with Leontief delayed model.
- The work [29] is devoted to interval observers design for discrete-time Linear Parameter-Varying (LPV) systems under the assumption that the vector of scheduling parameters is not available for measurements. Two problems are considered: a pure estimation problem and an output stabilizing feedback design problem where the stability conditions are expressed in terms of Linear Matrix Inequalities (LMIs).
- The paper [48] investigates the interval observer design for a class of nonlinear continuous systems, which can be represented as a superposition of a uniformly observable nominal subsystem with a Lipschitz nonlinear perturbation. It is shown in this case there exists an interval observer for the system that estimates the set of admissible values for the state consistent with the output measurements. In [77] similar methodology is extended to singular systems.
- A finite-time version, based on Implicit Lyapunov Functions, for the Attractive Ellipsoid Method is developed in [65]. Based on this, a robust control scheme [36] is presented to ensure finite-time convergence of the solutions of a chain of integrators with bounded output perturbations to a minimal ellipsoidal set. The control parameters are obtained by solving a minimization problem of the " size " of the ellipsoid subject to a set of Linear Matrix Inequalities, and by applying the implicit function theorem.
- In [78] we consider a problem of sliding mode control design for LTI systems with multiplicative disturbances of the input and noisy measurements of the output. We apply the minimax observer to provide the best possible estimate of the system's state. Then we solve a problem of optimal reaching for the observer: we design sub-optimal control algorithms generating continuous and discontinuous feedback controls that steer the observer as close as possible to a given sliding hyperplane in a finite time.

6.4. Observability And Observer Design For Nonlinear Systems

- In [18] a method to carried out the state estimation is proposed for a class of nonlinear systems with unknown inputs whose dynamics is governed by differential-algebraic equations (DAE). We achieve, under suitable conditions, to replace the original DAE for a system with differential equations only by using a zeroing manifold algorithm inducing a state space dimension reduction.
- In the paper [44], we investigate the estimation problem for a class of partially observable nonlinear systems. For the proposed Partial Observer Normal Form (PONF), necessary and sufficient conditions are deduced to guarantee the existence of a change of coordinates which can transform the studied system into the proposed PONF.
- Using the theory of non-commutative rings, the delay identification problem of nonlinear time-delay systems with unknown inputs is studied in the paper [82]. Necessary and sufficient conditions are proposed to judge the identifiability of the delay, where two different cases are discussed for the dependent and independent outputs, respectively. After that, necessary and sufficient conditions are given to analyze the causal and non-causal observability for nonlinear time-delay systems with unknown inputs.

- In the paper [58], we investigate the stabilization of a linear plant subject to network constraints, partial state knowledge and time varying bounded parameter uncertainties. An event–triggered version of the Luenberger observer is proposed, and necessary conditions on the uncertainties are given in term of LMI's to enable output– based stabilization under different triggering strategies.
- The papers [47], [76] investigate an unknown input observer design for a large class of linear systems with unknown inputs and commensurate delays. A Luenberger-like observer is proposed by involving only the past and actual values of the system output. The required conditions for the proposed observer are considerably relaxed in the sense that they coincide with the necessary and sufficient conditions for the unknown input observer design of linear systems without delays.
- The paper [71] deals with the problem to estimate some states of a multi-output nonlinear dynamical system which is partially observable. To address this problem, this paper provides a set of geometrical conditions that guarantee the existence of a change of coordinates which decomposes the studied nonlinear dynamical system into two dynamical subsystems, where the first one is of the well-known output injection form. This transformed form allows us to design a simple reduced-order (Luenberger-like) observer to estimate the observable state.

6.5. Model-Free Control

- In the paper [41] the Universal Integral Control, introduced by H.K. Khalil, is revisited by employing mollifiers instead of a high-gain observer for the differentiation of the output signal. The closed loop system is a classical functional differential equation with distributed delays on which standard Lyapunov arguments are applied to study the stability. Low-pass filtering capability of mollifiers is demonstrated for a high amplitude and rapidly oscillating noise.
- The paper [64] proposes an universal adaptive control structure for robot manipulators, without knowing the dynamic model of the system, as well it is robust to corrupt payload change and initial conditions.
- In [66], the control design of an artificial pancreas, a hot research topic in diabetology, is tackled via the newly introduced model-free control and its corresponding "intelligent" proportional controller, which were already quite successful in many concrete and diverse situations. It results in an insulin injection for type 1 diabetes which displays via constant references a good nocturnal/fasting response, but unfortunately a poor postprandial behavior due to long hyperglycemia. When a variable reference is introduced, that switches between a constant one, when glycemia is more or less normal or moderate, and an exponential decay reference path, when a high glycemia rate indicates a meal intake, the results in silico, which employ real clinical data, become excellent. We obtain a bolus-shaped insulin injection rate during postprandial phases. The hyperglycemic peaks are therefore lowered a lot.

6.6. Sliding Mode Control And Estimation

- The paper [22] addresses the problem of oscillatory failure case detection in the electrical flight control system of a generic commercial airplane. A non-homogeneous differentiator is first used to provide accurate derivatives in noisy environment and fast convergence time. In this study case, fault detection is addressed in the unknown input estimation issue for fault reconstruction with the same evaluation techniques currently employed in Airbus A380 airplanes. Performance and robustness of the developed monitoring strategy are assessed using a high-fidelity Airbus benchmark and a parametric test campaign for the flight scenarios defined in the EU-FP7 ADDSAFE project.
- A new sliding mode control approach is introduced in [26] with the dedicated mathematical tools. A time-delay modification/approximation of sign function is proposed in [57], and it is shown that by substituting this new "sign " realization in the conventional sliding mode algorithms the main advantages of the sliding mode tools are preserved (like rejection of matched disturbances and hyper-exponential convergence), while the chattering is reduced.

- The article [34] proposes a convex optimization approach for the design of relay feedback controllers. The case of linear systems is studied in the presence of matched perturbations. The system input is a generalized relay that may take values in a finite set of constant vectors. A simple design method is proposed using Linear Matrix Inequalities (LMIs).
- In the note [53] we study the effect of an implicit Euler time-discretization method on the stability of the discretization of a globally fixed-time stable, scalar differential inclusion representing a simple nonlinear system with a set-valued signum controller. The controller nonlinearity is a cubic term and it is shown that the fully-implicit method preserves the global Lyapunov stability property of the continuous-time system, contrarily the explicit discretization which does not. It allows to obtain finite-time convergence to the origin when the plant is undisturbed, while the cubic term provides the hyper-exponential convergence rate.
- The problem of finite-time stabilization of multi-input linear system by means of sliding mode relay feedback is considered in [68]. A new control design procedure, which combines convex embedding technique with implicit Lyapunov function method, is developed. The issues of practical implementation of the obtained implicit relay feedback are discussed. Theoretical result is supported by numerical simulation.

6.7. Non-Linear, Sampled-Data And Time-Delay Systems

- The method of Implicit Lyapunov-Krasovski Functional (ILKF) for stability analysis of time-delay systems is introduced in [39]. Theorems on Lyapunov, asymptotic, (hyper) exponential , finite-time and fixed-time stability analysis using ILKF are presented. The hyper exponential stabilization algorithm for a time-delay system is presented.
- A recent generalization of the classical ISS theory to multistable systems is presented in [17]. Based on it a robust synchronization protocols with respect to a compact invariant set of the unperturbed system are designed in [14], [49].
- The paper [21] deals with the design of an active fault-tolerant control strategy based on the supervisory control approach technique for linear time invariant MIMO systems affected by disturbances, measurement noise, and faults. From a bank of Luenberger observers that plays the role of a fault detection and isolation scheme, the supervisory algorithm selects the suitable fault-tolerant controller by means of a hysteresis-based switching mechanism based on the method proposed in this paper.
- In [30] motivated by the problem of phase-locking in droop-controlled inverter-based microgrids with delays, the recently developed theory of input-to-state stability (ISS) for multistable systems is extended to the case of multistable systems with delayed dynamics. Sufficient conditions for ISS of delayed systems are presented using Lyapunov-Razumikhin functions. It is shown that ISS multistable systems are robust with respect to delays in a feedback [55].
- The work [31] aims at enlarging the sampling intervals in several state feedback control situations by designing a sampling map in the state space. For linear time invariant (LTI) systems with state-bounded perturbations this guarantees exponential stability with a chosen decay-rate. The approach is based on linear matrix inequalities (LMIs) obtained thanks to Lyapunov-Razumikhin stability conditions and convexification arguments. Then, the obtained results are extended to design the sampling map in three dynamic sampling control situations: event-triggered control, self-triggered control, and state-dependent sampling.
- In the paper [43] the problem of discrete and continuous state estimation for a class of uncertain switched LPV systems is addressed. Parameter identification techniques are applied to realize an approximate identification of the scheduled parameters of a switched LPV system with certain uncertainties and/or disturbances. A discrete state estimation is achieved using the parameter identification. A Luenberger-like hybrid observer, based on discrete state information and LMIs approach, is used for the continuous state estimation.

- The paper [70] contributes to the exponential stability analysis for impulsive dynamical systems based on a vector Lyapunov function and its divergence operator. The method relies on a 2D time domain representation. The results are applied to analyze the exponential stability of linear impulsive systems based on LMIs.

6.8. Networked Systems

- The problem of phase synchronization for a population of genetic oscillators (circadian clocks, synthetic oscillators, etc.) is considered in the paper [13]. The proposed analysis approach is based on the Phase Response Curve model of an oscillator. The performance of the obtained solutions is demonstrated via computer experiments for two different models of circadian/genetic oscillators.
- The paper [23] focuses on the design of fixed-time consensus for first order multi-agent systems with unknown inherent nonlinear dynamics. A distributed control protocol, based on local information, is proposed to ensure the convergence of the tracking errors in finite time. Some conditions are derived to select the controller gains in order to obtain a prescribed convergence time regardless of the initial conditions.
- The problem of phase regulation for a population of oscillating systems is considered in [24] based on a Phase Response Curve (PRC) model of an oscillator. The problem of phase resetting for a network of oscillators is solved by applying a common control input. Performance of the obtained solutions is demonstrated via computer simulation for three different models of circadian/neural oscillators.

6.9. Applications

- The problem of avoiding obstacles while navigating within an environment for a Unicycle-like Wheeled Mobile Robot (WMR) is of prime importance in robotics. The work [32] solves such a problem proposing a perturbed version of the standard kinematic model able to compensate for the neglected dynamics of the robot. The effectiveness of the solution is proved, supported by experiments and finally compared with the Dynamic Window Approach (DWA) to show how the proposed method can perform better than standard methods. The paper [60] presents a decentralized solution to control a leader-follower formation of unicycle wheeled mobile robots allowing collision and obstacle avoidance. The work [62] solves the obstacle avoidance problem extending the Potential Field (PF) method for a mobile robot. The usual definition of the PF has been modified to have a field which is continuous everywhere. It is shown that the system has an attracting equilibrium at the target point, repelling equilibriums in the centers of the obstacles and saddle points on the borders. Those unstable equilibriums are avoided capitalizing on the established Input-to-State Stability (ISS) property of this multi-stable system. To escape a local minima this work makes the most of ISS property that is not lost for perturbations. And for small properly designed disturbances the global attractivity of the target point is proved.
- The paper [63] investigates the behavior of central Jacobi differentiator in robot identification applications. It is applied to compute acceleration from noisy position measurements. Its frequency domain property is analyzed via a finite impulse response (FIR) filter point of view, indicating clearly the differentiators performance. Two revolute joints planar robot parameter identification is done. Comparisons between the Jacobi differentiator and the Euler differentiation combined with Butterworth filter are drawn.
- In [50] the velocity of valve movement activity is estimated using three different differentiation schemes: an algebraic-based differentiator method, a non-homogeneous higher order sliding mode differentiator and a homogeneous finite-time differentiator. We demonstrate that this estimated velocity can be used for water quality monitoring as the differentiators can detect very rapid change in valve movements of the oyster population resulting from some external stimulus or common input.

- In the paper [15] the measurements of valve activity in a population of bivalves under natural environmental conditions (16 oysters in the Bay of Arcachon, France) are used for a physiological model identification. A nonlinear auto-regressive exogenous (NARX) model is designed and tested. Through this study, it is demonstrated that the developed dynamical model of the oyster valve movement can be used for estimating normal physiological rhythms of permanently immersed oysters and can be considered for detecting perturbations of these rhythms due to changes in the water quality, i.e. for ecological monitoring.
- Spawning observations are important in aquaculture and biological studies, and until now, such a detection is done through visual analysis by an expert. Using measurements of valve activity (i.e. the distance between the two valves) in populations of bivalves under natural environmental condition (16 oysters in the Bay of Arcachon, France, in 2007, 2013 and 2014), algorithms for an automatic detection of the spawning period of oysters are proposed in the paper [16], [51]. The fault detection method presented in the paper can also be used to detect complex oscillatory behavior which is of interest to control engineering community.
- The work presented in the paper [33] is undertaken within the European FP7 funded Advanced Fault Diagnosis for Sustainable Flight Guidance and Control (ADDSAFE) project. It proposes new fault detection and fault diagnosis techniques that could significantly help developing environmentally-friendlier aircraft. LPV model-based fault detection schemes are proposed and compared for robust and early detection of faults in aircraft control surfaces servo-loop. The proposed methodologies are based on a slight modification of the H_∞/H_- LPV optimization techniques for systems modelled in, first polytopic manner, second linear fractional representation fashion. It is shown that the proposed fault detection schemes can be embedded within the structure of in-service monitoring systems as a part of the Flight Control Computer software. Several important examples on model and signal based fault detection in aircraft Electrical Flight Control System are studied in [80].
- For analyzing the transients of induction heating systems, time-dependent phasor transformations were proposed so far in the literature. Applying these transformations to a linear R, L, C circuit equations leads to differential equations in the complex domain from which equivalent circuits modeling the envelopes of sinusoidal waveforms were derived. The work [46] proposes a phasor transformation which is based on fictitiously replacing the real voltage and current signals of a system by complex ones. It leads to transformed system equations in the real domain where instantaneous amplitudes, phases and frequencies appear explicitly, which makes the transformed equations suitable for the feedback control design. The methodology is applied to a parallel induction heating system in order to design a sliding mode controller.
- The problem of air-to-fuel ratio regulation for a direct injection engine is addressed in [54]. A LPV model of the engine is used, for which an interval observer is designed. The interval observer is applied for the model validation and control synthesis. The results of design are confirmed by implementation.
- Modular Robot Manipulators are user-configurable manipulators which provide rapid design and inexpensive implementation. To be easy-use, smart actuators embedded with position input and position feedback controller are adopted, these local controllers render the manipulators position controlled, but also result in limited performance and precision. The paper [72] targets the case that the built-in controller does not provide desirable precision for set-point regulation. Firstly a joint-level model is established, of which the nominal model can be identified with derivative observer based on the position feedback, then an auxiliary adaptive controller coping with parametric uncertainty is proposed which leads to an error close to zero, a switching control strategy is introduced considering the actuator saturation. The paper [73] addresses the set-point control of actuators integrated with built-in controller, which presents steady-state error (SSE) under certain load. To eliminate the SSE, a model of the actuator-plus-controller system is established and identified, a switched adaptive controller is developed to work with the embedded one, considering the physical constraints, a switching control strategy is proposed. The proposed algorithms are implemented on a 5-DOF modular manipulator, with comparison to classic integral controller.

- The communication [74] is devoted to a comparison between various meteorological forecasts, for the purpose of energy management, via different time series techniques. The first group of methods necessitates a large number of historical data. The second one does not and is much easier to implement, although its performances are today only slightly inferior. Theoretical justifications are related to methods stemming from a new approach to time series, artificial neural networks, computational intelligence and machine learning.
- ALINEA is a well known ramp metering closed-loop control the aim of which is to improve highway traffic. The report [84] shows that ALINEA may be slightly modified in order to be efficiently implemented without any need of crucial time-varying quantities, like the critical density and the free-flow speed, which are most difficult to estimate correctly online.
- For malaria patients, a usual observation problem consists in estimation of sequestered parasites Plasmodium falciparum from measurements of circulating ones. The model of an infected patient is rather uncertain, and for all rates (death, transition, recruitment and infection) in the model it is assumed that only intervals of admissible values are given. In addition, the measurements of the concentration of circulating parasites are subjected by a bounded noise, while some parameters, like the rate of infection of blood cells by merozoites, are completely unknown and highly time-varying. In order to evaluate the concentration of sequestered parasites, an interval observer is designed in [85], which provides intervals of admissible value for that concentration, with the interval width proportional to the model uncertainty.

QUANTIC Project-Team

6. New Results

6.1. Entanglement between stationary and propagating modes

Participants: B. Huard and F. Mallet.

The results of this section were published in [14].

Entanglement being instrumental in quantum machines, we have shown how a Josephson mixer can generate and distribute entangled microwave radiations on separated transmission lines and different frequencies by spontaneous parametric down-conversion in 2012. Using two Josephson mixers, we have provided the first demonstration of entanglement between spatially separated propagating fields in the microwave domain. Therefore, a new variety of entangled states, the so-called EPR states (after Einstein, Podolsky and Rosen), which are encoded on continuous variables, is now available in this frequency range.

In 2015, we have shown that it could constitute the central component of a potential quantum network based on continuous-variable entanglement. The device essentially acts as a regular mixer performing frequency conversion but without adding extra noise. Used as a switch, it is able to open and close the coupling to a high-quality factor cavity in a time-controlled way. We have demonstrated how this feature leads to a new kind of quantum memory. Coupled to its ability to generate entanglement, we have demonstrated the time-controlled generation, storage and on-demand release of an entangled state, which is the prerequisite for the node of a quantum network.

Several implementations of quantum memories for microwave radiation have been realized in the past few years. In order to store the state of microwave signals, some use spin ensembles [81], [130], [71], or mechanical oscillators [98], while others use superconducting cavities with tunable input coupling [124], [102]. Our own implementation is sketched in Fig. 3 b, where the Josephson Mixer allows an on-demand access to the long lived 3D cavity based on noiseless frequency conversion. Its main advantage consists in the ability to generate entanglement between the memory and the output port.

Noiseless frequency conversion is another regime of the Josephson mixer. The frequency of the pump tone is now chosen to be at the difference between the frequencies of the modes $\widehat{a}$ and $\widehat{b}$, $\Omega = |\omega_a - \omega_b|$. In the rotating frame, the effective Hamiltonian reduces to a beam-splitter Hamiltonian with an implicit frequency conversion:

$$H = \hbar\chi(\widehat{a}^\dagger\widehat{b}\widehat{c} + \widehat{a}\widehat{b}^\dagger\widehat{c}^\dagger).$$

The elementary process corresponds to the conversion of photons between the mode a and b mediated by the pump at a rate $\chi|\langle\widehat{c}\rangle|$ as sketched in Fig. 3 c. Therefore, the noiseless frequency conversion generates a coupling between the long lived cavity mode $\widehat{b}$ and the propagating modes at the input of mode $\widehat{a}$. This pump field can then be varied in time to switch on and off the coupling.

A first measurement consists in the capture, storage and retrieval of a microwave pulse. The protocol is quite simple, we turn the pump tone on when the incoming pulse reaches the memory input. The signal pulse has been designed such that it is optimally absorbed by the memory. The pump tone is turned off after the absorption and turned back on at a later time τ to retrieve the pulse in the transmission line. The measured output amplitude in time shown in Fig. 3 d demonstrate that this protocol can be performed with a great efficiency for a few microseconds.

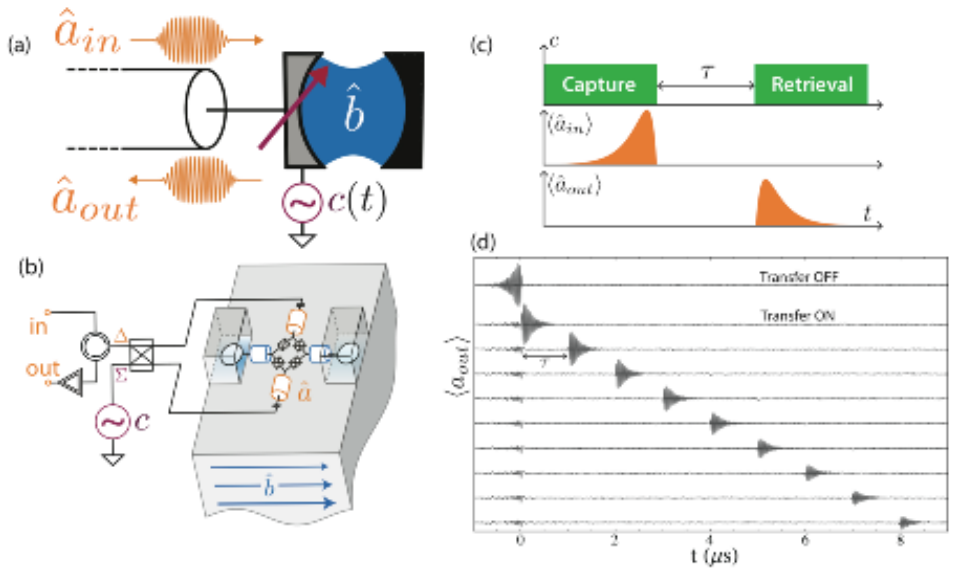


Figure 3. (a) Simplified schematics of the quantum memory. When the pump is driven at $\Omega = |\omega_a - \omega_b|$, the JRM behaves as a beam splitter with an implicit frequency conversion whose transparency depends on the pump amplitude. (b) Schematics of the device. The core of the device is similar to the usual design [107] excepted that one of the two transmission lines is replaced by a superconducting 3D cavity that defines the memory mode. (c) Protocol of the capture, storage and release of a incoming microwave pulse. (d) Measured output amplitude as a function of time. In the first trace, the pump is always turned off and the measured amplitude corresponds to the reflected incoming pulse. In the following traces, the pump is turned on and varied in time as indicated in (c). The storage time is varied from 0 μs to 8 μs.

However, the unique ability of this device lies in the possibility to combine this storage operation with the entanglement generation demonstrated previously. A second measurement consists in the generation, storage and characterization of an EPR state distributed between the memory and the transmission line. The protocol is sketched in Fig. 4 b. The pump is first applied at $\Omega = \omega_a + \omega_b$ to generate an EPR state shared between the memory and the propagating mode. The propagating mode complex amplitude is measured and at a later time, the pump is turned on again at $\Omega = |\omega_a - \omega_b|$ to activate the noiseless conversion. The memory mode is then retrieved in the transmission line and its complex amplitude is measured. By analyzing the cross-correlations between these two measurements, we have been able to show that the memory preserves the entanglement of the EPR state. Furthermore, the contours of the EPR state Wigner function have been inferred from this correlation measurement (Fig. 4 c) and the entanglement quantified.

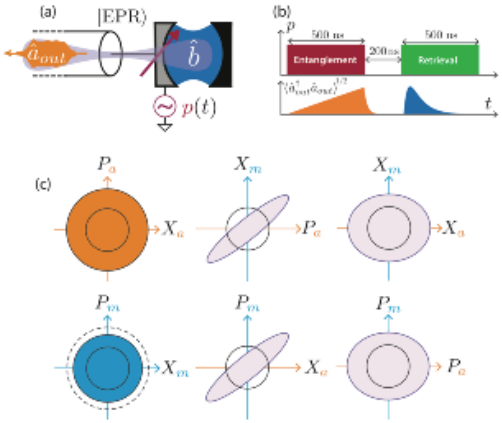


Figure 4. (a) When the pump is shined at $\Omega = \omega_a + \omega_b$, an EPR state is distributed between the transmission line and the memory. (b) Protocol for the entanglement distribution, storage and retrieval. (c) Contour of the marginal Wigner distributions reconstructed from the correlation measurements corresponding to the protocol (b).

6.2. Wideband Josephson mixer

Participants: B. Huard and F. Mallet.

The results of this section were published in [22].

For nearly a decade, the superconducting circuits community develops microwave amplifiers in the quantum regime, i.e. adding only a noise comparable to the vacuum fluctuations of the signal. We participated in this effort in 2012 [107] by adding frequency tunability to the only non-degenerate existing amplifier: the Josephson Parametric Converter (JPC) invented by the group of Michel Devoret at Yale.

However, this amplifier showed the defect of being limited to a few MHz bandwidth for a gain of 20 dB and a dynamic range (maximum input power before changing the gain) capable of amplifying signals typical of circuit-QED. We conducted a theoretical study to understand the various constraints involved in the manufacture of such an amplifier. This study has allowed us to make the first lumped element version of the JPC with bandwidth only limited by the mismatch between the characteristic impedance of the resonators and that of the transmission line.

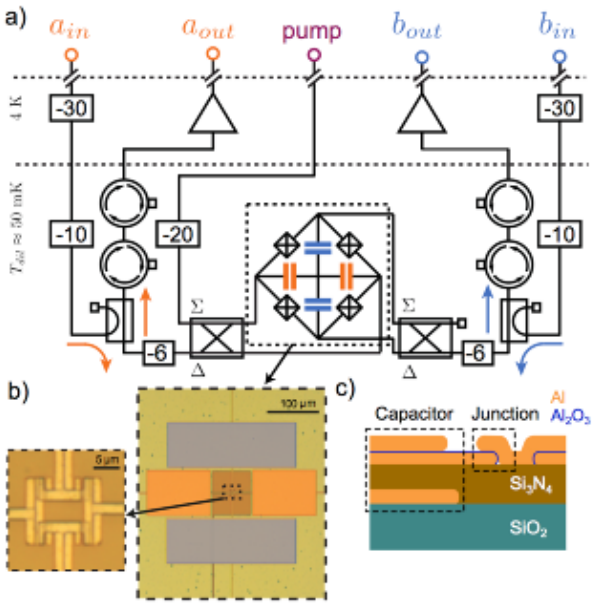


Figure 5. (a) Simplified schematic of the experimental setup. Differential a and b modes of the Josephson mixer are addressed in reflection through two 180 degree hybrid couplers. All input lines are filtered and attenuated (partially shown). Output signals are separated from input signals by a directional coupler and amplified by a low noise HEMT amplifier at 4K. (b) Optical microscope picture of the device showing the planar capacitors (right) and the Josephson junction ring (left). (c) Side view of the device. The thickness of the bottom plate of the capacitors is 35 nm and buried below 200 nm of silicon nitride, the top plate of the capacitors and the Josephson junctions are obtained by double angle deposition of 100 nm and 120 nm of aluminium with an intermediate oxidation.

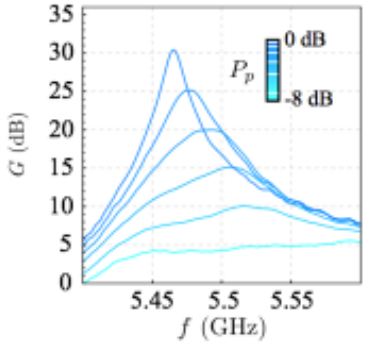


Figure 6. Gain in reflection as a function of frequency for various pump powers. The color bar encodes the pump power referred to the parametric oscillation threshold.

Finally we have measured the quantum efficiency of this amplifier and obtained almost 70%, which means that only 30% of the noise power observed at the end of line comes from technical noise while 70% is the signal, including quantum noise.

6.3. Quantum Zeno dynamics

Participants: B. Huard, L. Bretheau, P. Campagne-Ibarcq, F. Mallet.

The results of this section were published in [13].

Electromagnetic modes are instrumental for realizing quantum physics experiments and building quantum machines. Their manipulation usually involves the tailoring of their Hamiltonian in time. An alternative control scheme, called Quantum Zeno Dynamics (QZD), consists in restricting the evolution of a mode to a subset of possible states. This promising control scheme had been implemented in 2014 on atomic levels of Rb and of a Rydberg atom.

We have made the first observation of QZD of light, using superconducting circuits. By preventing the access to a single energy level, the dynamics of the field is dramatically changed. In this experiment, it was indeed possible to avoid a number of photons N, which was arbitrarily chosen between 2 and 5. Under this constraint, and starting in its ground state, a resonantly driven mode is confined to levels 0 to $N-1$. The level occupation is then found to oscillate in time, similarly to an N-level system. Performing a direct Wigner tomography of the field reveals its non-classical features. In particular, at half period in the evolution, it resembles a "Schrödinger cat state".

In its original definition, the quantum Zeno effect corresponds to the inhibition of coherent transitions from, or to, the pointer states of a strong measurement or dissipative process. Instead of freezing the dynamics, one can restrict it to a given subspace by choosing a measurement with degenerate eigenvalues.

Similar behavior can also be induced by rapid unitary "kicks", leaving the subspace to protect unaffected. It can be understood considering a model for the original Zeno measurement as a series of coherent interactions with ancillary systems. When the interactions are strong enough, departure from the subspace is perfectly suppressed, so that the outcome of the detector is always the same. Therefore, the ancillas are all left in the same state after the interaction and they do not need to be reset. One can then enforce Zeno dynamics by performing repeatedly unitary operations controlling the state of an auxiliary degree of freedom. This amounts

to re-using the same ancilla, at the condition that the unitary evolutions are fast enough to effectively randomize the phase of coherences created with the system. In that sense, QZD is a coherent feedback, which engineers the energy level landscape of a system or its environment by coherent coupling with an ancillary degree of freedom.

In the experiment, a qubit in the resolved photon number regime plays the role of the ancillary system. A strong Rabi drive is applied on its transition conditioned on the cavity mode hosting N photons (N = 3 on Fig. 7). The drive hybridizes the levels $|N, g\rangle$ and $|N, e\rangle$ that repel each other. The level $|N\rangle$ is then moved out from the harmonic ladder of the cavity mode. When starting in the vacuum and applying a coherent drive at ω_r, the generated state cannot contain N photons so that it is restricted to N levels.

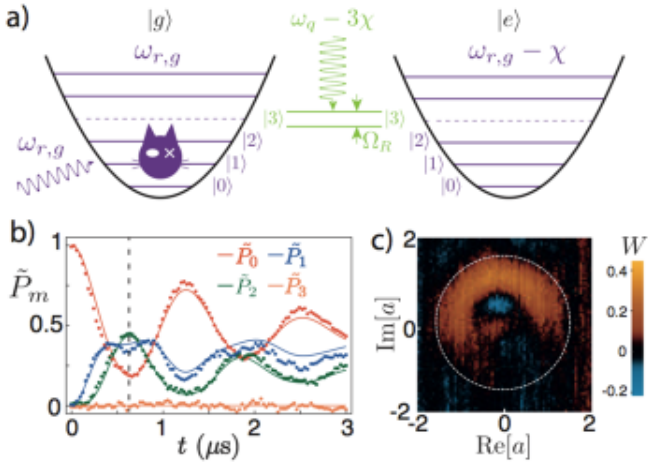


Figure 7. a) Combined energy level diagram for the qubit and cavity. By applying a strong Rabi drive on the $|3, g\rangle \longleftrightarrow |3, e\rangle$ transition, the $|2\rangle \longleftrightarrow |3\rangle$ transition of the cavity becomes off resonant at $\omega_{r,g}$. b) Oscillations of the Fock state occupation when driving the cavity mode from the vacuum and blocking $|3\rangle$. c) Wigner tomography of the field at half period of oscillation (dashed line in b). The quasi-probability density is confined within a circular barrier of radius $\sqrt{3}$ (white circle). Negativities (in blue) reveal a non classical state.

When measuring the Fock state occupation probabilities as a function of time for this effective driven N-level system, characteristic oscillations appear (see Fig. 7 b). Quantum coherence of the field is revealed by direct Wigner tomography (see Fig. 7 c). At half-period of the oscillations, fringes with negativities can be observed. This non classical state is similar to a "Schrödinger cat state", confined in phase space within a circular barrier of radius $\sqrt{N}$.

All these observations are well captured by a model based on N levels only. Our results demonstrate that QZD allows the direct control of the field state in its phase space. This experiment paves the way to the realization of various protocols, such as phase space tweezers, generation and protection of entanglement, and quantum logic operations.

6.4. Efficient quantum filtering for quantum feedback control

Participants: Pierre Rouchon

The results of this section were published in [23].

We discuss an efficient numerical scheme for the recursive filtering of diffusive quantum stochastic master equations. We show that the resulting quantum trajectory is robust and may be used for feedback based on inefficient measurements. The proposed numerical scheme is amenable to approximation, which can be used to further reduce the computational burden associated with calculating quantum trajectories and may allow real-time quantum filtering. We provide a two-qubit example where feedback control of entanglement may be within the scope of current experimental systems.

6.5. Adaptive low-rank approximation and denoised Monte-Carlo approach for high-dimensional Lindblad equations

Participants: Pierre Rouchon

The results of this section were published in [17].

We present a twofold contribution to the numerical simulation of Lindblad equations. First, an adaptive numerical approach to approximate Lindblad equations using low-rank dynamics is described: a deterministic low-rank approximation of the density operator is computed, and its rank is adjusted dynamically, using an on-the-fly estimator of the error committed when reducing the dimension. On the other hand, when the intrinsic dimension of the Lindblad equation is too high to allow for such a deterministic approximation, we combine classical ensemble averages of quantum Monte Carlo trajectories and a denoising technique. Specifically, a variance reduction method based upon the consideration of a low-rank dynamics as a control variable is developed. Numerical tests for quantum collapse and revivals show the efficiency of each approach, along with the complementarity of the two approaches.

This work results from a collaboration with Claude Le Bris of the Matherials project-team and in the framework of the ANR-project EMAQS entitled "Evaluation and Manipulation At Quantum Scale" coordinated by Karine Beauchard from ENS-Rennes.

6.6. Stabilization of photon-number states via single-photon corrections: a first convergence analysis under an ideal set-up

Participants: Pierre Rouchon

The results of this section were published in [33].

This work presents a first mathematical convergence analysis of a Fock states feedback stabilization scheme via single-photon corrections. This measurement-based feedback has been developed and experimentally tested in 2012 by the cavity quantum electrodynamics group of Serge Haroche and Jean-Michel Raimond. Here, we consider the infinite-dimensional Markov model corresponding to the ideal set-up where detection errors and feedback delays have been disregarded. In this ideal context, we show that any goal Fock state can be stabilized by a Lyapunov-based feedback for any initial quantum state belonging to the dense subset of finite rank density operators with support in a finite photon-number sub-space. Closed-loop simulations illustrate the performance of the feedback law.

Paulo Sergio Pereira da Silva and Pierre Rouchon are participants to the Inria associate Team CDSS with principal Inria investigator, François Dufour of the Inria Team Project CQFD on the topic "Control of dynamic systems subject to stochastic jumps".

6.7. Convergence and adiabatic elimination for a driven dissipative quantum harmonic oscillator

Participants: Rémi Azouit, Alain Sarlette, Pierre Rouchon

The results of this section were published in [30].

We prove that a harmonic oscillator driven by Lindblad dynamics where the typical drive and loss channels are two-photon processes instead of single-photon ones, converges to a protected subspace spanned by two coherent states of opposite amplitude. We then characterize the slow dynamics induced by a perturbative single-photon loss on this protected subspace, by performing adiabatic elimination in the Lindbladian dynamics.

6.8. Parameter estimation from measurements along quantum trajectories

Participants: Pierre Six, Ph. Campagne-Ibarcq, Benjamin Huard, Pierre Rouchon

The results of this section were published in [34].

The dynamics of many open quantum systems are described by stochastic master equations. In the discrete-time case, we recall the structure of the derived quantum filter governing the evolution of the density operator conditioned to the measurement outcomes. We then describe the structure of the corresponding particle quantum filters for estimating constant parameter and we prove their stability. In the continuous-time (diffusive) case, we propose a new formulation of these particle quantum filters. The interest of this new formulation is first to prove stability, and also to provide an efficient algorithm preserving, for any discretization step-size, positivity of the quantum states and parameter classical probabilities. This algorithm is tested on experimental data to estimate the detection efficiency for a superconducting qubit whose fluorescence field is measured using a heterodyne detector.

6.9. Adding a single state memory optimally accelerates symmetric linear maps

Participants: Alain Sarlette

The results of this section are to be published in IEEE Trans. Automatic Control [24].

This work is exploring the context and benefits of so-called “non-Markovian” dynamics, where the dynamics implied by hidden variables modifies the behavior of an iterative procedure. Such mechanisms appear in both classical and quantum systems, and one of our future goals is to better characterize the benefits of engineered non-Markovianity in terms of stabilizing power in very constrained systems. The precise setting here is a discrete-time linear map, which is unknown except for a lower and upper bound on its eigenvalues. By adding one memory slot to each coordinate, this map can be accelerated quadratically. We prove that by adding more memory slots, this cannot be further improved. This is reminiscent of the acceleration of random walks by lifting them or by quantizing them, which we are currently exploring.

6.10. A common symmetrization framework for iterative (linear) maps

Participants: Alain Sarlette

The results of this section were presented at [29].

We review a “symmetrization” abstraction of iterative consensus algorithms, which allows to generalize them to general discrete group operations including those acting on quantum systems and on sequences of control actions. We highlight a few new applications of the framework including: consensus networks with antagonistic interactions; sub-stochastic matrix iterations; and coordinate descent on (locally) quadratic functions. The purpose is to show which types of iterative dynamics can be covered by this group-theoretic framework, and potentially operationally generalized to non-classical systems.

6.11. Deterministic hidden coordinate for a qubit under fluorescence measurement

Participants: Alain Sarlette, Pierre Rouchon

The experimentalists in the group have set up an experiment with continuous heterodyne measurement of an energy loss operator on a superconducting qubit. We have observed that in the associated mathematical model, due to the degeneracy of the diffusion operator, the resulting quantum trajectories are supported not in the entire Bloch sphere, but instead they belong to the surface of a *deterministically* evolving ellipsoid. We have entirely characterized this fact and highlighted that such behavior is not generic. A paper comparing this to the experimental data and a more general theory about deterministic evolutions in quantum stochastic differential equations are being finalized. This work has been presented at [28].

6.12. Relations between quantum walks, open quantum walks, and lifted walks: the cycle graph

Participants: Alain Sarlette

The convergence time of a random walk on a graph towards its stationary distribution is an important indication of the efficiency of random algorithms based on it. Quantum random walks have been shown to allow quadratically accelerated convergence for large graphs, at least in some cases. The famous Grover search algorithm has been shown to actually fit this framework in an abstracted setting (it is doing the opposite of a random walk: converging from the uniform distribution towards a particular identified element). Yet also with classical dynamics, simple mechanisms have been proposed which allow to quadratically accelerate the convergence with respect to a standard random walk. Some basic principles have been conjectured to cause this acceleration, basically transforming a diffusion-like behavior into a more transport-like behavior, but with remaining trail. We are working towards formally characterizing the effect of these principles, and extracting similar principles in the quantum walks. This should help identify key effects to be protected in the associated quantum algorithms. We currently have worked out the equivalence of all these accelerating settings for the simplest example of the cycle graph. Quantum coherences turn out to play no major role and a classical feedback structure can be identified. We are now working towards other graphs, where the convergence effect of quantum coherences might be hidden in propagating classical information. This work has been presented at [35].

6.13. Confining the state of light to a quantum manifold by engineered two-photon loss

Participants: Zaki Leghtas and Mazyar Mirrahimi

Physical systems usually exhibit quantum behavior, such as superpositions and entanglement, only when they are sufficiently decoupled from a lossy environment. Paradoxically, a specially engineered interaction with the environment can become a resource for the generation and protection of quantum states. This notion can be generalized to the confinement of a system into a manifold of quantum states, consisting of all coherent superpositions of multiple stable steady states. In a collaboration with the team of Michel H. Devoret at Yale university, we have confined the state of a superconducting resonator to the quantum manifold spanned by two coherent states of opposite phases and have observed a Schrödinger cat state spontaneously squeeze out of vacuum before decaying into a classical mixture. As suggested by our earlier work [93], this experiment points toward robustly encoding quantum information in multidimensional steady-state manifolds and should lead to significant hardware shortcuts for quantum error correction and fault-tolerant quantum computation.

This experimental work was published in Science [18].

6.14. Single-Photon-Resolved Cross-Kerr Interaction for Autonomous Stabilization of Photon-Number States

Participants: Zaki Leghtas and Mazyar Mirrahimi

Quantum states can be stabilized in the presence of intrinsic and environmental losses by either applying active feedback conditioned on an ancillary system or through reservoir engineering. Reservoir engineering maintains a desired quantum state through a combination of drives and designed entropy evacuation. In a collaboration with the team of Robert J. Schoelkopf at Yale university, we propose and implement a quantum reservoir engineering protocol that stabilizes Fock states in a microwave cavity. This protocol is realized with a circuit quantum electrodynamics platform where a Josephson junction provides direct, nonlinear coupling between two superconducting waveguide cavities. The nonlinear coupling results in a single photon resolved cross-Kerr effect between the two cavities enabling a photon number dependent coupling to a lossy environment. The quantum state of the microwave cavity is discussed in terms of a net polarization and is analyzed by a measurement of its steady state Wigner function.

This work was published in Physical Review Letters [15].

6.15. Characterizing entanglement of an artificial atom and a cavity cat state with Bell's inequality

Participants: Zaki Leghtas and Mazyar Mirrahimi

The Schrödinger's cat thought experiment highlights the counterintuitive concept of entanglement in macroscopically distinguishable systems. The hallmark of entanglement is the detection of strong correlations between systems, most starkly demonstrated by the violation of a Bell inequality. No violation of a Bell inequality has been observed for a system entangled with a superposition of coherent states, known as a cat state. In a collaboration with the team of Robert J. Schoelkopf at Yale university, we use the Clauser-Horne-Shimony-Holt formulation of a Bell test to characterize entanglement between an artificial atom and a cat state, or a Bell-cat. Using superconducting circuits with high-fidelity measurements and real-time feedback, we detect correlations that surpass the classical maximum of the Bell inequality. We investigate the influence of decoherence with states up to 16 photons in size and characterize the system by introducing joint Wigner tomography. Such techniques demonstrate that information stored in superpositions of coherent states can be extracted efficiently, a crucial requirement for quantum computing with resonators.

This work was published in Nature Communications [25].

SPHINX Team

7. New Results

7.1. Analysis, control and stabilization of heterogeneous systems

Motivated by the collision problem for rigid bodies in a perfect fluid, Munnier and Ramdani investigated in [9] the asymptotics of a 2D Laplace Neumann problem in a domain with cusp. The small parameter involved in the problem is the distance between the solid and the cavity's bottom. Denoting by $\alpha > 0$ the tangency exponent at the contact point, the authors prove that the solid always reaches the cavity in finite time, but with a non zero velocity for $\alpha < 2$ (real shock case), and with null velocity for $\alpha \geqslant 2$ (smooth landing case). The proof is based on a suitable change of variables transforming the Laplace Neumann problem into a generalized Neumann problem set on a domain containing a horizontal rectangle whose length tends to infinity as the solid approached the cavity.

The paper [14] presents the first positive result on approximate controllability for bilinear Schrödinger equations in presence of mixed spectrum when the interaction term is unbounded.

In [15], Tucsnak, Valein and Wu study the numerical approximation of the solutions of a class of abstract parabolic time optimal control problems. The main results assert that, provided that the target is a closed ball centered at the origin and of positive radius, the optimal time and the optimal controls of the approximate time optimal problems converge to the optimal time and to the optimal controls of the original problem. This is based on a nonsmooth data error estimate for abstract parabolic systems.

A vesicle is an elastic membrane containing a liquid and surrounded by another liquid. Such a vesicle can be found in nature or it can be created in laboratory. They can store and/or transport substances. Modeling vesicles is also a first step in order to study and understand the behavior of more complex cells such as red cells. Their studies are important for many applications, in particular in biological and physiological subjects. Recent papers have been devoted to both experimental studies to the modeling and finally to the mathematical analysis of the obtained models. There are many different models to describe the motion of the membrane and one can for instance optimize the shape in order to minimize the elastic energy of the membrane. Such a problem is tackled in [4] in the 2D case and in [6] in the 3D case. In [4], the optimization is done among convex domains whereas in [6], the authors consider the problem of minimizing the total mean curvature in order to understand the differences between the Helfrich energy and the Willmore energy. Up to now, these models are considered without any fluid.

In [13], San Martin, Takahashi and Tucsnak consider a class of low Reynolds number swimmers, of prolate spheroidal shape, which can be seen as simplified models of ciliated microorganisms. Within this model, the form of the swimmer does not change, the propelling mechanism consisting in tangential displacements of the material points of swimmer's boundary. They obtain the exact controllability of the prolate spheroidal swimmer and the existence of an optimal control problem (in the sense of the efficiency during a stroke). They also provide a method to compute an approximation of the efficiency by using explicit formulas for the Stokes system at the exterior of a prolate spheroid, with some particular tangential velocities at the fluid-solid interface. They analyze the sensitivity of this efficiency with respect to the eccentricity of the considered spheroid and show that for small positive eccentricity, the efficiency of a prolate spheroid is better than the efficiency of a sphere. Finally, they use numerical optimization tools to investigate the dependence of the efficiency on the number of inputs and on the eccentricity of the spheroid.

7.2. Inverse problems for heterogeneous systems

In [7], David Dos Santos Ferreira *et al.* obtain global stability estimates for a potential in a Schrödinger equation on an open bounded set in dimension $n = 3$ from the Dirichlet-to-Neumann map with partial data. This improves previous results where local stability was proved : the region under control was the penumbra

delimited by a source of light outside of the convex hull of the open set. These local estimates provided stability of log-log type corresponding to the uniqueness results in Calderón's inverse problem with partial data proved by Kenig, Sjöstrand and Uhlmann. The corresponding global estimates are proved in all dimensions higher than three. The estimates are based on the construction of solutions of the Schrödinger equation by complex geometrical optics developed in the anisotropic setting by Dos Santos Ferreira, Kenig, Salo and Uhlmann to solve the Calderón problem in certain admissible geometries.

In [20], David Dos Santos Ferreira *et al.* proved uniform L^p resolvent estimates for the stationary damped wave operator. Uniform L^p resolvent estimates for the Laplace operator on a compact smooth Riemannian manifold without boundary were first established by Shen on the Torus, then by Dos Santos Ferreira-Kenig-Salo for general compact manifolds and advanced further by Bourgain-Shao-Sogge-Yao. An alternative proof relying on the techniques of semiclassical Strichartz estimates allows to handle non-self-adjoint perturbations of the Laplacian and embeds very naturally in the semiclassical spectral analysis framework, and applies in the damped wave context.

In [10], Munnier and Ramdani considered the 2D inverse problem of recovering the positions and the velocities of slowly moving small rigid disks in a bounded cavity filled with a perfect fluid. Using an integral formulation, they first derive an asymptotic expansion of the DtN map of the problem as the diameters of the disks tend to zero. Then, combining a suitable choice of exponential type data and the DORT method (french acronym for Diagonalization of the Time Reversal Operator), a reconstruction method for the unknown positions and velocities is proposed. Let us emphasize here that this reconstruction method uses in the context of fluid-structure interaction problems a method which is usually used for waves inverse scattering (the DORT method).

In [24], Munnier and Ramdani proposed a new method to tackle a geometric inverse problem related to Calderón's inverse problem. More precisely, they proposed an explicit reconstruction formula for the cavity inverse problem using conformal mapping. This formula is derived by combining two ingredients: a new factorization result of the DtN map and the so-called generalized Polia-Szegö tensors of the cavity.

In [11], Ramdani, Tucsnak and Valein tackled a state estimation problem for an infinite dimensional system arising in population dynamics (a linear model for age-structured populations with spatial diffusion). Assume the initial state to be unknown, the considered inverse problem is to estimate asymptotically on time the state of the system from a locally distributed observation in both age and space. This is done by designing a Luenberger observer for the system, taking advantage of the particular spectral structure of the problem (the system has a finite number of unstable eigenvalues).

In [12], San Martin, Schwindt and Takahashi consider the geometrical inverse problem consisting in recovering an unknown obstacle in a viscous incompressible fluid by measurements of the Cauchy force on the exterior boundary. They deal with the case where the fluid equations are the non stationary Stokes system and using the enclosure method, they can recover the convex hull of the obstacle and the distance from a point to the obstacle. With the same method, they can obtain the same result in the case of a linear fluid–structure system composed by a rigid body and a viscous incompressible fluid. They also tackle the corresponding nonlinear systems: the Navier–Stokes system and a fluid–structure system with free boundary. Using complex spherical waves, they obtain some partial information on the distance from a point to the obstacle.

7.3. Numerical analysis and simulation of heterogeneous systems

In optics, metamaterials (also known as negative or left-handed materials), have known a growing interest in the last two decades. These artificial composite materials exhibit the property of having negative dielectric permittivity and magnetic permeability in a certain range of frequency, leading hence to materials with negative refractive index and super lens effects. In [5], Bunoiu and Ramdani studied a complex wave system involving such materials. More precisely, they consider a periodic homogenization problem involving two isotropic materials with conductivities of different signs: a classical material and a metamaterial (or negative material). Combining the $\mathbf{T}-$coercivity approach and the unfolding method for homogenization, they prove well-posedness results for the initial and the homogenized problems and obtain a convergence result, provided that the contrast between the two conductivities is large enough (in modulus).

Several results on domain decomposition were obtained in the frame of the collaboration of Xavier Antoine with the team of Christophe Geuzaine (Belgium). The paper [3] deals with a Schwarz-type solver for domain decomposition, the paper [8] proposes a Schwarz-type domain decomposition for high frequency electromagnetism equations, the paper [1] exposes how to use of GPELab to solve Gross-Pitaevskii equations.

The paper [2] deals with domain decomposition for nonlinear Schrödinger equations and the book chapter [16] is focused on the modeling of Bose-Einstein condensates.

DOLPHIN Project-Team

7. New Results

7.1. Benchmarking Numerical Optimizers

Participants: D. Brockhoff, B. Derbel, A. Liefooghe, T.-D. Tran, D. Tušar, T. Tušar (DOLPHIN), O. Ait Elhara, A. Atamna, A. Auger, N. Hansen (TAO team, Inria Saclay), P. Preux (Univ. Lille 3), O. Mersmann, T. Wagner (TU Dortmund University, Germany), B. Bischl (LMU Munich, Germany), Y. Akimoto (Shinshu University, Japan)

In terms of benchmarking numerical optimization algorithms, our research effort went into two different directions. On the one hand, we continued our work on benchmarking single-objective optimization algorithms via the Coco platform in which we started to focus on algorithms for expensive optimization (problems for which only a few function evaluations are affordable). In particular, we benchmarked algorithm variants from the MATSuMoTo library [52], [50] and from the bandits-based global optimizer SOO (Simultaneous optimistic optimization) [33], and organized two workshops at CEC 2015 and GECCO 2015 (see also http://coco.gforge.inria.fr/). On the other hand, we started to develop an extension of the Coco platform towards multiobjective optimization and tried to establish the state of the art in single-objective benchmarking (target-based runtimes, data profiles, ...) also in the multi-objective case [30]. At the same time, we proposed a new bi-objective test suite, consisting of 300 well-understood, scalable test problems.

7.2. Handling numeric and temporal data in a local search-based classification algorithm

Participants: J. Jacques, L. Jourdan, C. Dhaenens, M. Vandomme

MOCA-I [20] is a highly efficient classification algorithm, primarily designed for knowledge extraction on large-scale, real-life medical data. This algorithm has been first extended to deal with numeric data [58], [46], through the definition of a model for classification rules on numeric attributes. Several neighborhood operators have been proposed, and compared, as components of the overarching local search metaheuristic guiding the discovery and optimization of these rules. A new model has also been proposed to handle temporal data. This model allows for the inclusion of sequences of events in classification rules, in addition to non-temporal attributes, thus building more informative classifiers. This model, along with various optimizations in the local search process, has been favorably compared to the previous MOCA-I algorithm and other standard classification algorithms. It is now used on real hospital data in order to evaluate its performance in a real environment.

7.3. MO-DYNAMOP

Participants: S. Jacquin, L. Jourdan, E-G. Talbi

The proposed method, MO-DYNAMOP generalize to multi-objective optimization, DYNAMOP, a state of the art optimizer, which was successfully applied to several MO problems. The specificity of this method is to combine aMO dynamic programming (MO-DP) with a MO evolutionary algorithm (MOEA). MO-DYNAMOP is applied to the first stage of the MO-UCP problem including minimization of gas emission. Since the second stage of the problem is now multi-objective, each solution of the first stage problem induces an entire Pareto front of the second stage problem. MO-UCP is solved by assigning an approximation of this Pareto front to each solution of the first stage problem. A comparison study with methods previously proposed in literature is performed. Experiments indicate that MO-DYNAMOP performs considerably better.

7.4. Decomposition-based multi-objective optimization

Participants: Dimo Brockhoff, Bilel Derbel, Arnaud Liefooghe, Gauvain Marquet, El-Ghazali Talbi, Saul Zapotecas-Martinez (external collaborators: Hernan Aguirre and Kiyoshi Tanaka, Shinshu Univ., Japan; Juan Palacios Alonso, Univ. Oviedo, Spain)

MOEA/D is an aggregation-based evolutionary algorithm which has been proved extremely efficient and effective for solving multi-objective optimization problems. It is based on the idea of decomposing the original multi-objective problem into several single-objective subproblems by means of well-defined scalarizing functions. Those single-objective subproblems are solved in a cooperative manner by defining a neighborhood relation between them. This makes MOEA/D particularly interesting when attempting to plug and to leverage single-objective optimizers in a multi-objective setting. For continuous optimization, we investigate in [49] the benefits that MOEA/D can achieve when coupled with CMA-ES, which is believed to be a powerful single-objective optimizer. We rely on the ability of CMA-ES to deal with injected solutions in order to update different covariance matrices with respect to each subproblem defined in MOEA/D. We show that by cooperatively evolving neighboring CMA-ES components, we are able to obtain competitive results for different multi-objective benchmark functions. Moreover, in the combinatorial case, we study in [48] the incorporation of geometric differential evolution (gDE), the discrete generalization of DE, into the MOEA/D framework. We conduct preliminary experiments in order to study the effectiveness of gDE when coupled with MOEA/D. Our results indicate that the proposed approach is highly competitive with respect to the original version of MOEA/D, when solving a combinatorial optimization problem having between two and four objective functions. In [36], we consider a bi-objective scheduling combinatorial problem in which task durations and due-dates are uncertain as a case study for MOEA/D. In particular, we investigate existing variants of MOEA/D and we propose a novel and simple alternative replacement component at the aim of maintaining population diversity. Through extensive experiments, we then provide a comprehensive analysis on the relative performance and the behavior of the considered algorithms. Besides being able to outperform existing MOEA/D variants, as well as the standard NSGA-II algorithm, our investigations provide new insights into the search ability of MOEA/D and highlight new research opportunities for improving its design components. At last, in [32], we propose the first large-scale message passing distributed scheme for parallelizing the computational flow of MOEA/D. We show how synchronicity and workload granularity can impact both quality and computing time, in an extremely fine-grained configuration. We deploy our distributed protocol using a large-scale environment of 128 computing cores. Besides being able to show significant speed-ups while maintaining competitive search quality, our experimental results provide insights into the behavior of the proposed scheme in terms of quality/speed-up trade-offs; thus pushing a step towards the achievement of effective and efficient parallel decomposition-based approaches for large-scale multi-objective optimization.

7.5. Fitness landscape analysis for multi-objective optimization

Participants: F. Daolio, A. Liefooghe (external collaborators: Sébastien Verel, Univ. Littoral Côte d'Opale, France; Hernan Aguirre and Kiyoshi Tanaka, Shinshu Univ., Japan)

Computationally hard multi-objective combinatorial optimization problems are common in practice, and numerous evolutionary multi-objective optimization (EMO) algorithms have been proposed to tackle them. Our aim is to understand which (and how) problem features impact the search performance of such approaches. In [38], we adopt a statistical approach, based on simple and multiple linear regression analysis, to enquire the expected running time of global SEMO with restart for identifying a $(1+\varepsilon)$-approximation of the Pareto set for small-size enumerable instances. Our analysis provides further insights on the EMO search behavior and on the most important features that characterize the difficulty of an instance for this class of problems and algorithms. In [31], we consider two prototypical dominance-based algorithms: a global EMO strategy using an ergodic variation operator (GSEMO) and a neighborhood-based local search heuristic (PLS). Their respective runtime is estimated on a benchmark of combinatorial problems with tunable ruggedness, objective space dimension, and objective correlation (ρMNK-landscapes). In other words, benchmark parameters define classes of instances with increasing empirical problem hardness; we enumerate and characterize the search space of small instances. Our study departs from simple performance comparison to systematically analyze

the correlations between runtime and problem features, contrasting their association with search performance within and across instance classes, for both chosen algorithms. A mixed-model approach then allows us to further generalize from the experimental design, supporting a sound assessment of the joint impact of instance features on EMO search performance. Next, in [28], we analyse the behavior and compares the performance of MOEA/D, IBEA using the binary additive epsilon and the hypervolume difference indicators, and AεSεH as representative algorithms of decomposition, indicators, and ε-dominance based approaches for many-objective optimization. We use small MNK-landscapes to trace the dynamics of the algorithms generating high-resolution approximations of the Pareto optimal set. Also, we use large MNK-landscapes to analyze their scalability to larger search spaces. At last, in [39], we report an experimental analysis on stochastic local search for approximating the Pareto set of bi-objective unconstrained binary quadratic programming problems. First, we investigate two scalarizing strategies that iteratively identify a high-quality solution for a sequence of sub-problems. Each sub-problem is based on a static or adaptive definition of weighted-sum aggregation coefficients, and is addressed by means of a state-of-the-art single-objective tabu search procedure. Next, we design a Pareto local search that iteratively improves a set of solutions based on a neighborhood structure and on the Pareto dominance relation. At last, we hybridize both classes of algorithms by combining a scalarizing and a Pareto local search in a sequential way. A comprehensive experimental analysis reveals the high performance of the proposed approaches, which substantially improve upon previous best-known solutions. Moreover, the obtained results show the superiority of the hybrid algorithm over non-hybrid ones in terms of solution quality, while requiring a competitive computational cost. In addition, a number of structural properties of the problem instances allow us to explain the main difficulties that the different classes of local search algorithms have to face.

7.6. Fitness Landscape of the Factoradic Representation on the PFSP

Participants: Marie-Eléonore Marmion (external collaborators: Olivier Regnier-Courdert, University of Aberdeen, UK)

Because permutation problems are particularly challenging to model and optimise, the possibility to represent solutions by means of factoradics has recently been investigated, allowing algorithms from other domains to be used. Initial results have shown that methods using factoradics can efficiently explore the search space, but also present difficulties to exploit the best areas. In [57], the fitness landscape of the factoradic representation and one of its simplest operator is studied on the Permutation Flowshop Scheduling Problem (PFSP). The analysis highlights the presence of many local optima and a high ruggedness, which confirms that the factoradic representations is not suited for local search. In addition, comparison with the classic permutation representation establishes that local moves on the factoradic representation are less able to lead to the global optima on the PFSP.

7.7. How Neutrality Helps Multiobjective Local Search Algorithms

Participants: Aymeric Blot, Clarisse Dhaenens, Laetitia Jourdan, Marie-Eléonore Marmion(external collaborators: Hernan Aguirre and Kiyoshi Tanaka, Shinshu Univ., Japan)

We extend the concept of neutrality used in single-objective optimization to the multi-objective context and investigate its effects on the performance of multi-objective dominance-based local search methods [29]. We discuss neutrality in single-objective optimization and fitness assignment in multi-objective algorithms to provide a general definition for neutrality applicable to multi-objective landscapes. We also put forward a definition of neutrality when Pareto dominance is used to compute fitness of solutions. Then, we focus on dedicated local search approaches that have shown good results in multi-objective combinatorial optimization. In such methods, particular attention is paid to the set of solutions selected for exploration, the way the neighborhood is explored, and how the candidate set to update the archive is defined. We investigate the last two of these three important steps from the perspective of neutrality in multi-objective landscapes, propose new strategies that take into account neutrality, and show that exploiting neutrality allows to improve the performance of dominance-based local search methods on bi-objective permutation flowshop scheduling problems. This work is a first step to integrate learning in strategies of local search algorithms.

7.8. Surrogate-assisted multiobjective evolutionary algorithm for fuzzy job shop problems

Participants: E-G. Talbi and Juan José Palacios, Jorge Puente, Camino R. Vela, Inés Gonzalez-Rodrıguez (Univ. Oviedo, Spain)

We have considered a job shop scheduling problem with uncertain processing times modelled as triangular fuzzy numbers and propose a multiobjective surrogate assisted evolutionary algorithm to optimise not only the schedule's fuzzy makespan but also the robustness of schedules with respect to different perturbations in the durations. The surrogate model is defined to avoid evaluating the robustness measure for some individuals and estimate it instead based on the robustness values of neighbouring individuals, where neighbour proximity is evaluated based on the similarity of fuzzy makespan values. The experimental results show that by using fitness estimation, it is possible to reach good fitness levels much faster than if all individuals are evaluated.

7.9. Bipartite matching approximation

Participants: F. Dufossé

Bipartite matching is a classical academic problem on bipartite graphs. Many iterative heuristics need an initial approximate matching with linear computational time. We have designed two randomized highly parallelizable algorithms with linear execution time and quality guarantee. The approximation guarantees have been proved to reach respectively 63demonstrate the speed-ups and validate the applicability and efficiency of these algorithms on general bipartite graphs. Comparisons with the more efficient suboptimal linear algorithms of bipartite matching demonstrate a lower efficiently in average but a similar execution time, and validate the quality guarantee on all experiments. This work has been published in [16].

7.10. Parallel B&B revisited for coprocessors using our new IVM data structure dedicated to permutation problems

Participants: J. Gmys, R. Leroy and N. Melab

This contribution is a joint work with M. Mezmaz and D. Tuyttens from University of Mons (UMONS).

Solving large permutation Combinatorial Optimization Problems (COPs) using Branch-and-Bound (B&B) algorithms results in the generation of a very large pool of subproblems. Therefore, defining a dedicated data structure is crucial to store and manage efficiently that pool. In the Ph.D thesis of R. Leroy [11], we have proposed an original data structure called Integer-Vector-Matrix (IVM) for permutation COPs based on the factorial number system. Consequently, we have redefined the operators of the B&B algorithm acting on it. For performance evaluation in terms of memory footprint and CPU time usage, we conduct a complexity analysis and an extensive experimentation using the permutation Flow-Shop Scheduling Problem (FSP) as a case study. Compared to the Head-Tail Linked List (LL) data structure often used for parallel B&B as in our work [11], IVM requires up to n times less memory than LL, n being the size of permutations. Moreover, the IVM-based B&B is up to one order of magnitude faster than its LL-based counterpart in managing the pool of subproblems. Another major contribution of this thesis is to revisit parallel B&B for multi-core processors and many-core coprocessors (GPU and MIC) using IVM and LL-based work stealing. Several challenging issues are addressed including work distribution using factoradic-based intervals on multi-core processors, thread/branch divergence and data placement optimization on GPU, and vectorization on Intel Xeon Phi. The contribution and some of its extensions have been published in [40], [18]. An extensive experimental study shows that the IVM-based approach outperforms its LL-based counterpart by a significant margin on multi-core processors as well as on coprocessors.

A major extension of this work has been proposed in [54] and awarded as a best paper consists in offloading all the operators of the B&B algorithm to the GPU. Four interval-based WS strategies have been investigated using IVM. An extensive experimentation allowed us to demontrate that the GPU-accelerated approach is 5 times faster than its multi-core counterpart.

7.11. large scale heterogeneous parallel B&B based on hybrid work-stealing

Participants: Bilel Derbel, Tuan Trong Vu

In [27], we investigate the design of parallel B&B in large scale heterogeneous compute environments where processing units can be composed of a mixture of multiple shared memory cores, multiple distributed CPUs and multiple GPUs devices. We describe two approaches based on hybrid work-stealing in shared and distributed memory systems, addressing the critical issue of how to map B&B workload with the different levels of parallelism exposed by the target compute platform. We also contribute a throughout large scale experimental study which allows us to derive a comprehensive and fair analysis of the proposed approaches under different system configurations using up to 16 GPUs and up to 512 distributed cores. Our results shed more light on the main challenges one has to face when tackling B&B algorithms while describing efficient techniques to address them. In particular, we are able to obtain linear speed-ups at moderate scales where adaptive load balancing among the heterogeneous compute resources is shown to have a significant impact on performance. At the largest scales, intra-node parallelism and hybrid decentralized load balancing is shown to have a crucial importance in order to alleviate locking issues among shared memory threads and to scale the distributed resources while optimizing communication costs and minimizing idle times.

7.12. A Multi-objective Evolutionary Algorithm for Cloud Platform Reconfiguration

Participants: F. Legillon, N. Melab and E-G. Talbi

This contribution published in [37] is a result of an industrial collaboration with Tasker Cloud services company.

Offers of public IAAS providers are dynamic: new providers enter the market, existing ones change their pricing or improve their offering. The decision on whether and how to improve already deployed platforms, either by reconfiguration or migration to another provider, can be modelled as an NP-hard optimization problem. In this paper, we define a new realistic model for this migration problem, based on a multi-objective Optimization formulation. An evolutionary approach is introduced to tackle the problem, using newly defined specific operators. Experiments are conducted on multiple realistic data-sets, showing that the evolutionary approach is viable to tackle real-size instances in a reasonable amount of time.

7.13. A multi-objective approach for energy-efficient scheduling of large workloads in multicore distributed systems

Participants: E-G. Talbi and B. Dorronsoro (Univ. Cadiz, Spain), S. Nesmachnow (Universidad de la República, Uruguay), J. Taheri, A. Zomaya (Univ. Sydney, Australia), P. Bouvry (Univ. Luxembourg

This work proposes a two-level strategy for scheduling large workloads of parallel applications in multicore distributed systems, taking into account the minimization of both the total computation time and the energy consumption of solutions. Nowadays, energy efficiency is of major concern when using large computing systems such as cluster, grid, and cloud computing facilities. In the approach proposed, a combination of higher-level (i.e., between distributed systems) and lower-level (i.e., within each data-center) schedulers are studied for finding efficient mappings of workflows into the resources in order to maximize the quality of service, while reducing the energy required to compute them. The experimental evaluation demonstrates that accurate schedules are computed by using combined list scheduling heuristics (accounting for both problem objectives) in the higher level, and ad-hoc scheduling techniques to take advantage of multicore infrastructures in the lower level. Solutions are also evaluated with two user- and administrator-oriented metrics. Significant improvements are reported on the two problem objectives when compared with traditional load-balancing and round-robin techniques [15].

GEOSTAT Project-Team

7. New Results

7.1. Super-resolution, multiscale data fusion and complex dynamics in Earth Observation and Universe Sciences

Participants: Hussein Yahia, Nicolas Brodu, Guillaume Attuel, Sylvain Bontemps, Nicola Schneider, Camila Artana, Dharmendra Singh, Joel Sudre, Véronique Garçon, Christine Provost, Anass El Aouni, Oriol Pont, Khalid Daoudi, Ayoub Tamim, Akankhsa Garg, Frédéric Frappart, Luc Bourrel.

In these thematics the following research is started or continued:

- Super-resolution and data fusion in Earth Observation. Important results obtained in validation either in ocean dynamics or partial pCO_2 pressures in ocean/atmosphere exchanges, coastal upwelling.
- Development of a new super-resolution model for multispectral images, demonstration on MODIS (NASA) and Sentinel-2 (ESA) data.
- Adaptive optics.
- Starting of a strong collaboration with Labroatoire d'Astrophysique de Bordeaux on the dynamics of galactic clouds.
- Supervised classification of ground terrain through multispectral imagery (with OPTIC associated team).
- Anomaly detection in SAR images, application to flood monitoring in Equator.
- Starting of a project on dune monitoring.

Publications: [21], [19], [29], [22], [25], [18] A. Tamim's PhD HAL link, IEEE TGRS article on AO [21].

7.2. Characterization of underlying stochastic dynamic of the cardiac muscle under fibrillation: singularity analysis and modeling

Participants: Guillaume Attuel, Binbin Xu, Oriol Pont, Hussein Yahia.

Signals of heart electrical activity obtained through invasive measurements show properties not compatible with the purely excitable nature of cellular dynamics. We have developed a synaptic perturbation model of that dynamics showing good properties. Pertubations propagate an inter-cell desynchronization formally like diffusion-coupled chaotic maps. The model enters the universality class of directed propagative fronts of the type random branching or directed polymer in a disordeRed medium in 1+1D and pinning-depinning contact lines in 1+2D. In the continuum limit, the universality class is supposed to be the one of KPZ (Kardar Parisi Zhang) or VM (Voter Model). This is a change in paradigm for the description of cardiac dynamics. We make use of this hypothesis to characterize precisely the state of the substratum through appropriate signal analysis, with the goal of being able to distinguish between different states or types in the pathology. We are involved in a technological transfert on this activity since summer 2015.
Publication: [26].

7.3. Classification of Cardiac Arrhythmia in vitro based on Multivariate Complexity Analysis

Participant: Binbin Xu.

Background: The animal models (in vitro or in vivo) provide an excellent tool to study heart diseases, among them the arrhythmia remains one of the most active research subjects. It can be induced or treated by drugs, electrical stimulation, hypothermia etc. **Problems:** However, the inducing or treating effects in cardiac culture often happened long after the initial applications or in some relatively short time windows. So, it is necessary to capture and classify rapidly the signal change. Human-assisted monitoring is time-consuming and less efficient. An automatic classification method for real-time use would be useful and necessary. **Methods:** Since electrocardiological signals are features by repetitive or similar patterns reflecting the intrinsic information about the patient (or culture), analyzing these patterns could help not only to monitor the status's change but also to evaluate/explore the physiologic control mechanisms. Methods based on complexity analysis are of considerable interest in this case. **Aims:** Compare different complexity analysis methods in order to find the most appropriate ones to discriminate the normal cardiac signals from arrhythmic ones acquired from a cardiac cell culture in vitro. The selected features are then used by a SVM classifier.

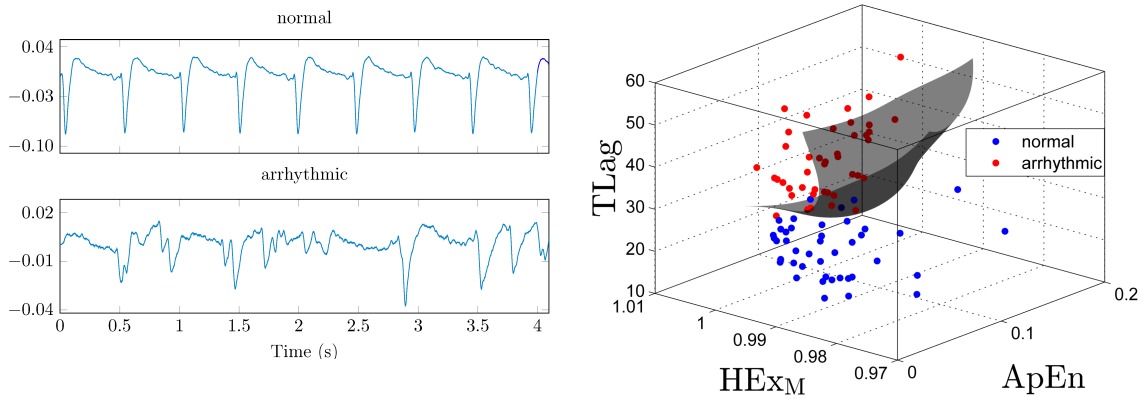


Figure 1. Left: Electrical field potential (EFP) of in vitro cardiac culture on Multielectrodes Array; Right: SVM classification of normal and arrhythmic EFP signals.

Results: Among the six complexity analysis methods, Time Lagging (TLag) method allowed obtaining the best discrimination index (normal vs. arrhythmic, p-value, 9e-23). The proposed Modified Hurst Exponent ($\mathrm{HEx_M}$) showed better performance than original Hurst Exponent with well-improved p-value (from 0.019 to 2e-9). The Approximate Entropy (ApEn), Sample Entropy (SampEn) and Detrended Fluctuation Analysis gave good discrimination ratio but with larger p-values (at order 10^{-3}). Combination of TLag, $\mathrm{HEx_M}$ and ApEn can provide a more robust classifier and allow monitoring and classifying in an automatic way the electrical activities' changes in the cardiac cultures.
Publication: [28].

7.4. Classification of Cardiac Arrhythmia in vitro based on Multivariate Complexity Analysis

Participant: Binbin Xu.

Physiological signals are temporal series containing a lot of information, and their analysis (either for diagnosis or evolution monitoring) necessitates tools that take into account their intrinsic characteristics, notably in terms of impredictability and high number of parameters. Methodologies coming from chaotic and nonlinear dynamical systems contain some useful building blocks in that perspective, and allow a qualitative link with phenomenological and bio-inspired models. The objective of this work is to introduce some methods in nonlinear dynamics useful for the processing of these types of signals. An application of these tools is

illustrated in the processing of potential electrical fields acquired from in vitro culture cells on newborn rats. Both normal (regular contraction of cells) and arrythmic (disordoned contractions) cases are contemplated.

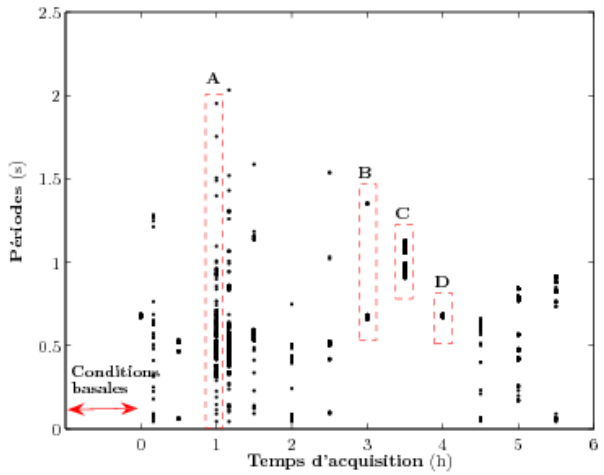


Figure 2. CPE period bifurcartion diagram. Cells are stimulated by M1 electrode during 5 minutes with an impulsion train of $200\mu m$ *and frequency* 100Hz*. Three particular phenomena in cell behaviour:* ***A*** *(*$t = 1$ *hour) chaotic state,* ***B*** *(*$t = 3$ *hour) and* ***C*** *(*$t = 3.5$ *hour) period doubling phase,* ***D*** *(*$t = 4$ *hour) regular and stable rythm.*

The bifurcation diagram is an example of a tool that can be used in the temporal analysis of an experimental system.
Publication: [32].

7.5. Nonlinear trend removal should be carefully performed in heart rate variability analysis

Participants: Binbin Xu, Oriol Pont, Hussein Yahia, Rémi Dubois.

Background : In Heart rate variability analysis, the rate-rate time series suffer often from aperiodic non-stationarity, presence of ectopic beats etc. It would be hard to extract helpful information from the original signals. **Problem** : Trend removal methods are commonly practiced to reduce the influence of the low frequency and aperiodic non-stationary in RR data. This can unfortunately affect the signal and make the analysis on detrended data less appropriate. **Objective** : Investigate the detrending effect (linear & nonlinear) in temporal / nonliear analysis of heart rate variability of long-term RR data (in normal sinus rhythm, atrial fibrillation, congestive heart failure and ventricular premature arrhythmia conditions). **Methods** : Temporal method : standard measure SDNN; Nonlinear methods : multi-scale Fractal Dimension (FD), Detrended Fluctuation Analysis (DFA) & Sample Entropy (SampEn) analysis.

Results : The linear detrending affects little the global characteristics of the RR data, either in temporal analysis or in nonlinear complexity analysis. After linear detrending, the SDNNs are just slightly shifted and all distributions are well preserved. The cross-scale complexity remained almost the same as the ones for original RR data or correlated. Nonlinear detrending changed not only the SDNNs distribution, but also the order among different types of RR data. After this processing, the SDNN became indistinguishable between SDNN for normal sinus rhythm and ventricular premature beats. Different RR data has different complexity signature. Nonlinear detrending made the all RR data to be similar, in terms of complexity. It is thus impossible

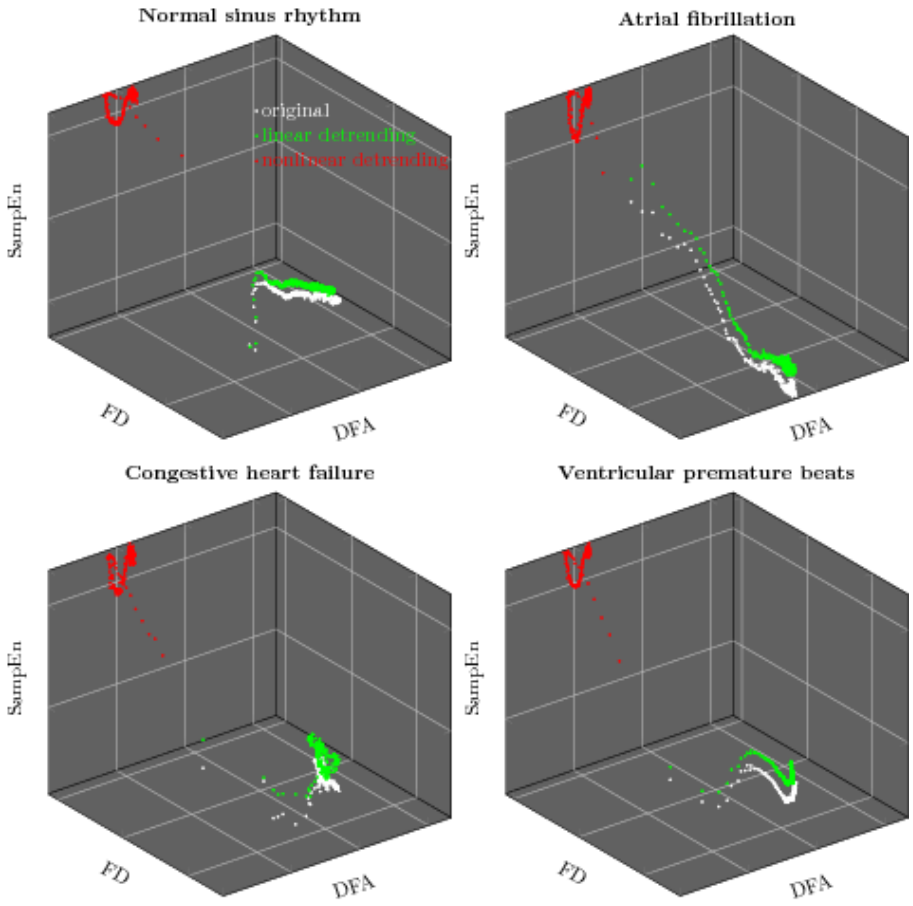


Figure 3. Complexity Space based on FD, DFA & SampEn, for RR data in NSR, AF, CHF & VPB conditions.

to distinguish them. The FD showed that nonlinearly detrended RR data has a dimension close to 2, the exponent from DFA is close to zero and SampEn is larger than 1.5 – these complexity values are very close to those for random signal. **Conclusions** : Pre-processing by linear detrending can be performed on RR data, which has little influence on the corresponding analysis. Nonlinear detrending could be harmful and it is not advisable to use this type of pre-processing. Exceptions do exist, but only combined with other appropriate techniques to avoid complete change of the signal's intrinsic dynamics.
One submitted publication.

7.6. Quantification of Heart's Recover by Multiscale Complexity Analysis of Heart Rate: a Validation Study

Participants: Binbin Xu, Hussein Yahia, Rémi Dubois.

Background : Heart rate analysis is the common analysis of heart's function. After the drug treatment of cardiac arrhythmia, the heart rate looks like the same as the group with normal sinus rhythm.

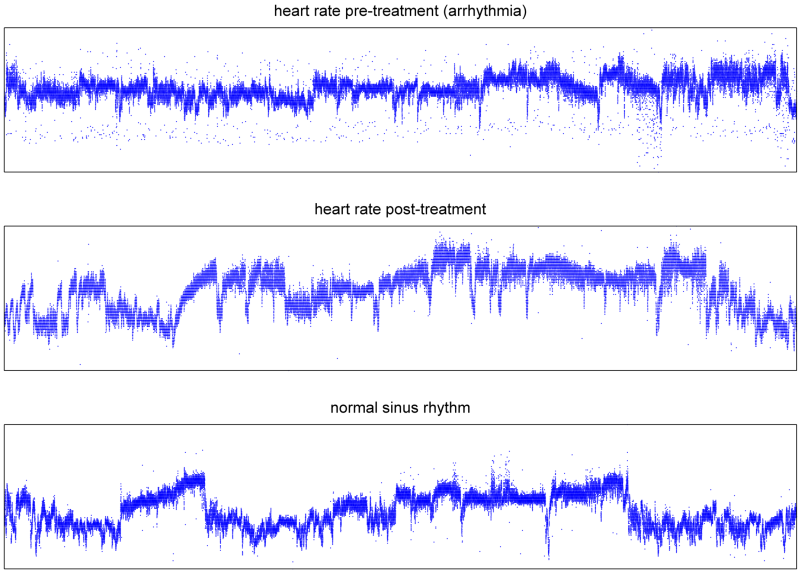


Figure 4. Heart rate RR time series in three cases : (1) arrhythmia, pre-treatment; (2) arrhythmia suppressed, post-treatment; (3) normal healthy group.

Problem : However, the visibly "same dynamics" for post-treatment & normal group does not reflect the true intrinsic dynamics of the heart. **Methods** : Using multi-scale complexity analysis to quantify and qualify the heart rate's dynamics.

Results : Thought the analysis shown in time domain that the dynamics of post-treatment and normal group looked similar. Their dynamics is completely different : (1) for normal heart rate, the multiscale fractal dimension is almost linearly decreased – invariance; (2) for arrhythmic heart rate before and after treatment, they converged to a certain value. All these suggested that item after the drug treatments, the heart's function is not still fully restored and more recovering time is needed. The multiscale complexity analysis can be used to quantify the heart function's recovering and optimize the post-treatment.
One submitted publication.

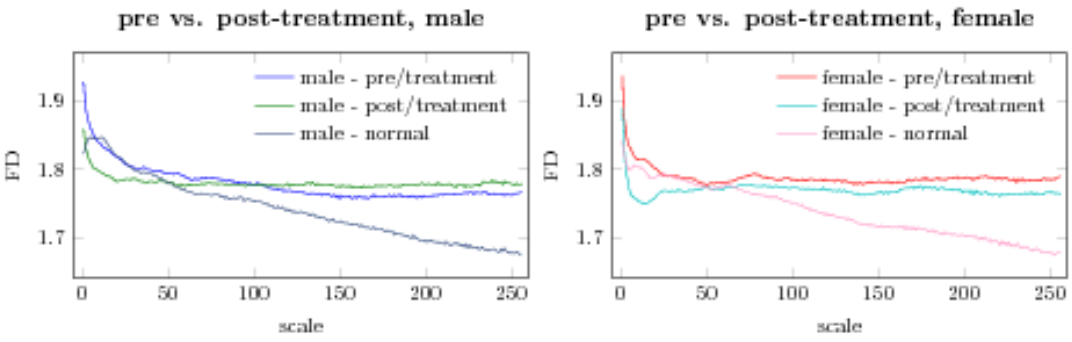


Figure 5. Analysis of heart rate variation by multiscale (coarse-graining) fractal dimension

7.7. Quantification and Its Approximate Solution of Action Potential in Neuron Models by Anharmonicity Analysis

Participants: Binbin Xu, Hussein Yahia, Rémi Dubois.

Action potential (AP) plays an important role to initiate and maintain the cell-cell communication. The nerve impulses are extensively studied but the action potential is less investigated as in other types of cells (for example, cardiac action potential). The AP can tell more about the state of the cell. It reflects the physical / chemical intracellular exchanges. Any changes in the cell would change the form/geometry of AP, or a more relevant term the *harmony*. The intrinsic changes would modify the harmony of the impulses train. The broken harmony (form/geometry change) of the impulse train means that there would be some problems in the cell. This provides an indirect way to study the intrinsic dynamics the cells.

In the work of P. Hanusse proposed a very interesting signal analyzing approach by anharmonicity, especially for signals with nonlinear oscillations properties exhibited in many physical / biological systems. This is exactly the case for neuron impulses trains. The principle is to describing the signal with their harmonic behaviors by solving the nonlinear phase equation. The obtained phase is thus used to reconstruct a solution of the original signal. The key notion is the nonlinear trigonometry that they developed. According to this approach, for any periodic signal $x(t) = x_0 + x_1 \cos(\phi(t))$, its phase can be obtained by the proposed general solution $t(\phi) = \phi + \sum_{k=1}^{n} a_k \mathrm{hpsin}_1(\phi - p_k, r_k) - b_k \mathrm{hpcos}_1(\phi - p_k, r_k)$ which can be used to reconstruct the original signal $x(t)$.

There is no practical implementation in their papers. Here we propose a first order solution of the original analytical equation. It can be used to quantify the harmonicity of the action potential.

$$\mathrm{hpsin}_1 = \frac{-i\left(-\ln\left(1-\mathrm{e}^{it}r\right)+\ln\left(1-r\mathrm{e}^{-it}\right)\right)}{2\,r},\quad \mathrm{hpcos}_1 = -\frac{\ln\left(1-\mathrm{e}^{it}r\right)+\ln\left(1-r\mathrm{e}^{-it}\right)}{2\,r}$$

The phase of a signal can be solved as : $\phi(t) = t - t_0 + a_1 \mathrm{hpsin}_1(t - t_1, r) - a_2 \mathrm{hpsin}_1(t - t_2, r)$, so the signal can be reconstructed as $x(t) = \cos(\phi(t))$. The related parameters can be obtained by regression or nonlinear optimization methods. In consequence, all AP can be quantified by the anharmonicity parameter r.

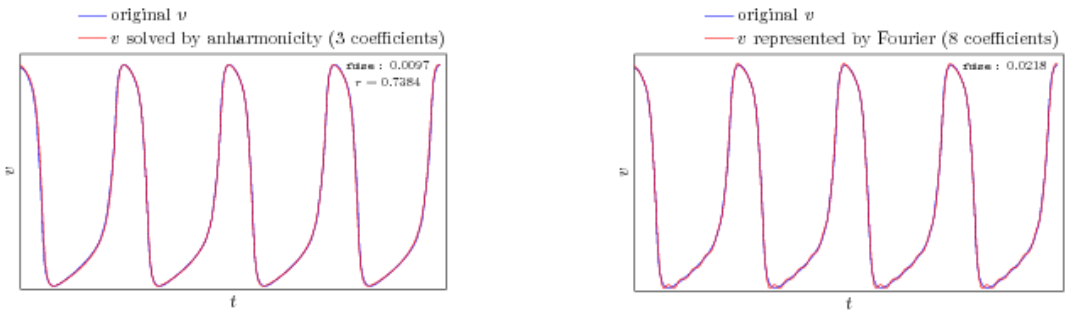


Figure 6. Quantification of action potential in FitzHugh-Nagumo (FHN) model by anharmonicity analysis

FitzHugh-Nagumo (FHN) model has been one of the basic models to study the action potential's dynamics. It's derived from the Hodgkin-Huxley model and is physiologically correct. We take here dynamics of APs from FHN model to illustrate the anharmonicity analysis. As shown in the following figure, anharmonicity analysis is far more efficient than Fourier representation. Even with 8 Fourier terms, the signal is ill-represented with Gibbs phenomena. In contrast, 3 anharmonic terms exhibit a quasi-identical fit. These AP are quantified with an anharmonicity $r = 0.7384$.

More development of anharmonicity analysis on AP is ongoing in order to provide a more efficient way to generalize the practices and for better solutions. We believe that anharmonicity analysis can help to quantify/qualify the AP in a different yet efficient way than conventional analysis.
One submitted publication.

7.8. Image Reconstruction from Highly Corrupted Gradients

Participants: Hicham Badri, Hussein Yahia, Driss Aboutajdine.

Surface-from-Gradients (SfG) is an important step in many imaging applications. It consists in reconstructing an image/surface from corrupted gradient fields, which results in an ill-posed problem. We propose to use sparsity to regularize the problem. The first approach uses sparsity in the gradient field together with a robust norm on the data-fitting term and was presented at CVPR 2014. The new approach uses a non-local regularization that manipulates non-local similar patches of the corrupted gradient and forcing them to be low-rank. The two approaches significantly outperform previous optimization-based SfG methods on both synthetic and real data.
One submitted publication.

7.9. Fast Image Edge-Aware Processing

Participants: Hicham Badri, Hussein Yahia, Driss Aboutajdine.

We present a framework for fast edge-aware processing of images and videos. This is an extension of our previous SIGGRAPH Asia 2013 paper. The proposed approach uses non-convex sparsity on the gradients of the latent smooth image to better preserve sharp edges. We develop tools based on first order proximal estimation for fast processing. We also propose fast and efficient numerical solutions based on separable filters estimation, which enables our method to perform fast high-quality smoothing on large-scale images. Extensive experiments show that the proposed method produces high-quality smoothing compared to state-of-the-art methods, while being fast and simple to implement.
Publication: [15].

7.10. Low-Rankness Transfer for Realistic Denoising

Participants: Hicham Badri, Hussein Yahia.

Image restoration is a very challenging task in low-level vision and is extensively used in many imaging applications. Sparsity in various forms (dictionary learning, low-rank estimation,...) has shown to be the key for successful image denoising. However, the standard noise model used to validate the results is mainly Gaussian and uniform, with known standard deviation. Unfortunately, these assumptions do not hold for real camera noise. Instead of using sparsity to model the singular values of non-local clean similar patches, we use a learning model that trains a mapping between the noisy and ground-truth clean singular values. The training is performed on real camera noise, contrary to previous methods. Experiments show that the proposed method significantly outperforms previous denoising works on real non-uniform noise and does not require estimating the standard deviation of the corruption.
One publication accepted with minor revision at IEEE Transactions on Image Processing, publication date: 2016.

7.11. Turbulent Flow Estimation

Participants: Hicham Badri, Hussein Yahia.

We use singularity exponents (SE) to regularize the problem of turbulent flow estimation under the assumption that the brightness constancy constraint holds also for (SE). We also use weighted filtering (Lucas–Kanade's solution) and sparsity on the data-fitting term to improve robustness to outliers. The proposed motion estimation is built on a Gaussian pyramid and uses the theory of warping for a better estimation of large displacements. Experiments on synthetic data show that the proposed method outperforms sophisticated methods while being simple.

Work in progress.

7.12. Pathological voice classification

Participants: Khalid Daoudi, Nicolas Brodu.

Based on our GCI detection algorithm, we redefined the classical pitch perturbation measures that are widely used in voice quality assessment. We showed that our perturbation measures yield significantly better performance in pathological voice classification than classical measures. We also showed that some matching pursuit features can allow good performances in discrimination between pathological voice categories.
Publications: [31], [30].

7.13. Emotion detection: project with Batvoice start-up

Participants: Khalid Daoudi, Nicolas Brodu.

Geostat has been granted in 2015 a Carnot-Inria contact to fund a 1 year engineer to develop a prototype of a speech emotion detection system.

7.14. Heartbeat signal analysis: Proof of Concept with IHU LIRYC

Participants: Hussein Yahia, Guillaume Attuel, Oriol Pont, Binbin Xu.

Geostat has been granted in 2015 a fund from Inria DGT to conduct pre-clinical vlidation from patient database acquired by IHU LIRYC.

INOCS Team (section vide)

MISTIS Project-Team

7. New Results

7.1. Mixture models

7.1.1. Taking into account the curse of dimensionality

Participants: Stéphane Girard, Alessandro Chiancone, Seydou-Nourou Sylla.

Joint work with: C. Bouveyron (Univ. Paris 5), M. Fauvel (ENSAT Toulouse) and J. Chanussot (Gipsa-lab and Grenoble-INP)

In the PhD work of Charles Bouveyron (co-advised by Cordelia Schmid from the Inria LEAR team) [61], we proposed new Gaussian models of high dimensional data for classification purposes. We assume that the data live in several groups located in subspaces of lower dimensions. Two different strategies arise:

- the introduction in the model of a dimension reduction constraint for each group
- the use of parsimonious models obtained by imposing to different groups to share the same values of some parameters

This modelling yields a supervised classification method called High Dimensional Discriminant Analysis (HDDA) [4]. Some versions of this method have been tested on the supervised classification of objects in images. This approach has been adapted to the unsupervised classification framework, and the related method is named High Dimensional Data Clustering (HDDC) [3]. Our recent work consists in adding a kernel in the previous methods to deal with nonlinear data classification and heterogeneous data [13]. We first investigate the use of kernels derived from similary measures on binary data [30]. The targeted application is the analysis of verbal autopsy data (PhD thesis of N. Sylla): Indeed, health monitoring and evaluation make more and more use of data on causes of death from verbal autopsies in countries which do not keep records of civil status or with incomplete records. The application of verbal autopsy method allows to discover probable cause of death. Verbal autopsy has become the main source of information on causes of death in these populations. Second, the kernel classification method is applied to three real hyperspectral data sets,and compared with three others classifiers. The proposed models show good results in terms of classification accuracy and processing time [21].

7.2. Semi and non-parametric methods

7.2.1. Conditional extremal events

Participant: Stéphane Girard.

Joint work with: L. Gardes (Univ. Strasbourg), G. Mazo (Univ. Catholique de Louvain), J. Elmethni (Univ. Paris 5) and S. Louhichi (Univ. Grenoble 1)

The goal of the PhD theses of Alexandre Lekina and Jonathan El Methni was to contribute to the development of theoretical and algorithmic models to tackle conditional extreme value analysis, *ie* the situation where some covariate information X is recorded simultaneously with a quantity of interest Y. In such a case, the tail heaviness of Y depends on X, and thus the tail index as well as the extreme quantiles are also functions of the covariate. We combine nonparametric smoothing techniques [63] with extreme-value methods in order to obtain efficient estimators of the conditional tail index and conditional extreme quantiles. The strong consistency of such an estimator is established in [53]. When the covariate is functional and random (random design) we focus on kernel methods [23].

Conditional extremes are studied in climatology where one is interested in how climate change over years might affect extreme temperatures or rainfalls. In this case, the covariate is univariate (time). Bivariate examples include the study of extreme rainfalls as a function of the geographical location. The application part of the study is joint work with the LTHE (Laboratoire d'étude des Transferts en Hydrologie et Environnement) located in Grenoble [20] and the "département Génie urbain" of "Université Paris-Est Marne-la-vallée" [11].

7.2.2. Estimation of extreme risk measures

Participant: Stéphane Girard.

Joint work with: A. Daouia (Univ. Toulouse), E. Deme (Univ. Gaston-Berger, Sénégal), A. Guillou (Univ. Strasbourg) and G. Stupfler (Univ. Aix-Marseille).

One of the most popular risk measures is the Value-at-Risk (VaR) introduced in the 1990's. In statistical terms, the VaR at level $\alpha \in (0,1)$ corresponds to the upper α-quantile of the loss distribution. The Value-at-Risk however suffers from several weaknesses. First, it provides us only with a pointwise information: VaR(α) does not take into consideration what the loss will be beyond this quantile. Second, random loss variables with light-tailed distributions or heavy-tailed distributions may have the same Value-at-Risk . Finally, Value-at-Risk is not a coherent risk measure since it is not subadditive in general. A first coherent alternative risk measure is the Conditional Tail Expectation (CTE), also known as Tail-Value-at-Risk, Tail Conditional Expectation or Expected Shortfall in case of a continuous loss distribution. The CTE is defined as the expected loss given that the loss lies above the upper α-quantile of the loss distribution. This risk measure thus takes into account the whole information contained in the upper tail of the distribution. It is frequently encountered in financial investment or in the insurance industry. In [51], we have established the asymptotic properties of the CTE estimator in case of extreme losses, *i.e.* when $\alpha \to 0$ as the sample size increases. We have exhibited the asymptotic bias of this estimator, and proposed a bias correction based on extreme-value techniques. A second possible coherent alternative risk measure is based on expectiles [59]. Compared to quantiles, the family of expectiles is based on squared rather than absolute error loss minimization. The flexibility and virtues of these least squares analogues of quantiles are now well established in actuarial science, econometrics and statistical finance. Both quantiles and expectiles were embedded in the more general class of M-quantiles as the minimizers of a generic asymmetric convex loss function. It has been proved very recently that the only M-quantiles that are coherent risk measures are the expectiles.

7.2.3. Multivariate extremal events

Participants: Stéphane Girard, Florence Forbes.

Joint work with: F. Durante (Univ. Bolzen-Bolzano, Italy) L. Gardes (Univ. Strasbourg) and G. Mazo (Univ. Catholique de Louvain, Belgique).

Copulas are a useful tool to model multivariate distributions [67].

However, while there exist various families of bivariate copulas, much fewer has been done when the dimension is higher. To this aim an interesting class of copulas based on products of transformed copulas has been proposed in the literature. The use of this class for practical high dimensional problems remains challenging. Constraints on the parameters and the product form render inference, and in particular the likelihood computation, difficult. We proposed a new class of high dimensional copulas based on a product of transformed bivariate copulas [26]. No constraints on the parameters refrain the applicability of the proposed class which is well suited for applications in high dimension. Furthermore the analytic forms of the copulas within this class allow to associate a natural graphical structure which helps to visualize the dependencies and to compute the likelihood efficiently even in high dimension. The extreme properties of the copulas are also derived and an R package has been developed.

As an alternative, we also proposed a new class of copulas constructed by introducing a latent factor. Conditional independence with respect to this factor and the use of a nonparametric class of bivariate copulas lead to interesting properties like explicitness, flexibility and parsimony. In particular, various tail behaviours are exhibited, making possible the modeling of various extreme situations [19], [27], [52]. A pairwise moment-based inference procedure has also been proposed and the asymptotic normality of the corresponding estimator has been established [28].

In collaboration with L. Gardes, we investigate the estimation of the tail copula, which is widely used to describe the amount of extremal dependence of a multivariate distribution. In some situations such as risk management, the dependence structure can be linked with some covariate. The tail copula thus depends on this covariate and is referred to as the conditional tail copula. The aim of our work is to propose a nonparametric estimator of the conditional tail copula and to establish its asymptotic normality [22].

7.2.4. Level sets estimation

Participant: Stéphane Girard.

Joint work with: G. Stupfler (Univ. Aix-Marseille)

The boundary bounding the set of points is viewed as the larger level set of the points distribution. This is then an extreme quantile curve estimation problem. We proposed estimators based on projection as well as on kernel regression methods applied on the extreme values set, for particular set of points [10]. We also investigate the asymptotic properties of existing estimators when used in extreme situations. For instance, we have established in collaboration with G. Stupfler that the so-called geometric quantiles have very counter-intuitive properties in such situations [24], [25] and thus should not be used to detect outliers.

7.2.5. Retrieval of Mars surface physical properties from OMEGA hyperspectral images.

Participants: Stéphane Girard, Alessandro Chiancone.

Joint work with: J. Chanussot (Gipsa-lab and Grenoble-INP).

Visible and near infrared imaging spectroscopy is one of the key techniques to detect, to map and to characterize mineral and volatile (eg. water-ice) species existing at the surface of planets. Indeed the chemical composition, granularity, texture, physical state, etc. of the materials determine the existence and morphology of the absorption bands. The resulting spectra contain therefore very useful information. Current imaging spectrometers provide data organized as three dimensional hyperspectral images: two spatial dimensions and one spectral dimension. Our goal is to estimate the functional relationship F between some observed spectra and some physical parameters. To this end, a database of synthetic spectra is generated by a physical radiative transfer model and used to estimate F. The high dimension of spectra is reduced by Gaussian regularized sliced inverse regression (GRSIR) to overcome the curse of dimensionality and consequently the sensitivity of the inversion to noise.
In his PhD thesis work, Alessandro Chiancone studies the extension of the SIR method to different sub-populations. The idea is to assume that the dimension reduction subspace may not be the same for different clusters of the data [14].

7.2.6. Robust Sliced Inverse Regression.

Participants: Stéphane Girard, Alessandro Chiancone, Florence Forbes.

Sliced Inverse Regression (SIR) has been extensively used to reduce the dimension of the predictor space before performing regression. Recently it has been shown that this techniques is, not surprisingly, sensitive to noise. Different approaches has been proposed to robustify SIR, in this work, we start considering an inverse problem proposed by R.D. Cook and we show that the framework can be extended to take into account a non-Gaussian noise. Generalized Student distribution are considered and all parameters are estimated via EM algorithm. The algorithm is outlined and tested comparing the results with different approaches on simulated data. Results on a real dataset shows the interest of this technique in presence of outliers.

7.2.7. Robust Locally linear mapping with mixtures of Student distributions

Participants: Florence Forbes, Emeline Perthame, Brice Olivier, Leo Nicoletti.

The standard GLLiM model [17] for high dimensional regression assumes Gaussian noise models and is in its unconstrained version equivalent to a joint GMM. The fact that response and independent variables (X, Y) are jointly a mixture of Gaussian distribution is the key for all derivations in the model. In this work, we show that similar developments are possible based on a joint Student Mixture model, joint SMM. It follows a new model referred to as SLLiM for Student Locally linear mapping for which we investigate the robustness to outlying data in a high dimensional regression context.

7.3. Markov models

7.3.1. Change-point models for tree-structured data

Participant: Jean-Baptiste Durand.

Joint work with: Pierre Fernique (Inria) and Yann Guédon (CIRAD), Inria Virtual Plants.

In the context of plant growth modelling, methods to identify subtrees of a tree or forest with similar attributes have been developed. They rely either on hidden Markov modelling or multiple change-point approaches. The latter are well-developed in the context of sequence analysis, but their extensions to tree-structured data are not straightforward. Their advantage on hidden Markov models is to relax the strong constraints regarding dependencies induced by parametric distributions and local parent-children dependencies. Heuristic approaches for change-point detection in trees were proposed and applied to the analysis of patchiness patterns (consisting of canopies made of clumps of either vegetative or flowering botanical units) in mango trees [45].

7.3.2. Hidden Markov models for the analysis of eye movements

Participants: Jean-Baptiste Durand, Brice Olivier.

This research theme is supported by a LabEx PERSYVAL-Lab project-team grant.

Joint work with: Marianne Clausel (LJK) Anne Guérin-Dugué (GIPSA-lab) and Benoit Lemaire (Laboratoire de Psychologie et Neurocognition)

In the last years, GIPSA-lab has developed computational models of information search in web-like materials, using data from both eye-tracking and electroencephalograms (EEGs). These data were obtained from experiments, in which subjects had to make some kinds of press reviews. In such tasks, reading process and decision making are closely related. Statistical analysis of such data aims at deciphering underlying dependency structures in these processes. Hidden Markov models (HMMs) have been used on eye movement series to infer phases in the reading process that can be interpreted as steps in the cognitive processes leading to decision. In HMMs, each phase is associated with a state of the Markov chain. The states are observed indirectly through eye-movements. Our approach was inspired by Simola *et al.* (2008) [68], but we used hidden semi-Markov models for better characterization of phase length distributions. The estimated HMM highlighted contrasted reading strategies (i.e., state transitions), with both individual and document-related variability.

However, the characteristics of eye movements within each phase tended to be poorly discriminated. As a result, high uncertainty in the phase changes arose, and it could be difficult to relate phases to known patterns in EEGs.

This is why, as part of Brice Olivier's PhD thesis, we are developing integrated models coupling EEG and eye movements within one single HMM for better identification of the phases. Here, the coupling should incorporate some delay between the transitions in both (EEG and eye-movement) chains, since EEG patterns associated to cognitive processes occur lately with respect to eye-movement phases. Moreover, EEGs and scanpaths were recorded with different time resolutions, so that some resampling scheme must be added into the model, for the sake of synchronizing both processes.

7.3.3. Lossy compression of tree structures

Participant: Jean-Baptiste Durand.

Joint work with: Christophe Godin (Inria, Virtual Plants) and Romain Azais (Inria BIGS)

In a previous work [65], a method to compress tree structures and to quantify their degree of self-nestedness was developed. This method is based on the detection of isomorphic subtrees in a given tree and on the construction of a DAG (Directed Acyclic Graph), equivalent to the original tree, where a given subtree class is represented only once (compression is based on the suppression of structural redundancies in the original tree). In the lossless compressed graph, every node representing a particular subtree in the original tree has exactly the same height as its corresponding node in the original tree. A lossy version of the algorithm consists in coding the nearest self-nested tree embedded in the initial tree. Indeed, finding the nearest self-nested tree of a structure without more assumptions is conjectured to be an NP-complete or NP-hard problem. We improved this lossy compression method by computing a self-nested reduction of a tree that better approximates the initial tree. The algorithm has polynomial time complexity for trees with bounded outdegree. This approximation relies on an indel edit distance that allows (recursive) insertion and deletion of leaf vertices only. We showed in a conference paper accepted at DCC'2016 [55] with a simulated dataset that the error rate of this lossy compression method is always better than the loss based on the nearest embedded self-nestedness tree [65] while the compression rates are equivalent. This procedure is also a keystone in our new topological clustering algorithm for trees. In addition, we obtained new theoretical results on the combinatorics of self-nested structures. The redaction of an article is currently in progress.

7.4. Statistical models for Neuroscience

7.4.1. Comparison of stochastic and variational solutions to ASL fMRI data analysis

Participants: Florence Forbes, Aina Frau Pascual.

Joint work with: Philippe Ciuciu from Team Parietal and Neurospin, CEA Saclay.

Functional Arterial Spin Labeling (fASL) MRI can provide a quantitative measurement of changes of cerebral blood flow induced by stimulation or task performance. fASL data is commonly analysed using a general linear model (GLM) with regressors based on the canonical hemodynamic response function. In this work [37], we consider instead a joint detection-estimation (JDE) framework which has the advantage of allowing the extraction of both task-related perfusion and hemodynamic responses not restricted to canonical shapes. Previous JDE attempts for ASL have been based on computer intensive sampling (MCMC) methods. Our contribution is to provide a comparison with an alternative variational expectation-maximization (VEM) algorithm on synthetic and real data. Other investigations were related to the use of appropriate physiological information and priors [39], [38].

7.4.2. A differential evolution-based approach for fitting a nonlinear biophysical model to fMRI BOLD data

Participants: Florence Forbes, Pablo Mesejo.

Joint work with: Jan Warnking from Grenoble Institute of Neuroscience.

Physiological and biophysical models have been proposed to link neuronal activity to the Blood Oxygen Level-Dependent (BOLD) signal in functional MRI (fMRI). Those models rely on a set of parameter values that cannot always be extracted from the literature. In some applications, interesting insight into the brain physiology or physiopathology can be gained from an estimation of the model parameters from measured BOLD signals. This estimation is challenging because there are more than 10 potentially interesting parameters involved in nonlinear equations and whose interactions may result in identifiability issues. However, the availability of statistical prior knowledge about these parameters can greatly simplify the estimation task. In this work we focus on the extended Balloon model and propose the estimation of 15 parameters using two stochastic approaches: an Evolutionary Computation global search method called Differential Evolution (DE)

and a Markov Chain Monte Carlo version of DE. To combine both the ability to escape local optima and to incorporate prior knowledge, we derive the target function from Bayesian modeling. The general behavior of these algorithms is analyzed and compared with the *de facto* standard Expectation Maximization Gauss-Newton (EM/GN) approach, providing very promising results on challenging real and synthetic fMRI data sets involving rats with epileptic activity. These stochastic optimizers provided a better performance than EM/GN in terms of distance to the ground truth in 4 out of 6 synthetic data sets and a better signal fitting in 12 out of 12 real data sets. Non-parametric statistical tests showed the existence of statistically significant differences between the real data results obtained by DE and EM/GN. Finally, the estimates obtained from DE for these parameters seem both more realistic and more stable or at least as stable across sessions as the estimates from EM/GN. This work will appear in [29]. A preliminary version has also been accepted at the conference MICCAI 2015 [40].

7.4.3. Multi-subject joint parcelation detection estimation in functional MRI

Participant: Florence Forbes.

Joint work with: Lotfi Chaari, Mohanad Albughdadi, Jean-Yves Tourneret from IRIT-ENSEEIHT in Toulouse and Philippe Ciuciu from Neurospin, CEA Saclay.

fMRI experiments are usually conducted over a population of interest for investigating brain activity across different regions, stimuli and subjects. Multi-subject analysis usually proceeds in two steps: an intra-subject analysis is performed sequentially on each individual and then a group-level analysis is carried out to report significant results at the population level. This work considers an existing Joint Parcellation Detection Estimation (JPDE) model which performs joint hemodynamic parcellation, brain dynamics estimation and evoked activity detection. The hierarchy of the JPDE model is extended for multi-subject analysis in order to perform group-level parcellation. Then, the corresponding underlying dynamics is estimated in each parcel while the detection and estimation steps are iterated over each individual. Validation on synthetic and real fMRI data shows its robustness in inferring group-level parcellation and the corresponding hemodynamic profiles. This work has been accepted at ISBI 2016.

7.4.4. Tumor classification and prediction using robust multivariate clustering of multiparametric MRI

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Emmanuel Barbier and Benjamin Lemasson from Grenoble Institute of Neuroscience.

Advanced statistical clustering approaches are promising tools to better exploit the wealth of MRI information especially on large cohorts and multi-center studies. In neuro-oncology, the use of multiparametric MRI may better characterize brain tumor heterogeneity. To fully exploit multiparametric MRI (e.g. tumor classification), appropriate analysis methods are yet to be developed. They offer improved data quality control by allowing automatic outlier detection and improved analysis by identifying discriminative tumor signatures with measurable predictive power. In this work, we show on small animals data that advanced statistical learning approaches can help 1) in organizing existing data by detecting and excluding outliers and 2) in building a dictionary of tumor fingerprints from a clustering analysis of their microvascular features. The work also now includes the integration in a joint statistical model of both automatic ROI delineation and clustering for whole brain data analysis. A preliminary version of this work has been accepted to the ISMRM 2015 conference and in the SFMRMB 2015 conference [41].

7.4.5. Functional specifications of a brain segmentation software

Participants: Florence Forbes, Priscillia Previtero.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience and Senan Doyle from Pixyl.

The goal of P. Previtero's internship was to help with a number of software engineering tasks and communications actions around the P-Locus software and the Pixyl start-up. The internship resulted in particular in a new web site for Pixyl.

MODAL Project-Team

7. New Results

7.1. Functional data analysis applied to hydrological or environnemental data

Participant: Sophie Dabo.

The new results concern particularly functional data analysis applied to hydrological or environnemental data. First in a recent paper ([16]), two statistical techniques from the theory of functional data classification are adapted and applied for the analysis of flood hydrographs. Functional classification directly employs all data of a discharge time series and thus contains all available information on shape, peak, and timing. This potentially allows a better understanding and treatment of floods as well as other hydrological phenomena.

7.2. New functional regression model when data are auto-correlated

Participant: Sophie Dabo.

We develop a new functional regression model when data are auto-correlated, in collaboration with Serge Guillas (University of College London) and Camille Ternynck (University of Lille 2). This work will appear in Journal of Multivariate Analysis. (Dabo-Niang, S, Guillas, S et Ternynck, C. (2016). More efficient kernel functional spatial regression estimation with autocorrelated errors. *Journal of Multivariate Analysis*). In this work we introduce a new procedure for the estimation in the nonlinear functional regression model where the explanatory variable takes values in an abstract function space and the residual process is autocorrelated. The procedure consists in a pre-whitening transformation of the dependent variable based on the estimated autocorrelation. We establish both consistency and asymptotic normality of the regression function estimate. For kernel methods encountered in the literature, the correlation structure is commonly ignored (the so-called "working independence estimator"); we show here that there is a strong benefit in taking into account the autocorrelation in the error process. We also find that the improvement in efficiency can be large in our functional setting, up to 25% in the presence of high autocorrelation levels. Concerning spatial data, we develop a new spatial prediction method that takes into account the spatial dependence. This work will appear in Journal of Nonparametric Statistics (Dabo-Niang, Ternynck, C., Yao, A.-F. (2016). Nonparametric prediction in the multivariate spatial context. *Journal of Nonparametric Statistics*)

7.3. Differential gene expression analysis

Participant: Guillemette Marot.

The use of empirical Bayesian techniques implemented in the Bioconductor package `limma` has enabled to better understand Waldenstrom's macroglobulinemia. Gene Set enrichment analysis was also performed after differential analysis. The new findings in Biology have been published in [21].

7.4. Evolutionary clustering for categorical data

Participant: Julien Jacques.

This is a joint work with Md Abul Hasnat, Julien Velcin and Stephane Bonnevay (Univ. de Lyon).

An evolutionary clustering algorithm for categorical data has been developed, based on parametric links between multinomial mixture models. This model has been used to study the evolution of opinions in Twitter data. A Preprint of this work is available [54].

7.5. Clustering categorical functional data: Application to medical discharge letters

Participants: Cristian Preda, Cristina Preda, Vincent Vandewalle.

Categorical functional data represented by paths of a stochastic jump process are considered for clustering. For paths of the same length, the extension of the multiple correspondence analysis allows the use of well-known methods for clustering finite dimensional data. When the paths are of different lengths, the analysis is more complex. In this case, for Markov models we have proposed an EM algorithm to estimate a mixture of Markov processes. This work has been presented in a conference [34].

7.6. Degeneracy in Gaussian Mixtures with missing data

Participants: Christophe Biernacki, Vincent Vandewalle.

The missing data problem is well-known for statisticians but its frequency increases with the growing size of modern datasets. In Gaussian model-based clustering, the EM algorithm easily takes into account such data by dealing with two kinds of latent levels: the components and the variables. However, the quite familiar degeneracy problem in Gaussian mixtures is aggravated during the EM runs. Indeed, numerical experiments clearly reveal that degeneracy is quite slow and also more frequent than with complete data. In practice, such situations are difficult to detect efficiently. Consequently, degenerated solutions may be confused with valuable solutions and, in addition, computing time may be wasted through wrong runs. A simple condition on the latent partition to avoid degeneracy has been exhibited, and a constrained version of the Stochastic EM (SEM) algorithm satisfying this condition has been proposed. This work has been presented in a conference [33].

7.7. Model for conditionally correlated categorical data

Participants: Christophe Biernacki, Vincent Vandewalle, Matthieu Marbac-Lourdelle.

An extension of the latent class model is proposed for clustering categorical data by relaxing the classical class conditional independence assumption of variables. In this model (called CCM for Conditional Correlated Model), variables are grouped into inter-independent and intra-dependent blocks in order to consider the main intra-class correlations. The dependence between variables grouped into the same block is taken into account by mixing two extreme distributions, which are respectively the independence and the maximum dependence ones. In the conditionally correlated data case, this approach is expected to reduce biases involved by the latent class model and to produce a meaningful model with few additional parameters. The parameters estimation by maximum likelihood is performed by an EM algorithm while a MCMC algorithm avoiding combinatorial problems involved by the block structure search is used for model selection. Applications on sociological and biological data sets bring out the proposed model interest. These results strengthen the idea that the proposed model is meaningful and that biases induced by the conditional independence assumption of the latent class model are reduced. This work is published [20] . Furthermore, an R package (Clustericat) is available on Rforge(see https://github.com/rforge/clustericat).

7.8. Model-based clustering for multivariate partial ordinal data

Participants: Christophe Biernacki, Julien Jacques.

We design the first univariate probability distribution for ordinal data which strictly respects the ordinal nature of data. More precisely, it relies only on order comparisons between modalities, the proposed distribution being obtained by modeling the data generating process which is assumed, from optimality arguments, to be a stochastic binary search algorithm in a sorted table. The resulting distribution is natively governed by two meaningful parameters (position and precision) and has very appealing properties: decrease around the mode, shape tuning from uniformity to a Dirac, identifiability. Moreover, it is easily estimated by an EM algorithm since the path in the stochastic binary search algorithm is missing. Using then the classical latent class assumption, the previous univariate ordinal model is straightforwardly extended to model-based clustering for multivariate ordinal data. Again, parameters of this mixture model are estimated by an EM algorithm. Both simulated and real data sets illustrate the great potential of this model by its ability to parsimoniously identify particularly relevant clusters which were unsuspected by some traditional competitors. This work is now published in an international journal [12] and is also currently available in the MixtComp software at https://modal-research.lille.inria.fr/BigStat/

7.9. Semi-Linear Auto-Associative Model

Participant: Serge Iovleff.

We design a new model for data analysis which is a generalization of the probabilistic PCA. The interpretation properties of the PCA are preserved while presence of non-linear repartitions in data can be detected and adjusted using B-spline regression. This model has been published in [18].

REALOPT Project-Team

7. New Results

7.1. Improving Branch-and-Price Methods

We have made progress on stabilization techniques and math-heuristics that have become essential components for Branch-and-Price methods.
Smoothing and proximal methods based on penalizing the deviation from the incumbent dual solution have become standards of the domain. Interpreting column generation as cutting plane strategies in the dual problem, we analyze in [26] the mechanisms on which stabilization relies. In particular, the link is established between smoothing and in-out separation strategies to derive generic convergence properties. For penalty function methods as well as for smoothing, we describe proposals for parameter self-adjusting schemes. Such schemes make initial parameter tuning less of an issue as corrections are made dynamically. Such adjustments also allow to adapt the parameters to the phase of the algorithm. We provide extensive test reports that validate our self-adjusting parameter scheme and highlight their performances. Our results also show that using smoothing in combination with penalty function yields a cumulative effect on convergence speed-ups.
Effects of stabilization techniques can be seen in practice. Routing and logistics applications are often viewed as intractable for exact optimization tools. Although such problems are naturally suited for a decomposition approach, branch-and-price-and-cut algorithms of the literature typically do not scale to the size of real-life instances. Some recent progress in stabilization techniques amongst other advances (such as diving heuristics, strong branching, and the combination with cutting plane approaches) generate new ambitions for column generation approach in solving approximately very large scale instances. Let us for instance point to the new benchmarks for the Capacitated Vehicle Routing Problem (CVRP) in [62]. The paper [24] illustrates this trend, showing exact results for freight transportation instances of a scale never considered before. Our column generation algorithm yields dual bounds and serves as the core procedure for a primal heuristic. The overal procedure is quite competitive in great part due to the convergence speed-ups resulting from efficient stabilization schemes. It typically provides optimal solutions as primal and dual bounds tend to be equal. The very large scale freight transportation instances (with up to 1,025 stations, 5,300 demands, and 12,651 rail cars) were submitted to us by our Russian partner Freight-One.
Math-heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending generic MIP heuristics, our study in [28] outlines generic procedures to build primal solutions in the context of a Branch-and-Price approach and reports on their performance. Rounding the linear relaxation solution of the Dantzig-Wolfe reformulation, which is typically tighter than that of the original compact formulation, sometimes produces better solutions than state-of-the-art specialised heuristics as revealed by our numerical experiments. We focus on the so-called diving methods and their combination with diversification-intensification paradigms such as Limited Discrepancy Search, sub-MIPing, relaxation induced neighbourhood search, local branching, and strong branching. The dynamic generation of variables inherent to a column generation approach requires specific adaptation of heuristic paradigms. Our contribution lies in proposing 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.

7.2. Dual feasible functions

Dual-feasible functions have proved to be very effective for generating fast lower bounds and valid inequalities for integer linear programs with knapsack constraints. However, a significant limitation is that they are defined only for positive arguments. Extending the concept of dual-feasible function to the general domain and range R is not straightforward. In [10], we propose the first construction principles to obtain general functions with domain and range R, and we show that they lead to non-dominated maximal functions.

7.3. Allocation algorithms in Cloud platforms

In the context of service hosting in large-scale datacenters, we provide [11] a deep analysis of a cluster data trace recently released by Google and we focus on a number of questions which have not been addressed in previous studies. In particular, we describe the characteristics of job resource usage in terms of dynamics (how it varies with time), of correlation between jobs (identify daily and/or weekly patterns), and correlation inside jobs between the different resources (dependence of memory usage on CPU usage). From this analysis, we derive scalable formalizations of the allocation problem which encompass most job features. In [19], [22], we study one such model, where long-running services experience demand variations with a periodic (daily) pattern. Such services account for most of the overall CPU demand. This leads to an allocation problem where the classical Bin-Packing issue is augmented with the possibility to co-locate jobs whose peaks occur at different times of the day, which is bound to be more efficient than the usual approach that consists in over-provisioning for the maximum demand. We propose mathematical formulations, column generation approaches, and analyze their performance compared to standard packing heurisics (such as Best-Fit or First-Fit Decreasing). We show that taking periodicity of demand into account allows for a substantial improvement on machine utilization in the context of large-scale, state-of-the-art production datacenters, and that column generation allows to obtain quasi-optimal solutions in reasonable time.

7.4. Scheduling and placement for HPC

With the complexification of the architecture of HPC nodes (multicores, non uniform memory access, GPU and accelerators), a recent trend in application development is to explicitely express the computations as a task graph, and rely on a specialized middleware stack to make scheduling decisions and implement them. Traditional algorithms used in this community are dynamic heuristics, to cope with the unpredictability of execution times. In [17], [18] we analyze the performance of static and hybrid strategies, obtained by adding more static (resp. dynamic) features into dynamic (resp. static) strategies. Our conclusions are somehow unexpected in the sense that we prove that static-based strategies are very efficient, even in a context where performance estimations are not very good.

Another study [13] focuses on the memory-constrained case, where tasks may produce large data. A task can only be executed if all input and output data fit into memory, and a data can only be removed from memory after the completion of the task that uses it as an input data. Trees of such tasks arise in the multifrontal method of sparse matrix factorization. Minimizing the peak memory required on a single processor is well studied, [13] extends the problem to multiple processors, where both makespan and memory need to be minimized. We study the computational complexity of this problem and provide inapproximability results even for unit weight trees. We design a series of practical heuristics achieving different trade-offs between the minimization of peak memory usage and makespan. Some of these heuristics are able to process a tree while keeping the memory usage under a given memory limit. The different heuristics are evaluated in an extensive experimental evaluation using realistic trees.

In [20], we perform another study of static, dynamic and hybrid strategies in the context of load balancing and data placement for matrix multiplication in heterogeneous machines. Through a set of extensive simulations, we analyze the behavior of static, dynamic, and hybrid strategies, and we assess the possible benefits of introducing more static knowledge and allocation decisions in runtime libraries. In [21], we consider the purely static problem, modeled as a partitioning of a square into a set of zones of prescribed areas, while minimizing the overall size of their projections onto horizontal and vertical axes. We combine two ideas from the literature (recursive partitioning, and optimal solution structure for low number of processors) to obtain a non-rectangular recursive partitioning (NRRP), whose approximation ratio is $\frac{2}{\sqrt{3}} \simeq 1.15$, improving over the previous 1.25 ratio. Moreover, we observe on a large set of realistic platforms built from CPUs and GPUs that this proposed NRRP algorithm allows to achieve very efficient partitionings on all considered cases.

7.5. Production scheduling

Together with Shunji Tanaka, from Kyoto University, we developed Lagrangian relaxation-based methods for solving min-sum shop scheduling problems. In our studies, large scale network flow formulations of the problems are suggested together with strong Lagrangian bounds based on these formulations.

In [23], we consider the flow-shop problem on two machines with sequence-independent setup times to minimize total completion time. To cope with the size of the network, filtering procedures are developed. To solve the problem to optimality, we embed the Lagrangian bounds into two branch-and-bound algorithms. The best algorithm is able to solve all 100-jobs instances of our testbed with and without setup times, thus significantly outperforming the best algorithms in the literature, which were limited to instances with 30 and 45 jobs respectively.

In [25], we propose a new dual bound for the job-shop problem with the objective of minimizing the sum of completion costs of the operations. The bound is obtained by a Lagrangian relaxation that decomposes the problem into two types of large network flow problems: one dealing with the precedence constraints among operations of a same job, and the other one satisfying the disjunctive constraints related to the machines. Numerical experiments on the just-in-time job-shop problem show that the method is able to improve the existing lower bounds significantly.

7.6. Clustering problems

Clustering problems, and in particular partitionning problems, are widespread in combinatorial optimization. The goal is to partition a set of items in subset satisfying various constraints such as knapsack constraints, cardinality constraints, connectivity constraints, and so on. Beside the PhD thesis of Jérémy Guillot that aims to develop aggregating techniques to handles large scale instances for partitionning problems, the team also study some particular versions.

In [15] we present the application of branch-and-price approaches to the automatic version of the Software Clustering Problem. To tackle this problem, we apply the Dantzig-Wolfe decomposition to a formulation from literature. Given this, we present two Column Generation (CG) approaches to solve the linear programming relaxation of the resulting reformulation: the standard CG approach, and a new approach, which we call Staged Column Generation (SCG). Also, we propose a modification to the pricing subproblem that allows to add multiple columns at each iteration of the CG. We test our algorithms in a set of 45 instances from the literature. The proposed approaches were able to improve the literature results solving all these instances to optimality. Furthermore, the SCG approach presented a considerable performance improvement regarding computational time, number of iterations and generated columns when compared with the standard CG as the size of the instances grows.

In collaboration with researchers from University Paris 6 and Paris 13, we also study the problem of partitionning a geographical area in connected parcels. A first step of this study was to cut the area in two connected parcels while minimizing the dissimilarities inside each parcels. Such partitionning is also called a bond. It happens that in series-parallel garph, a bond correspond to a circuit in the dual graph. In [12], we give a full description of the circuit polytope on series–parallel graphs. We first show the existence of a compact extended formulation. Though not being explicit, its construction process helps us to inductively provide the description in the original space. As a consequence, using the link between bonds and circuits in planar graphs, we also describe the bond polytope on series–parallel graphs.

7.7. Tour scheduling with multi-skill heterogeneous workforce

In [14], we address a multi-activity tour scheduling problem with time varying demand. The objective is to compute a team schedule for a fixed roster of employees in order to minimize the over-coverage and the under-coverage of different parallel activity demands along a planning horizon of one week. Numerous complicating constraints are present in our problem: all employees are different and can perform several different activities during the same day-shift, lunch breaks and pauses are flexible, demand is given for 15 minutes periods. Employees have feasibility and legality rules to be satisfied, but the objective function does not account for any quality measure associated with each individual's schedule. More precisely, the problem mixes simultaneously

days-off scheduling, shift scheduling, shift assignment, activity assignment, pause and lunch break assignment. To solve this problem, we developed four methods: a compact Mixed Integer Linear Programming model, a branch-and-price like approach with a nested dynamic program to solve heuristically the subproblems, a diving heuristic and a greedy heuristic based on our subproblem solver. The computational results, based on both real cases and instances derived from real cases, demonstrate that our methods are able to provide good quality solutions in a short computing time. Our algorithms are now embedded in a commercial software, which is already in use in a mini-mart company.

7.8. Traffic routing in optical networks

In [16], we consider a multi-layer network design model arising from a real-life telecommunication application where traffic routing decisions imply the installation of expensive nodal equipment. Customer requests come in the form of bandwidth reservations for a given origin destination pair. Bandwidth demands are expressed as multiples of nominal granularities. Each request must be single-path routed. Grooming several requests on the same wavelength and multiplexing wavelengths in the same optical stream allow a more efficient use of network capacity. However, each addition or withdrawal of a request from a wavelength requires optical to electrical conversion and the use of cross-connect equipment with expensive ports of high densities. The objective is to minimize the number of required ports of the cross-connect equipment. We deal with backbone optical networks, therefore with networks with a moderate number of nodes (14 to 20) but thousands of requests. Further difficulties arise from the symmetries in wavelength assignment and traffic loading. Traditional multi-commodity network flow approaches are not suited for this problem. Instead, four alternative models relying on Dantzig-Wolfe and/or Benders' decomposition are introduced and compared. The formulations are strengthened using symmetry breaking restrictions, variable domain reduction, zero-one discretization of integer variables, and cutting planes. The resulting dual bounds are compared to the values of primal solutions obtained through hierarchical optimization and rounding procedures. For realistic size instances, our best approaches provide solutions with optimality gap of approximately 5% on average in around two hours of computing time.

7.9. Dense sphere packing

In [27], we consider the sphere packing problem in arbitrary dimension: what is the maximum fraction Δ_n of the Euclidean space $\mathbb{R}_n$ that can be covered by unit balls with pairwise disjoint interiors?

Δ_n is known for only for some small values of n , and when n grows, we only have lower bounds. A trivial lower bound states that for every n, $\Delta_n \geq 2^{-n}$. Minkowski and Hlwaka's Theorem (1905) improves this lower bound by a factor 2: $\Delta_n \geq 2 \times 2^{-n}$. Asymptotic improvements of this bound were obtained (from Rogers, 1947 up to Ball, 1992), all of them being of the form $\Delta_n \geq cn2^{-n}$ where c is a constant.

This problem has a natural reformulation in graph theoretic terms as follows: let G denote the graph whose vertices are the points of the Euclidean space and edges are pair of vertices at distance at most 2 one from the other. The independent sets of G are the sphere packings: so, finding a maximum-density sphere packing is the same as finding a maximum-density independent set in this infinite graph. By using graph theoretic arguments only, Krivelevich et al. established that $\Delta_n \geq 0.01n2^{-n}$ for sufficiently large n.

In a recent breakthrough, Venkatesh introduced the first superlinear improvement: there are infinitely many n such that $\Delta_n \geq cn \log\log n2^{-n}$, where c is a constant. Venkatesh's result is however non-constructive.

In this joint work with C. Bachoc and P. Moustrou, we give a constructive proof of Venkatesh's lower bound.

This study has been carried out with financial support from the French State, managed by the French National Research Agency (ANR) in the frame of the " Investments for the future " Programme IdEx Bordeaux - CPU (ANR-10-IDEX-03-02).

SELECT Project-Team

6. New Results

6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, Serge Cohen, Erwan Le Pennec, Pascal Massart, Kevin Bleakley.

The well-documented and consistent variable selection procedure in model-based cluster analysis and classification that Cathy Maugis (INSA Toulouse) designed during her PhD thesis in SELECT, makes use of stepwise algorithms which are painfully slow in high dimension. In order to circumvent this drawback, Gilles Celeux, in collaboration with Mohammed Sedki (Université Paris XI) and Cathy Maugis), proposed to sort the variables using a lasso-like penalization adapted to the Gaussian mixture model context. Using this ranking to select variables, they avoid the combinatory problem of stepwise procedures. After tests on challenging simulated and real data sets, their algorithm has shown encouraging performance. Moreover, the possibility to sort the variables with their marginal likelihoods is under study. The first results are encouraging, and this approach requires no regularization hyperparameters, and is much more rapid.

In collaboration with Jean-Michel Marin (Université de Montpellier) and Olivier Gascuel (LIRMM), Gilles Celeux has continued research aiming to select a short list of models rather a single model. This short list is declared to be compatible with the data using a p-value derived from the Kullback-Leibler distance between the model and the empirical distribution. Furthermore, the Kullback-Leibler distances at hand are estimated through nonparametric and parametric bootstrap procedures. Different strategies are compared through numerical experiments on simulated and real data sets.

Emilie Devijver, Yannig Goude and Jean-Michel Poggi have proposed a new methodology for customer segmentation, in the context of load profiles in energy consumption. The method is based on high-dimensional regression models which perform clustering and model selection at the same time. They have focused on uncovering classes corresponding to different regression models ,and compute clustering and model identification in each cluster simultaneously. They have shown the feasibility of the approach on a real data set of Irish customers.

Emilie Devijver has studied a dimension-reduction method for finite mixtures of multivariate response regression models in high-dimension. The size of the response and the number of predictors may exceed the sample size. She considers jointly predictor selection and rank reduction to obtain lower-dimensional approximations of parameter matrices. A penalty, for which the model selected by penalized likelihood satisfies an oracle inequality, is given.

The detection of change-points in a spatially or time-ordered data sequence is an important problem in many fields such as genetics and finance. Kevin Bleakley, with Gérard Biau (LSTA, Paris 6 University) and David Mason (University of Delaware), has found asymptotic distributions of statistics used to detect change-points, and developed methods to provide stopping criteria (model selection) for the number of change-points found.

6.2. Statistical learning methodology and theory

Participants: Gilles Celeux, Christine Keribin, Erwan Le Pennec, Michel Prenat, Solenne Thivin, Kevin Bleakley.

Gilles Celeux has started a collaboration with Jean-Patrick Baudry on strategies to avoid traps in the EM algorithm in mixture analysis. They analyze the effect of spurious local maximizers, and regularized algorithms to avoid such solutions. They show the link that exists between the degree of regularization and slope heuristics. Moreover, their strategy to initiate the EM algorithm, embedding the solution with K components and the starting position with $K+1$ components to avoid suboptimal solutions, has been proved to be efficient, and is extended to a more complex framework of latent block models.

In the context of algorithms that depend on distributed computing and collaborative inference, Kevin Bleakley, with with Gérard Biau (LSTA, Paris 6) and Benoït Cadre (ENS Rennes), have proposed a collaborative framework that aims to estimate the unknown mean θ of a random variable X. In the model they present, a certain number of calculation units, distributed across a communication network represented by a graph, participate in the estimation of θ by sequentially receiving independent data from X while exchanging messages via a stochastic matrix A defined over the graph. They give precise conditions on the matrix A under which the statistical precision of the individual units is comparable to that of a (gold standard) virtual centralized estimate, even though each unit does not have access to all of the data.

6.3. Reliability

Participants: Yves Auffray, Gilles Celeux, Florence Ducros, Patrick Pamphile, Jana Kalawoun.

Since June 2015, in the framework of a CIFRE convention with Nexter, Florence Ducros has commenced a thesis on the modeling of aging of vehicles, supervised by Gilles Celeux and Patrick Pamphile. This thesis should lead to designing an efficient maintenance strategy according to vehicle use profiles. It will involve the estimation of mixtures and competing risk models in a highly censored setting.

Janan Kalawoun has defended her thesis supervised by Gilles Celeux, Patrick Pamphile and Maxime Montaru (CEA) on the estimation of the battery State of Charge (SoC). For vehicles powered by an electric motor, SoC estimation is essential to guarantee vehicle autonomy, as well as safe utilization. The aim is to create a reliable SoC model to closely fit battery dynamics in embedded applications (e.g., electric vehicles). The SoC is modeled by a switching Markov state-space model. Parameters are estimated by combining the EM algorithm and particle filter methods. The model is validated using real-world electric vehicle data. This model has been proved to be highly superior to a simple state space model. The optimal number of battery modes is then identified, using model selection criteria such as AIC and BIC, which has proved to be superior to cross-validation in this particular context.

In the framework of a study on the dispatch availability of Dassault Aviation business jets, Yves Auffray and Gilles Celeux have contributed to methodology aiming to discover the root causes of reliability flaws.

6.4. Statistical analysis of genomic data

Participants: Gilles Celeux, Mélina Gallopin, Christine Keribin, Yann Vasseur.

Mélina Gallopin defended her thesis supervised by Gilles Celeux, Florence Jaffrezic and Andrea Rau (INRA, animal genetics department), This thesis was concerned with modeling and model selection in the analysis of RNA-seq data. Its highlights are the following:

- Presentation of a model selection criterion for model-based clustering of annotated gene expression data. This criterion is an ICL-like criterion taking into account annotation.
- An objective comparison of discrete and continuous modeling after transformations for RNA-seq data based on a comparison of likelihoods (possibly penalized) of the possible models.
- A block diagonal covariance selection method for high dimensional Gaussian graphical models. This non-asymptotic model selection procedure is supported by strong theoretical guarantees, based on an oracle inequality and a minimax lower bound. This work was in collaboration with Emilie Devijver.

The subject of Yann Vasseur's PhD Thesis, supervised by Gilles Celeux and Marie-Laure Martin-Magniette (INRA URGV), is the inference of a regulatory network on Transcriptions Factors (TFs), which are specific genes, of *Arabidopsis thaliana*. To that purpose, a transciptome dataset with a similar number of TFs and statistical units is available. The first aim consists of reducing the dimension of the network to avoid high-dimensional difficulties. Representing this network with a Gaussian graphical model, the following procedure has been defined:

1. *Selection step*: choose the set of TF regulators (supports) of each TF.
2. *Classification step*: deduce co-factors groups (TFs with similar expression levels) from these supports.

Thus, the reduced network would be built on the co-factors groups. Currently, several selection methods based on Gauss-LASSO and resampling procedures have been applied to the dataset. The study of stability and parameter calibration of these methods is in progress. The TFs are clustered with the Latent Block Model in a number of co-factor groups, selected with BIC or the exact ICL criterion.

In a collaboration with Marie-Laure Martin-Magniette, Cathy Maugis and Andrea Rau, Gilles Celeux has studied gene expression obtained from high-throughput sequencing technology. The focus is on the question of clustering gene expression profiles as a means to discover groups of co-expressed genes. A Poisson mixture model is proposed, using a rigorous framework for parameter estimation as well as for the choice of the appropriate number of clusters. They illustrate co-expression analyses using this approach on two real RNA-seq datasets. A set of simulation studies also compares the performance of the proposed model with that of several related approaches developed to cluster RNA-seq and serial analysis of gene expression data. The proposed method is implemented in the open-source R package `HTSCluster`, available on CRAN. It can now be compared with Gaussian mixtures obtained after relevant data transformations.

6.5. Model based-clustering for pharmacovigilance data

Participants: Gilles Celeux, Christine Keribin, Valérie Robert.

In collaboration with Pascale Tubert-Bitter, Ismael Ahmed and Mohamed Sedki, Gilles Celeux and Christine Keribin have started research concerning the detection of associations between drugs and adverse events in the framework of the PhD of Valerie Robert. At first, this team developed a model-based clustering inspired by latent block models, which consists of co-clustering rows and columns of two binary tables, imposing the same row ranking. This enables it to highlight subgroups of individuals sharing the same drug profile, and subgroups of adverse effects and drugs with strong interactions. Furthermore, some sufficient conditions are provided to obtain the identifiability of the model, and some results are shown for simulated data. This year, the exact ICL criterion has been extended to this double block latent model. Moreover, the possible added value of this model, compared with standard contingency table analysis, is currently under scrutiny.

SEQUEL Project-Team

7. New Results

7.1. Decision-making Under Uncertainty

7.1.1. Reinforcement Learning

Nonparametric multiple change point estimation in highly dependent time series [7]

Given a heterogeneous time-series sample, the objective is to find points in time, called change points, where the probability distribution generating the data has changed. The data are assumed to have been generated by arbitrary unknown stationary ergodic distributions. No modelling, independence or mixing assumptions are made. A novel, computationally efficient, nonparametric method is proposed, and is shown to be asymptotically consistent in this general framework. The theoretical results are complemented with experimental evaluations.

Explore no more: Improved high-probability regret bounds for non-stochastic bandits [26]

This work addresses the problem of regret minimization in non-stochastic multi-armed bandit problems, focusing on performance guarantees that hold with high probability. Such results are rather scarce in the literature since proving them requires a large deal of technical effort and significant modifications to the standard, more intuitive algorithms that come only with guarantees that hold on expectation. One of these modifications is forcing the learner to sample arms from the uniform distribution at least $\Omega(\sqrt{T})$ times over T rounds, which can adversely affect performance if many of the arms are suboptimal. While it is widely conjectured that this property is essential for proving high-probability regret bounds, we show in this paper that it is possible to achieve such strong results without this undesirable exploration component. Our result relies on a simple and intuitive loss-estimation strategy called Implicit eXploration (IX) that allows a remarkably clean analysis. To demonstrate the flexibility of our technique, we derive several improved high-probability bounds for various extensions of the standard multi-armed bandit framework. Finally, we conduct a simple experiment that illustrates the robustness of our implicit exploration technique.

First-order regret bounds for combinatorial semi-bandits [27]

We consider the problem of online combinatorial optimization under semi-bandit feedback, where a learner has to repeatedly pick actions from a combinatorial decision set in order to minimize the total losses associated with its decisions. After making each decision, the learner observes the losses associated with its action, but not other losses. For this problem, there are several learning algorithms that guarantee that the learner's expected regret grows as $O(\sqrt{T})$ with the number of rounds T. In this paper, we propose an algorithm that improves this scaling to $O(\sqrt{L * T})$, where L * T is the total loss of the best action. Our algorithm is among the first to achieve such guarantees in a partial-feedback scheme, and the first one to do so in a combinatorial setting.

Random-Walk Perturbations for Online Combinatorial Optimization [4]

We study online combinatorial optimization problems where a learner is interested in minimizing its cumulative regret in the presence of switching costs. To solve such problems, we propose a version of the follow-the-perturbed-leader algorithm in which the cumulative losses are perturbed by independent symmetric random walks. In the general setting, our forecaster is shown to enjoy near-optimal guarantees on both quantities of interest, making it the best known efficient algorithm for the studied problem. In the special case of prediction with expert advice, we show that the forecaster achieves an expected regret of the optimal order $O(\sqrt{n \log N})$ where n is the time horizon and N is the number of experts, while guaranteeing that the predictions are switched at most $O(\sqrt{n \log N})$ times, in expectation.

Qualitative Multi-Armed Bandits: A Quantile-Based Approach [32]

We formalize and study the multi-armed bandit (MAB) problem in a generalized stochastic setting, in which rewards are not assumed to be numerical. Instead, rewards are measured on a qualitative scale that allows for comparison but invalidates arithmetic operations such as averaging. Correspondingly, instead of characterizing an arm in terms of the mean of the underlying distribution, we opt for using a quantile of that distribution as a representative value. We address the problem of quantile-based online learning both for the case of a finite (pure exploration) and infinite time horizon (cumulative regret minimization). For both cases, we propose suitable algorithms and analyze their properties. These properties are also illustrated by means of first experimental studies.

Predicting the outcomes of every process for which an asymptotically accurate stationary predictor exists is impossible [30]

The problem of prediction consists in forecasting the conditional distribution of the next outcome given the past. Assume that the source generating the data is such that there is a stationary predictor whose error converges to zero (in a certainsense). The question is whether there is a universal predictor for all such sources, that is, a predictor whose error goes to zero if any of the sources that have this property is chosen to generate the data. This question is answered in the negative, contrasting a number of previously established positive results concerning related but smaller sets of processes.

Improved Regret Bounds for Undiscounted Continuous Reinforcement Learning [22]

We consider the problem of undiscounted reinforcement learning in continuous state space. Regret bounds in this setting usually hold under various assumptions on the structure of the reward andtransition function. Under the assumption that the rewards andtransition probabilities are Lipschitz, for 1-dimensional state space a regret bound of $\widetilde{O}(T^{\frac{3}{4}})$ after any T steps has been given by.Here we improve upon this result by using non-parametric kernel density estimation for estimating the transition probability distributions,and obtain regret bounds that depend on the smoothness of the transition probability distributions.In particular, under the assumption that the transition probability functions are smoothly differentiable, the regret bound is shown to be $\widetilde{O}(T^{\frac{2}{3}})$ asymptotically for reinforcement learning in 1-dimensional state space. Finally, we also derive improved regret bounds for higher dimensional state space.

Maximum Entropy Semi-Supervised Inverse Reinforcement Learning [9]

A popular approach to apprenticeship learning (AL) is to formulate itas an inverse reinforcement learning (IRL) problem. The MaxEnt-IRL algorithm successfully integrates the maximum entropy principleinto IRL and unlike its predecessors, it resolves theambiguity arising from the fact that a possibly large number of policies couldmatch the expert's behavior. In this paper, we study an AL setting in which inaddition to the expert's trajectories,a number of unsupervised trajectories is available. We introduce MESSI,a novel algorithm that combines MaxEnt-IRLwith principles coming from semi-supervised learning. In particular, MESSIintegrates the unsupervised data intothe MaxEnt-IRL framework using a pairwise penalty on trajectories. Empirical-results in a highway driving and grid-world problems indicate that MESSI is able to take advantage of the unsupervised trajectories and improve the performance ofMaxEnt-IRL.

Direct Policy Iteration with Demonstrations [12]

We consider the problem of learning the optimal policy of an unknown Markov decision process (MDP) when expert demonstrations are available along with interaction samples. We build on classification-based policy iteration to perform a seamless integration of interaction and expert data, thus obtaining an algorithm which can benefit from both sources of information at the same time. Furthermore , we provide a full theoretical analysis of the performance across iterations providing insights on how the algorithm works. Finally, we report an empirical evaluation of the algorithm and a comparison with the state-of-the-art algorithms.

Approximate Modified Policy Iteration and its Application to the Game of Tetris [8]

Modified policy iteration (MPI) is a dynamic programming (DP) algorithm that contains the two celebrated policy and value iteration methods. Despite its generality, MPI has not been thoroughly studied, especially its approximation form which is used when the state and/or action spaces are large or infinite. In this

paper, we propose three implementations of approximate MPI (AMPI) that are extensions of the well-known approximate DP algorithms: fitted-value iteration, fitted-Q iteration, and classification-based policy iteration. We provide error propagation analysis that unify those for approximate policy and value iteration. We develop the finite-sample analysis of these algorithms, which highlights the influence of their parameters. In the classification-based version of the algorithm (CBMPI), the analysis shows that MPI's main parameter controls the balance between the estimation error of the classifier and the overall value function approximation. We illustrate and evaluate the behavior of these new algorithms in the Mountain Car and Tetris problems. Remarkably, in Tetris, CBMPI outperforms the existing DP approaches by a large margin, and competes with the current state-of-the-art methods while using fewer samples.

7.1.2. Multi-arm Bandit Theory

Simple regret for infinitely many armed bandits [11]

We consider a stochastic bandit problem with infinitely many arms. In this setting, the learner has no chance of trying all the arms even once and has to dedicate its limited number of samples only to a certain number of arms. All previous algorithms for this setting were designed for minimizing the cumulative regret of the learner. In this paper, we propose an algorithm aiming at minimizing the simple regret. As in the cumulative regret setting of infinitely many armed bandits , the rate of the simple regret will depend on a parameter β characterizing the distribution of the near-optimal arms. We prove that depending on β, our algorithm is minimax optimal either up to a multiplicative constant or up to a log(n) factor. We also provide extensions to several important cases: when β is unknown, in a natural setting where the near-optimal arms have a small variance , and in the case of unknown time horizon.

Black-box optimization of noisy functions with unknown smoothness [20]

We study the problem of black-box optimization of a function f of any dimension, given function evaluations perturbed by noise. The function is assumed to be locally smooth around one of its global optima, but this smoothness is unknown. Our contribution is an adaptive optimization algorithm, POO or parallel optimistic optimization, that is able to deal with this setting. POO performs almost as well as the best known algorithms requiring the knowledge of the smoothness. Furthermore, POO works for a larger class of functions than what was previously considered, especially for functions that are difficult to optimize, in a very precise sense. We provide a finite-time analysis of POO's performance, which shows that its error after n evaluations is at most a factor of $\sqrt{\ln n}$ away from the error of the best known optimization algorithms using the knowledge of the smoothness.

Cheap Bandits [21]

We consider stochastic sequential learning problems where the learner can observe the average reward of several actions. Such a setting is interesting in many applications involving monitoring and surveillance, where the set of the actions to observe represent some (geographical) area. The importance of this setting is that in these applications , it is actually cheaper to observe average reward of a group of actions rather than the reward of a single action. We show that when the reward is smooth over a given graph representing the neighboring actions, we can maximize the cumulative reward of learning while minimizing the sensing cost. In this paper we propose CheapUCB, an algorithm that matches the regret guarantees of the known algorithms for this setting and at the same time guarantees a linear cost again over them. As a by-product of our analysis , we establish a (p dT) lower bound on the cumulative regret of spectral bandits for a class of graphs with effective dimension d.

Truthful Learning Mechanisms for Multi–Slot Sponsored Search Auctions with Externalities [5]

Sponsored Search Auctions (SSAs) constitute one of the most successful applications of microeconomic mechanisms. In mechanism design, auctions are usually designed to incentivize advertisers to bid their truthful valuations and, at the same time, to guarantee both the advertisers and the auctioneer a non–negative utility. Nonetheless, in sponsored search auctions, the Click–Through–Rates (CTRs) of the advertisers are often unknown to the auctioneer and thus standard truthful mechanisms cannot be directly applied and must be

paired with an effective learning algorithm for the estimation of the CTRs. This introduces the critical problem of designing a learning mechanism able to estimate the CTRs at the same time as implementing a truthful mechanism with a revenue loss as small as possible compared to the mechanism that can exploit the true CTRs. Previous work showed that, when dominant–strategy truthfulness is adopted, in single–slot auctions the problem can be solved using suitable exploration–exploitation mechanisms able to achieve a cumulative regret (on the auctioneer's revenue) of order $O(T^{(2/3)})$, where T is the number of times the auction is repeated. It is also known that, when truthfulness in expectation is adopted, a cumulative regret (over the social welfare) of order $O(T^{(1/2)})$ can be obtained. In this paper, we extend the results available in the literature to the more realistic case of multi–slot auctions. In this case, a model of the user is needed to characterize how the CTR of an ad changes as its position in the allocation changes. In particular, we adopt the cascade model, one of the most popular models for sponsored search auctions, and we prove a number of novel upper bounds and lower bounds on both auctioneer's revenue loss and social welfare w.r.t. to the Vickrey–Clarke–Groves (VCG) auction. Furthermore, we report numerical simulations investigating the accuracy of the bounds in predicting the dependency of the regret on the auction parameters.

A Relative Exponential Weighing Algorithm for Adversarial Utility-based Dueling Bandits *[37]*

We study the K-armed dueling bandit problem which is a variation of the classical Multi-Armed Bandit (MAB) problem in which the learner receives only relative feedback about the selected pairs of arms. We propose a new algorithm called Relative Exponential-weight algorithm for Exploration and Exploitation (REX3) to handle the adversarial utility-based formulation of this problem. This algorithm is a non-trivial extension of the Exponential-weight algorithm for Exploration and Exploitation (EXP3) algorithm. We prove a finite time expected regret upper bound of order O(sqrt(K ln(K)T)) for this algorithm and a general lower bound of order omega(sqrt(KT)). At the end, we provide experimental results using real data from information retrieval applications.

Simultaneous Optimistic Optimization on the Noiseless BBOB Testbed [15]

We experiment the SOO (Simultaneous Optimistic Optimization) global optimizer on the BBOB testbed. We report results for both the unconstrained-budget setting and the expensive setting, as well as a comparison with the DiRect algorithm to which SOO is mostly related. Overall, SOO is shown to perform rather poorly in the highest dimensions while agreeably exhibiting interesting performance for the most difficult functions, which is to be attributed to its global nature and to the fact that its design was guided by the goal of obtaining theoretically provable performance. The greedy exploration-exploitation sampling strategy underlying SOO design is also shown to be a viable alternative for the expensive setting which gives rooms for further improvements in this direction.

7.1.3. Recommendation systems

Bandits and Recommender Systems [23]

This paper addresses the on-line recommendation problem facing new users and new items; we assume that no information is available neither about users, nor about the items. The only source of information is a set of ratings given by users to some items. By on-line, we mean that the set of users, and the set of items, and the set of ratings is evolving along time and that at any moment, the recommendation system has to select items to recommend based on the currently available information, that is basically the sequence of past events. We also mean that each user comes with her preferences which may evolve along short and longer scales of time; so we have to continuously update their preferences. When the set of ratings is the only available source of information , the traditional approach is matrix factorization. In a decision making under uncertainty setting, actions should be selected to balance exploration with exploitation; this is best modeled as a bandit problem. Matrix factors provide a latent representation of users and items. These representations may then be used as contextual information by the bandit algorithm to select items. This last point is exactly the originality of this paper: the combination of matrix factorization and bandit algorithms to solve the on-line recommendation problem. Our work is driven by considering the recommendation problem as a feedback controlled loop. This leads to interactions between the representation learning, and the recommendation policy.

Collaborative Filtering as a Multi-Armed Bandit [35]

Recommender Systems (RS) aim at suggesting to users one or several items in which they might have interest. Following the feedback they receive from the user, these systems have to adapt their model in order to improve future recommendations. The repetition of these steps defines the RS as a sequential process. This sequential aspect raises an exploration-exploitation dilemma, which is surprisingly rarely taken into account for RS without contextual information. In this paper we present an explore-exploit collaborative filtering RS, based on Matrix Factor-ization and Bandits algorithms. Using experiments on artificial and real datasets, we show the importance and practicability of using sequential approaches to perform recommendation. We also study the impact of the model update on both the quality and the computation time of the recommendation procedure.

AUC Optimisation and Collaborative Filtering [39]

In recommendation systems, one is interested in the ranking of the predicted items as opposed to other losses such as the mean squared error. Although a variety of ways to evaluate rankings exist in the literature, here we focus on the Area Under the ROC Curve (AUC) as it widely used and has a strong theoretical underpinning. In practical recommendation, only items at the top of the ranked list are presented to the users. With this in mind, we propose a class of objective functions over matrix factorisations which primarily represent a smooth surrogate for the real AUC, and in a special case we show how to prioritise the top of the list. The objectives are differentiable and optimised through a carefully designed stochastic gradient-descent-based algorithm which scales linearly with the size of the data. In the special case of square loss we show how to improve computational complexity by leveraging previously computed measures. To understand theoretically the underlying matrix factorisation approaches we study both the consistency of the loss functions with respect to AUC, and generalisation using Rademacher theory. The resulting generalisation analysis gives strong motivation for the optimisation under study. Finally, we provide computation results as to the efficacy of the proposed method using synthetic and real data.

Collaborative Filtering with Localised Ranking [16]

In recommendation systems, one is interested in the ranking of the predicted items as opposed to other losses such as the mean squared error. Although a variety of ways to evaluate rankings exist in the literature, here we focus on the Area Under the ROC Curve (AUC) as it widely used and has a strong theoretical underpinning. In practical recommendation, only items at the top of the ranked list are presented to the users. With this in mind we propose a class of objective functions which primarily represent a smooth surrogate for the real AUC, and in a special case we show how to prioritise the top of the list. This loss is differentiable and is optimised through a carefully designed stochastic gradient-descent-based algorithm which scales linearly with the size of the data. We mitigate sample bias present in the data by sampling observations according to a certain power-law based distribution. In addition, we provide computation results as to the efficacy of the proposed method using synthetic and real data.

Collaborative Filtering with Stacked Denoising AutoEncoders and Sparse Inputs [36]

Neural networks have not been widely studied in Collaborative Filtering. For instance, no paper using neural networks was published during the Net-flix Prize apart from Salakhutdinov et al's work on Restricted Boltzmann Machine (RBM) [14]. While deep learning has tremendous success in image and speech recognition, sparse inputs received less attention and remains a challenging problem for neural networks. Nonetheless, sparse inputs are critical for collaborative filtering. In this paper, we introduce a neural network architecture which computes a non-linear matrix factorization from sparse rating inputs. We show experimentally on the movieLens and jester dataset that our method performs as well as the best collaborative filtering algorithms. We provide an implementation of the algorithm as a reusable plugin for Torch [4], a popular neural network framework.

7.1.4. Nonparametric statistics of time series

The Replacement Bootstrap for Dependent Data [31]

Applications that deal with time-series data often require evaluating complex statistics for which each time series is essentially one data point. When only a few time series are available, bootstrap methods are used to generate additional samples that can be used to evaluate empirically the statistic of interest. In this work a novel bootstrap method is proposed, which is shown to have some asymptotic consistency guarantees under the only assumption that the time series are stationary and ergodic. This contrasts previously available results that impose mixing or finite-memory assumptions on the data. Empirical evaluation on simulated and real data, using a practically relevant and complex extrema statistic is provided.

7.1.5. Imitation and Inverse Reinforcement Learning

Inverse Reinforcement Learning in Relational Domains [24]

In this work, we introduce the first approach to the Inverse Reinforcement Learning (IRL) problem in relational domains. IRL has been used to recover a more compact representation of the expert policy leading to better generalization performances among different contexts. On the other hand, rela-tional learning allows representing problems with a varying number of objects (potentially infinite), thus provides more generalizable representations of problems and skills. We show how these different formalisms allow one to create a new IRL algorithm for relational domains that can recover with great efficiency rewards from expert data that have strong generalization and transfer properties. We evaluate our algorithm in representative tasks and study the impact of diverse experimental conditions such as : the number of demonstrations, knowledge about the dynamics, transfer among varying dimensions of a problem, and changing dynamics.

Imitation Learning Applied to Embodied Conversational Agents [29]

Embodied Conversational Agents (ECAs) are emerging as a key component to allow human interact with machines. Applications are numerous and ECAs can reduce the aversion to interact with a machine by providing user-friendly interfaces. Yet, ECAs are still unable to produce social signals appropriately during their interaction with humans, which tends to make the interaction less instinctive. Especially, very little attention has been paid to the use of laughter in human-avatar interactions despite the crucial role played by laughter in human-human interaction. In this paper, methods for predicting when and how to laugh during an interaction for an ECA are proposed. Different Imitation Learning (also known as Apprenticeship Learning) algorithms are used in this purpose and a regularized classification algorithm is shown to produce good behavior on real data.

7.1.6. Stochastic Games

Optimism in Active Learning [3]

Active learning is the problem of interactively constructing the training set used in classification in order to reduce its size. It would ideally successively add the instance-label pair that decreases the classification error most. However, the effect of the addition of a pair is not known in advance. It can still be estimated with the pairs already in the training set. The online minimization of the classification error involves a tradeoff between exploration and exploitation. This is a common problem in machine learning for which multiarmed bandit, using the approach of Optimism int the Face of Uncertainty, has proven very efficient these last years. This paper introduces three algorithms for the active learning problem in classification using Optimism in the Face of Uncertainty. Experiments lead on built-in problems and real world datasets demonstrate that they compare positively to state-of-the-art methods.

Bayesian Credible Intervals for Online and Active Learning of Classification Trees [13]

Classification trees have been extensively studied for decades. In the online learning scenario, a whole class of algorithms for decision trees has been introduced, called incremental decision trees. In the case where subtrees may not be discarded, an incremental decision tree can be seen as a sequential decision process, consisting in deciding to extend the existing tree or not. This problem involves an trade-off between exploration and exploitation, which is addressed in recent work with the use of Hoeffding's bounds. This paper proposes to use Bayesian Credible Intervals instead, in order to get the most out of the knowledge of the output's

distribution's shape. It also studies the case of Active Learning in such a tree following the Optimism in the Face of Uncertainty paradigm. Two novel algorithms are introduced for the online and active learning problems. Evaluations on real-world datasets show that these algorithms compare positively to state-of-the-art.

Optimism in Active Learning with Gaussian Processes [14]

In the context of Active Learning for classification, the classification error depends on the joint distribution of samples and their labels which is initially unknown. The minimization of this error requires estimating this distribution. Online estimation of this distribution involves a trade-off between exploration and exploitation. This is a common problem in machine learning for which multi-armed bandit theory, building upon Optimism in the Face of Uncertainty, has been proven very efficient these last years. We introduce two novel algorithms that use Optimism in the Face of Uncertainty along with Gaussian Processes for the Active Learning problem. The evaluation lead on real world datasets shows that these new algorithms compare positively to state-of-the-art methods.

Approximate Dynamic Programming for Two-Player Zero-Sum Markov Games [28]

This paper provides an analysis of error propagation in Approximate Dynamic Programming applied to zero-sum two-player Stochastic Games. We provide a novel and unified error propagation analysis in L p-norm of three well-known algorithms adapted to Stochastic Games (namely Approximate Value Iteration, Approximate Policy Iteration and Approximate Generalized Policy Iteratio,n). We show that we can achieve a stationary policy which is 2γ+ $(1-\gamma)$ 2-optimal, where is the value function approximation error and is the approximate greedy operator error. In addition , we provide a practical algorithm (AGPI-Q) to solve infinite horizon γ-discounted two-player zero-sum Stochastic Games in a batch setting. It is an extension of the Fitted-Q algorithm (which solves Markov Decisions Processes from data) and can be non-parametric. Finally, we demonstrate experimentally the performance of AGPI-Q on a simultaneous two-player game, namely Alesia.

7.2. Statistical analysis of time series

7.2.1. Automata Learning

Non-negative Spectral Learning for Linear Sequential Systems [18]

Method of moments (MoM) has recently become an appealing alternative to standard iterative approaches like Expectation Maximization (EM) to learn latent variable models. In addition, MoM-based algorithms come with global convergence guarantees in the form of finite sample bounds. However, given enough computation time, by using restarts and heuristics to avoid local optima, iterative approaches often achieve better performance. We believe that this performance gap is in part due to the fact that MoM-based algorithms can output negative probabilities. By constraining the search space, we propose a non-negative spectral algorithm (NNSpectral) avoiding computing negative probabilities by design. NNSpectral is compared to other MoM-based algorithms and EM on synthetic problems of the PAutomaC challenge. Not only, NNSpectral outperforms other MoM-based algorithms, but also, achieves very competitive results in comparison to EM.

Learning of scanning strategies for electronic support using predictive state representations [17]

In Electronic Support, a receiver must monitor a wide frequency spectrum in which threatening emitters operate. A common approach is to use sensors with high sensitivity but a narrow band-width. To maintain surveillance over the whole spectrum, the sensor has to sweep between frequency bands but requires a scanning strategy. Search strategies are usually designed prior to the mission using an approximate knowledge of illumination patterns. This often results in open-loop policies that cannot take advantage of previous observations. As pointed out in past researches, these strategies lack of robustness to the prior. We propose a new closed loop search strategy that learns a stochastic model of each radar using predic-tive state representations. The learning algorithm benefits from the recent advances in spectral learning and rank minimization using nuclear norm penalization.

Spectral learning with proper probabilities for finite state automation [19]

Probabilistic Finite Automaton (PFA), Probabilistic Finite State Transducers (PFST) and Hidden Markov Models (HMM) are widely used in Automatic Speech Recognition (ASR), Text-to-Speech (TTS) systems and Part Of Speech (POS) tagging for language mod-eling. Traditionally, unsupervised learning of these latent variable models is done by Expectation-Maximization (EM)-like algorithms, as the Baum-Welch algorithm. In a recent alternative line of work, learning algorithms based on spectral properties of some low order moments matrices or tensors were proposed. In comparison to EM, they are orders of magnitude faster and come with theoretical convergence guarantees. However, returned models are not ensured to compute proper distributions. They often return negative values that do not sum to one, limiting their applicability and preventing them to serve as an initialization to EM-like algorithms. In this paper, we propose a new spectral algorithm able to learn a large range of models constrained to return proper distributions. We assess its performances on synthetic problems from the PAutomaC challenge and real datasets extracted from Wikipedia. Experiments show that it outperforms previous spectral approaches as well as the Baum-Welch algorithm with random restarts, in addition to serve as an efficient initialization step to EM-like algorithms.

7.3. Statistical Learning and Bayesian Analysis

7.3.1. Prediction of Sequences of Structured and Unstructured Data

Operator-valued Kernels for Learning from Functional Response Data [6]

In this paper we consider the problems of supervised classification and regression in the case where attributes and labels are functions: a data is represented by a set of functions, and the label is also a function. We focus on the use of reproducing kernel Hilbert space theory to learn from such functional data. Basic concepts and properties of kernel-based learning are extended to include the estimation of function-valued functions. In this setting, the representer theorem is restated, a set of rigorously defined infinite-dimensional operator-valued kernels that can be valuably applied when the data are functions is described, and a learning algorithm for nonlinear functional data analysis is introduced. The methodology is illustrated through speech and audio signal processing experiments.

7.4. Applications

7.4.1. Software development

An Experimental Protocol for Analyzing the Accuracy of Software Error Impact Analysis [25]

In software engineering, error impact analysis consists in predicting the software elements (e.g. modules, classes, methods) potentially impacted by a change. Impact analysis is required to optimize the testing effort. In this paper we present a new protocol to analyze the accuracy of impact analysis. This protocol uses mutation testing to simulate changes that introduce errors. To this end, we introduce a variant of call graphs we name the ”use graph” of a software which may be computed efficiently. We apply this protocol to two open-source projects and correctly predict the impact of 30

A Learning Algorithm for Change Impact Prediction: Experimentation on 7 Java Applications [41]

Change impact analysis consists in predicting the impact of a code change in a software application. In this paper, we take a learning perspective on change impact analysis and consider the problem formulated as follows. The artifacts that are considered are methods of object-oriented software; the change under study is a change in the code of the method, the impact is the test methods that fail because of the change that has been performed. We propose an algorithm, called LCIP that learns from past impacts to predict future impacts. To evaluate our system, we consider 7 Java software applications totaling 214,000+ lines of code. We simulate 17574 changes and their actual impact through code mutations, as done in mutation testing. We find that LCIP can predict the impact with a precision of 69

7.4.2. Spoken Dialogue Systems

Human-Machine Dialogue as a Stochastic Game [10]

In this paper, an original framework to model human-machine spoken dialogues is proposed to deal with co-adaptation between users and Spoken Dialogue Systems in non-cooperative tasks. The conversation is modeled as a Stochastic Game: both the user and the system have their own preferences but have to come up with an agreement to solve a non-cooperative task. They are jointly trained so the Dialogue Manager learns the optimal strategy against the best possible user. Results obtained by simulation show that non-trivial strategies are learned and that this framework is suitable for dialogue modeling.

SIERRA Project-Team

7. New Results

7.1. On the Global Linear Convergence of Frank-Wolfe Optimization Variants

Participant: Simon Lacoste-Julien [correspondent].

Collaboration with Martin Jaggi (ETH Zurich).

The Frank-Wolfe (FW) optimization algorithm has lately re-gained popularity thanks in particular to its ability to nicely handle the structured constraints appearing in machine learning applications. However, its convergence rate is known to be slow (sublinear) when the solution lies at the boundary. A simple less-known fix is to add the possibility to take 'away steps' during optimization, an operation that importantly does not require a feasibility oracle. In this paper [17], we highlight and clarify several variants of the Frank-Wolfe optimization algorithm that have been successfully applied in practice: away-steps FW, pairwise FW, fully-corrective FW and Wolfe's minimum norm point algorithm, and prove for the first time that they all enjoy global linear convergence, under a weaker condition than strong convexity of the objective. The constant in the convergence rate has an elegant interpretation as the product of the (classical) condition number of the function with a novel geometric quantity that plays the role of a 'condition number' of the constraint set. We provide pointers to where these algorithms have made a difference in practice, in particular with the flow polytope, the marginal polytope and the base polytope for submodular optimization.

7.2. Barrier Frank-Wolfe for Marginal Inference

Participant: Simon Lacoste-Julien [correspondent].

Collaboration with Rahul G. Krishnan [correspondent] and David Sontag (NYU).

In [16], we introduce a globally-convergent algorithm for optimizing the tree-reweighted (TRW) variational objective over the marginal polytope. The algorithm is based on the conditional gradient method (Frank-Wolfe) and moves pseudomarginals within the marginal polytope through repeated maximum a posteriori (MAP) calls. This modular structure enables us to leverage black-box MAP solvers (both exact and approximate) for variational inference, and obtains more accurate results than tree-reweighted algorithms that optimize over the local consistency relaxation. Theoretically, we bound the sub-optimality for the proposed algorithm despite the TRW objective having unbounded gradients at the boundary of the marginal polytope. Empirically, we demonstrate the increased quality of results found by tightening the relaxation over the marginal polytope as well as the spanning tree polytope on synthetic and real-world instances.

7.3. Sequential Kernel Herding: Frank-Wolfe Optimization for Particle Filtering

Participants: Simon Lacoste-Julien [correspondent], Francis Bach.

Collaboration with Fredrik Lindsten (University of Cambridge).

Recently, the Frank-Wolfe optimization algorithm was suggested as a procedure to obtain adaptive quadrature rules for integrals of functions in a reproducing kernel Hilbert space (RKHS) with a potentially faster rate of convergence than Monte Carlo integration (and "kernel herding" was shown to be a special case of this procedure). In this paper [18], we propose to replace the random sampling step in a particle filter by Frank-Wolfe optimization. By optimizing the position of the particles, we can obtain better accuracy than random or quasi-Monte Carlo sampling. In applications where the evaluation of the emission probabilities is expensive (such as in robot localization), the additional computational cost to generate the particles through optimization can be justified. Experiments on standard synthetic examples as well as on a robot localization task indicate indeed an improvement of accuracy over random and quasi-Monte Carlo sampling.

7.4. Variance Reduced Stochastic Gradient Descent with Neighbors

Participant: Simon Lacoste-Julien [correspondent].

Collaboration with Thomas Hofmann [correspondent], Aurelien Lucchi and Brian McWilliams (ETH Zurich).

Stochastic Gradient Descent (SGD) is a workhorse in machine learning, yet its slow convergence can be a computational bottleneck. Variance reduction techniques such as SAG, SVRG and SAGA have been proposed to overcome this weakness, achieving linear convergence. However, these methods are either based on computations of full gradients at pivot points, or on keeping per data point corrections in memory. Therefore speed-ups relative to SGD may need a minimal number of epochs in order to materialize. This paper [15] investigates algorithms that can exploit neighborhood structure in the training data to share and re-use information about past stochastic gradients across data points, which offers advantages in the transient optimization phase. As a side-product we provide a unified convergence analysis for a family of variance reduction algorithms, which we call memorization algorithms. We provide experimental results supporting our theory.

7.5. Rethinking LDA: Moment Matching for Discrete ICA

Participants: Anastasia Podosinnikova [correspondent], Francis Bach, Simon Lacoste-Julien.

In [21], we consider moment matching techniques for estimation in latent Dirichlet allocation (LDA). By drawing explicit links between LDA and discrete versions of independent component analysis (ICA), we first derive a new set of cumulant-based tensors, with an improved sample complexity. Moreover, we reuse standard ICA techniques such as joint diagonalization of tensors to improve over existing methods based on the tensor power method. In an extensive set of experiments on both synthetic and real datasets, we show that our new combination of tensors and orthogonal joint diagonalization techniques outperforms existing moment matching methods.

7.6. Tensorizing Neural Networks

Participant: Anton Osokin [correspondent].

Collaboration with Alexander Novikov, Dmitry Podoprikhin and Dmitry Vetrov.

Deep neural networks currently demonstrate state-of-the-art performance in several domains. At the same time, models of this class are very demanding in terms of computational resources. In particular, a large amount of memory is required by commonly used fully-connected layers, making it hard to use the models on low-end devices and stopping the further increase of the model size. In this paper [20], we convert the dense weight matrices of the fully-connected layers to the Tensor Train format such that the number of parameters is reduced by a huge factor and at the same time the expressive power of the layer is preserved. In particular, for the Very Deep VGG networks we report the compression factor of the dense weight matrix of a fully-connected layer up to 200000 times leading to the compression factor of the whole network up to 7 times.

7.7. Context-Aware CNNs for Person Head Detection

Participant: Anton Osokin [correspondent].

Collaboration with Tuan-Hung Vu [correspondent] and Ivan Laptev from the Willow project-team.

Person detection is a key problem for many computer vision tasks. While face detection has reached maturity, detecting people under a full variation of camera view-points, human poses, lighting conditions and occlusions is still a difficult challenge. In this work [23], we focus on detecting human heads in natural scenes. Starting from the recent local R-CNN object detector, we extend it with two types of contextual cues. First, we leverage person-scene relations and propose a Global CNN model trained to predict positions and scales of heads directly from the full image. Second, we explicitly model pairwise relations among objects and train a Pairwise CNN model using a structured-output surrogate loss. The Local, Global and Pairwise models are combined into a joint CNN framework. To train and test our full model, we introduce a large dataset composed of 369,846 human heads annotated in 224,740 movie frames. We evaluate our method and demonstrate improvements of person head detection against several recent baselines in three datasets. We also show improvements of the detection speed provided by our model.

7.8. Unsupervised Learning from Narrated Instruction Videos

Participants: Jean-Baptiste Alayrac [correspondent], Simon Lacoste-Julien.

Collaboration with Piotr Bojanowski, Josef Sivic and Ivan Laptev from the Willow project-team, and Nishant Agrawal.

In [29], we address the problem of automatically learning the main steps to complete a certain task, such as changing a car tire, from a set of narrated instruction videos. The contributions of this paper are three-fold. First, we develop a new unsupervised learning approach that takes advantage of the complementary nature of the input video and the associated narration. The method solves two clustering problems, one in text and one in video, applied one after each other and linked by joint constraints to obtain a single coherent sequence of steps in both modalities. Second, we collect and annotate a new challenging dataset of real-world instruction videos from the Internet. The dataset contains about 800,000 frames for five different tasks that include complex interactions between people and objects, and are captured in a variety of indoor and outdoor settings. Third, we experimentally demonstrate that the proposed method can automatically discover, in an unsupervised manner, the main steps to achieve the task and locate the steps in the input videos.

7.9. On Pairwise Cost for Multi-Object Network Flow Tracking

Participant: Simon Lacoste-Julien.

Collaboration with Visesh Chari, Ivan Laptev [correspondent] and Josef Sivic from the Willow project-team.

Multi-object tracking has been recently approached with the min-cost network flow optimization techniques. Such methods simultaneously resolve multiple object tracks in a video and enable modeling of dependencies among tracks. Min-cost network flow methods also fit well within the "tracking-by-detection" paradigm where object trajectories are obtained by connecting per-frame outputs of an object detector. Object detectors, however, often fail due to occlusions and clutter in the video. To cope with such situations, we propose in [13] an approach that regularizes the tracker by adding second order costs to the min-cost network flow framework. While solving such a problem with integer variables is NP-hard, we present a convex relaxation with an efficient rounding heuristic which empirically gives certificates of small suboptimality. Results are shown on real-world video sequences and demonstrate that the new constraints help selecting longer and more accurate tracks improving over the baseline tracking-by-detection method.

7.10. Multi-utility Learning: Structured-Output Learning with Multiple Annotation-Specific Loss Functions

Participant: Anton Osokin [correspondent].

Collaboration with Roman Shapovalov, Dmitry Vetrov and Pushmeet Kohli.

Structured-output learning is a challenging problem; particularly so because of the difficulty in obtaining large datasets of fully labelled instances for training. In this paper [22], we try to overcome this difficulty by presenting a multi-utility learning framework for structured prediction that can learn from training instances with different forms of supervision. We propose a unified technique for inferring the loss functions most suitable for quantifying the consistency of solutions with the given weak annotation. We demonstrate the effectiveness of our framework on the challenging semantic image segmentation problem for which a wide variety of annotations can be used. For instance, the popular training datasets for semantic segmentation are composed of images with hard-to-generate full pixel labellings, as well as images with easy-to-obtain weak annotations, such as bounding boxes around objects, or image-level labels that specify which object categories are present in an image. Experimental evaluation shows that the use of annotation-specific loss functions dramatically improves segmentation accuracy compared to the baseline system where only one type of weak annotation is used.

7.11. Convex Optimization for Parallel Energy Minimization

Participants: K. S. Sesh Kumar [correspondent], Francis Bach.

Collaboration with Alvaro Barbero, Stefanie Jegelka and Suvrit Sra.

Energy minimization has been an intensely studied core problem in computer vision. With growing image sizes (2D and 3D), it is now highly desirable to run energy minimization algorithms in parallel. But many existing algorithms, in particular, some efficient combinatorial algorithms, are difficult to parallelize. By exploiting results from convex and submodular theory, we reformulate in [47] the quadratic energy minimization problem as a total variation denoising problem, which, when viewed geometrically, enables the use of projection and reflection based convex methods. The resulting min-cut algorithm (and code) is conceptually very simple, and solves a sequence of TV denoising problems. We perform an extensive empirical evaluation comparing state-of-the-art combinatorial algorithms and convex optimization techniques. On small problems the iterative convex methods match the combinatorial max-flow algorithms, while on larger problems they offer other flexibility and important gains: (a) their memory footprint is small; (b) their straightforward parallelizability fits multi-core platforms; (c) they can easily be warm-started; and (d) they quickly reach approximately good solutions, thereby enabling faster "inexact" solutions. A key consequence of our approach based on submodularity and convexity is that it is allows to combine *any arbitrary combinatorial or convex methods as subroutines*, which allows one to obtain hybrid combinatorial and convex optimization algorithms that benefit from the strengths of both.

7.12. Active-set Methods for Submodular Optimization

Participants: K. S. Sesh Kumar [correspondent], Francis Bach.

In [46], we consider submodular optimization problems such as submodular function minimization (SFM) and quadratic problems regularized by the Lovász extension; for cut functions, this corresponds respectively to graph cuts and total variation (TV) denoising. Given a submodular function with an SFM oracle, we propose a new active-set algorithm for total variation denoising, which is more flexible than existing ones; the algorithm may be seen as a local descent algorithm over ordered partitions with explicit convergence guarantees. For functions that decompose into the sum of two functions F_1 and F_2 with efficient SFM oracles, we propose a new active-set algorithm for total variation denoising (and hence for SFM by thresholding the solution at zero). This algorithm also optimizes over ordered partitions and improves over existing ones based on TV or SFM oracles for F_1 and F_2.

7.13. Spectral Norm Regularization of Orthonormal Representations for Graph Transduction

Participant: Francis Bach [correspondent].

Collaboration with the Indian Institute of Science, Bangalore, India.

Recent literature suggests that embedding a graph on an unit sphere leads to better generalization for graph transduction. However, the choice of optimal embedding and an efficient algorithm to compute the same remains open. In this paper [25], we show that orthonormal representations, a class of unit-sphere graph embeddings are PAC learnable. Existing PAC-based analysis do not apply as the VC dimension of the function class is infinite. We propose an alternative PAC-based bound, which do not depend on the VC dimension of the underlying function class, but is related to the famous Lovasz function. The main contribution of the paper is SPORE, a SPectral regularized ORthonormal Embedding for graph transduction, derived from the PAC bound. SPORE is posed as a non-smooth convex function over an elliptope. These problems are usually solved as semi-definite programs (SDPs) with time complexity $O(n^6)$. We present, Infeasible Inexact proximal (IIP): an Inexact proximal method which performs subgradient procedure on an approximate projection, not necessarily feasible. IIP is more scalable than SDP, has an $O(1/\sqrt{T})$ convergence, and is generally applicable whenever a suitable approximate projection is available. We use IIP to compute SPORE where the approximate projection step is computed by FISTA, an accelerated gradient descent procedure. We show that the method has a convergence rate of $O(1/\sqrt{T})$. The proposed algorithm easily scales to 1000's of vertices, while the standard SDP computation does not scale beyond few hundred vertices. Furthermore, the analysis presented here easily extends to the multiple graph setting.

7.14. On the Equivalence between Quadrature Rules and Random Features

Participant: Francis Bach [correspondent].

In [31], we show that kernel-based quadrature rules for computing integrals can be seen as a special case of random feature expansions for positive definite kernels, for a particular decomposition that always exists for such kernels. We provide a theoretical analysis of the number of required samples for a given approximation error, leading to both upper and lower bounds that are based solely on the eigenvalues of the associated integral operator and match up to logarithmic terms. In particular, we show that the upper bound may be obtained from independent and identically distributed samples from a specific non-uniform distribution, while the lower bound if valid for any set of points. Applying our results to kernel-based quadrature, while our results are fairly general, we recover known upper and lower bounds for the special cases of Sobolev spaces. Moreover, our results extend to the more general problem of full function approximations (beyond simply computing an integral), with results in L_2- and L_infty-norm that match known results for special cases. Applying our results to random features, we show an improvement of the number of random features needed to preserve the generalization guarantees for learning with Lipschitz-continuous losses.

7.15. Preconditioning of a Generalized Forward-Backward Splitting and Application to Optimization on Graphs

Participant: Loïc Landrieu [correspondent].

Collaboration with Hugo Raguet.

In [41], we present a preconditioning of a generalized forward-backward splitting algorithm for finding a zero of a sum of maximally monotone operators $\sum_{i=1}^{n} A_i + B$ with B cocoercive, involving only the computation of B and of the resolvent of each A_i separately. This allows in particular to minimize functionals of the form $\sum_{i=1}^{n} g_i + f$ with f smooth, using only the gradient of f and the proximity operator of each g_i separately. By adapting the underlying metric, such preconditioning can serve two practical purposes: first, it might accelerate the convergence, or second, it might simplify the computation of the resolvent of A_i for some i. In addition, in many cases of interest, our preconditioning strategy allows the economy of storage and computation concerning some auxiliary variables. In particular, we show how this approach can handle large-scale, non-smooth, convex optimization problems structured on graphs, which arises in many image processing or learning applications, and that it compares favourably to alternatives in the literature.

7.16. A Riemannian Low-Rank Method for Optimization over Semidefinite Matrices with Block-Diagonal Constraints

Participant: Nicolas Boumal [correspondent].

In [34], we propose a new algorithm to solve optimization problems of the form $\min f(X)$ for a smooth function f under the constraints that X is positive semidefinite and the diagonal blocks of X are small identity matrices. Such problems often arise as the result of relaxing a rank constraint (lifting). In particular, many estimation tasks involving phases, rotations, orthonormal bases or permutations fit in this framework, and so do certain relaxations of combinatorial problems such as Max-Cut. The proposed algorithm exploits the facts that (1) such formulations admit low-rank solutions, and (2) their rank-restricted versions are smooth optimization problems on a Riemannian manifold. Combining insights from both the Riemannian and the convex geometries of the problem, we characterize when second-order critical points of the smooth problem reveal KKT points of the semidefinite problem. We compare against state of the art, mature software and find that, on certain interesting problem instances, what we call the staircase method is orders of magnitude faster, is more accurate and scales better. Code is available.

7.17. Tightness of the Maximum Likelihood Semidefinite Relaxation for Angular Synchronization

Participant: Nicolas Boumal [correspondent].

Collaboration with Afonso S. Bandeira and Amit Singer.

Many maximum likelihood estimation problems are, in general, intractable optimization problems. As a result, it is common to approximate the maximum likelihood estimator (MLE) using convex relaxations. Semidefinite relaxations are among the most popular. Sometimes, the relaxations turn out to be tight. In this paper [33], we study such a phenomenon. The angular synchronization problem consists in estimating a collection of n phases, given noisy measurements of some of the pairwise relative phases. The MLE for the angular synchronization problem is the solution of a (hard) non-bipartite Grothendieck problem over the complex numbers. It is known that its semidefinite relaxation enjoys worst-case approximation guarantees. In this paper, we consider a stochastic model on the input of that semidefinite relaxation. We assume there is a planted signal (corresponding to a ground truth set of phases) and the measurements are corrupted with random noise. Even though the MLE does not coincide with the planted signal, we show that the relaxation is, with high probability, tight. This holds even for high levels of noise. This analysis explains, for the interesting case of angular synchronization, a phenomenon which has been observed without explanation in many other settings. Namely, the fact that even when exact recovery of the ground truth is impossible, semidefinite relaxations for the MLE tend to be tight (in favorable noise regimes).

7.18. Coherent Diffractive Imaging Using Randomly Coded Masks

Participant: Alexandre d'Aspremont [correspondent].

Collaboration with Matthew H. Seaberg and Joshua J. Turner.

Coherent diffractive imaging (CDI) provides new opportunities for high resolution X-ray imaging with simultaneous amplitude and phase contrast. Extensions to CDI broaden the scope of the technique for use in a wide variety of experimental geometries and physical systems. Here [44], we experimentally demonstrate a new extension to CDI that encodes additional information through the use of a series of randomly coded masks. The information gained from the few additional diffraction measurements removes the need for typical object-domain constraints; the algorithm uses prior information about the masks instead. The experiment is performed using a laser diode at 532.2 nm, enabling rapid prototyping for future X-ray synchrotron and even free electron laser experiments. Diffraction patterns are collected with up to 15 different masks placed between a CCD detector and a single sample. Phase retrieval is performed using a convex relaxation routine known as "PhaseCut" followed by a variation on Fienup's input-output algorithm. The reconstruction quality is judged via calculation of phase retrieval transfer functions as well as by an object-space comparison between reconstructions and a lens-based image of the sample. The results of this analysis indicate that with enough masks (in this case 3 or 4) the diffraction phases converge reliably, implying stability and uniqueness of the retrieved solution.

7.19. Renegar's Condition Number and Compressed Sensing Performance

Participants: Vincent Roulet, Nicolas Boumal, Alexandre d'Aspremont [correspondent].

Renegar's condition number is a data-driven computational complexity measure for convex programs, generalizing classical condition numbers in linear systems. In [42], we provide evidence that for a broad class of compressed sensing problems, the worst case value of this algorithmic complexity measure taken over all signals matches the restricted eigenvalue of the observation matrix, which controls compressed sensing performance. This means that, in these problems, a single parameter directly controls computational complexity and recovery performance.

7.20. Supervised Clustering in the Data Cube

Participants: Vincent Roulet [correspondent], Fajwel Fogel, Alexandre d'Aspremont, Francis Bach.

In [43], we study a supervised clustering problem seeking to cluster either features, tasks or sample points using losses extracted from supervised learning problems. We formulate a unified optimization problem handling these three settings and derive algorithms whose core iteration complexity is concentrated in a k-means clustering step, which can be approximated efficiently. We test our methods on both artificial and realistic data sets extracted from movie reviews and 20NewsGroup.

7.21. Convex Relaxations for Permutation Problems

Participants: Fajwel Fogel [correspondent], Francis Bach, Alexandre d'Aspremont.

Collaboration with Rodolphe Jenatton.

Seriation seeks to reconstruct a linear order between variables using unsorted similarity information. It has direct applications in archeology and shotgun gene sequencing for example. In [4], we prove the equivalence between the seriation and the combinatorial 2-sum problem (a quadratic minimization problem over permutations) over a class of similarity matrices. The seriation problem can be solved exactly by a spectral algorithm in the noiseless case and we produce a convex relaxation for the 2-sum problem to improve the robustness of solutions in a noisy setting. This relaxation also allows us to impose additional structural constraints on the solution, to solve semi-supervised seriation problems. We present numerical experiments on archeological data, Markov chains and gene sequences.

7.22. Phase Recovery, MaxCut and Complex Semidefinite Programming

Participant: Alexandre d'Aspremont [correspondent].

Collaboration with Irène Waldspurger and Stéphane Mallat.

Phase retrieval seeks to recover a signal x from the amplitude $|Ax|$ of linear measurements. We cast the phase retrieval problem as a non-convex quadratic program over a complex phase vector and formulate a tractable relaxation (called PhaseCut) similar to the classical MaxCut semidefinite program. In [10], we solve this problem using a provably convergent block coordinate descent algorithm whose structure is similar to that of the original greedy algorithm in Gerchberg-Saxton, where each iteration is a matrix vector product. Numerical results show the performance of this approach over three different phase retrieval problems, in comparison with greedy phase retrieval algorithms and matrix completion formulations.

7.23. Choice of V for V-Fold Cross-Validation in Least-Squares

Participant: Sylvain Arlot [correspondent].

Collaboration with Matthieu Lerasle.

The paper [30] studies V-fold cross-validation for model selection in least-squares density estimation. The goal is to provide theoretical grounds for choosing V in order to minimize the least-squares loss of the selected estimator. We first prove a non-asymptotic oracle inequality for V-fold cross-validation and its bias-corrected version (V-fold penalization). In particular, this result implies that V-fold penalization is asymptotically optimal in the nonparametric case. Then, we compute the variance of V-fold cross-validation and related criteria, as well as the variance of key quantities for model selection performance. We show that these variances depend on V like $1 + 4/(V - 1)$, at least in some particular cases, suggesting that the performance increases much from $V = 2$ to $V = 5$ or 10, and then is almost constant. Overall, this can explain the common advice to take $V = 5$—at least in our setting and when the computational power is limited—, as supported by some simulation experiments. An oracle inequality and exact formulas for the variance are also proved for Monte-Carlo cross-validation, also known as repeated cross-validation, where the parameter V is replaced by the number B of random splits of the data.

7.24. Gains and Losses are Fundamentally Different in Regret Minimization: The Sparse Case

Participant: Vianney Perchet [correspondent].

Collaboration with Joon Kwon.

In [38], we demonstrate that, in the classical non-stochastic regret minimization problem with d decisions, gains and losses to be respectively maximized or minimized are fundamentally different. Indeed, by considering the additional sparsity assumption (at each stage, at most s decisions incur a nonzero outcome), we derive optimal regret bounds of different orders. Specifically, with gains, we obtain an optimal regret guarantee after T stages of order $\sqrt{T \log s}$, so the classical dependency in the dimension is replaced by the sparsity size. With losses, we provide matching upper and lower bounds of order $\sqrt{Ts \log(d)/d}$, which is decreasing in d. Eventually, we also study the bandit setting, and obtain an upper bound of order $\sqrt{Ts \log(d/s)}$ when outcomes are losses. This bound is proven to be optimal up to the logarithmic factor $\sqrt{\log(d/s)}$.

7.25. Batched Bandit Problems

Participant: Vianney Perchet [correspondent].

Collaboration with Philippe Rigollet, Sylvain Chassang and Erik Snowberg.

Motivated by practical applications, chiefly clinical trials, we study in [39] the regret achievable for stochastic bandits under the constraint that the employed policy must split trials into a small number of batches. Our results show that a very small number of batches gives close to minimax optimal regret bounds. As a byproduct, we derive optimal policies with low switching cost for stochastic bandits.

7.26. Online Learning in Repeated Auctions

Participant: Vianney Perchet [correspondent].

Collaboration with Jonathan Weed and Philippe Rigollet.

Motivated by online advertising auctions, in [40] we consider repeated Vickrey auctions where goods of unknown value are sold sequentially and bidders only learn (potentially noisy) information about a good's value once it is purchased. We adopt an online learning approach with bandit feedback to model this problem and derive bidding strategies for two models: stochastic and adversarial. In the stochastic model, the observed values of the goods are random variables centered around the true value of the good. In this case, logarithmic regret is achievable when competing against well behaved adversaries. In the adversarial model, the goods need not be identical and we simply compare our performance against that of the best fixed bid in hindsight. We show that sublinear regret is also achievable in this case and prove matching minimax lower bounds. To our knowledge, this is the first complete set of strategies for bidders participating in auctions of this type.

TAO Project-Team

7. New Results

7.1. Optimal Decision Making under Uncertainty

The Tao-uct-sig is working mainly on mathematical programming tools useful for power systems. In particular, we advocate a data science approach, in order to reduce the model error - which is much more critical than the optimization error, in most cases. Real data are the best way for handling uncertainties. Our main works are as follows:

- **Noisy optimization** In the context of stochastic uncertainties, noisy optimization handles the model error by simulation-based optimization. Our results include:
  - A formalization of noisy optimization in continuous domains, often poorly modeled in the evolutionary computation community [64], [6]. We also proposed heuristic rules for reaching slope -1/2 in log-log scale [34]. We also show that in some settings the slope -1 (classical in mathematical programming) can be recoved in evolution strategies (unpublished: http://www.lri.fr/~teytaud/mca.pdf), and we provided complexity bounds [20].
  - An extension of portfolio algorithms for noisy optimization. Portfolio methods are already usual in combinatorial optimization, some works exists in the continuous case, this is the first work in the noisy case[8].
  - Pragmatic approaches of noisy optimization, for improving robustness and for taking into account human expertise, including: Applying sieves methods in noisy optimization [27], paired optimization [35], and combining various policies [25].
  - Upper bounds on noisy optimization in discrete domains [5].
- **Quasi-random numbers** Continuous optimization is a key component of our works, hence we improve evolution strategies (which have simplicity and convenience qualities) by quasi-random numbers (showing that even in simple cases it is beneficial[52], and provides great improvements in highly multimodal cases (unpublished, http://www.lri.fr/~teytaud/qrr.pdf)). We also developped criteria and testbeds, pointing out some key points not widely studied in the optimization literature[26]. We also extended our earlier results in parallel optimization to additional algorithms[30], and used cutting planes as in the ellipsoid method, hence combining the best of both worlds, i.e. fast rates from cutting planes methodologies and parallel behavior as in evolution strategies[36].
- **Dynamical problems** The dynamical nature of power systems is critical, as transient regimes, ramping constraints are ubiquitous in unit commitment and dispatch. Optimizing policies, with their temporal components, is a challenge when the high dimension and the nonlinearities are taken into account. Games provide a nice testbed for experiments and are used in several of our works. We provided:
  - An original algorithm for learning opening books, by an unexpected use of random seeds[32]. The principle is to randomly sample policies, by modifying the random seed. This can be used for any stochastic policy: we generate thousands of deterministic policies (by setting the random seed to arbitrary values) and select the best ones. This can be applied for games (always the most convincing application for a proof of concept), and any control problem where stochastic policies are available.
  - An extension of the previous work for dynamically adapting the probability distribution for specific positions[51]. This work provides a MCTS without the scalability limitations of MCTS. This work might give birth to many future works.

7.2. Continuous Optimization

- **Markov Chain Analysis of Evolution Strategies** The theory of Markov chains with discrete time and continuous state space turns out to be very useful to analyze the convergence of adaptive evolution strategies (including simplified versions of the state-of-the are CMA-ES). Exploiting invariance of the algorithms, we can indeed construct homogeneous Markov chains underlying the algorithms whose stability implies the linear convergence of the algorithm [65]. We have also shown how the convergence on constrained problems can be analyzed with Markov chains theory [10].

  However the stability can be very difficult to prove; even the irreducibility can be very challenging to prove with current Markov chain theory. We have hence been developing new theoretical tools exploiting deterministic control models to prove more easily the irreducibility and T-chain property of general Markov chains [67]. Those theoretical tools can be applied to the optimization algorithms we are interested in, and trivialize some stability proofs [1], [10].
- **Benchmarking of continuous optimizers** We have been pursuing our effort towards improving the standards in benchmarking of continuous optimizers. We tackled the benchmarking of bi-objective problems and transferred and adapted standard benchmarking techniques from the single-objective optimization and classical derivative free optimization community to the field of EMO [28]. In addition, we have been rewritting part of the COCO platform to improve its modularity and make it less error prone and started its extension to multiobjective optimization.
- **Concentration inequalities for sampling without replacement** We studied the concentration of measure phenomenon in the case of sampling without replacement, which is directly relevant for a recent MCMC techique for large data sets, see [7] accepted to the Bernoulli journal.
- **Random projections for confident MCMC** In the paper [66] accepted at the NIPS "Bayesian Optimization Workshop", we study the benefit of replacing uniform subsampling by random projections in recent MCMC techniques for linear regression of tall datasets.
- **Automatic step size adaptation** We have derived a new, low-cost strategy for online adaptation of the step size in stochastic gradient descent and related algorithms [72]. This problem is of crucial importance in many machine learning algorithms, as current approaches often rely on exploring a grid of step sizes and performing a full optimization for each of them, a lengthy process.

7.3. Data Science

- **High Energy Physics** The success of the 2014 HiggsML challenge has created a willingness for structured collaboration from the High Energy Physics experiments. A working group has been set up and new challenges are currently explored. A yearly workshop has been decided, with a first edition at CERN 9-13 Nov. 2015, *DataScience@LHC*.

  The challenge exemplifies a new machine learning task [58][56]: *learning to discover* evaluating the significance of a scientific discovery. It can be formally casted into a two-class classification problem, but with two major departures from a regular setting. 1) Discovery: labeled training examples of the positive class (signals) are not available and must be obtained from simulation. The learning machine can then address the “inverse problem” of predicting which events are signals in real data. 2) Evaluation: because the classes are enormously imbalanced and overlapping, the objective function of the classifier is a metric of a statistical test.
- **Personal Semantics** Our algorithm for inducing a taxonomy from a set of domain terms placed first in the international Taxonomy Induction task, part of the SemEval 2015 conference in Denver. Since then, we have developed a robust technique for discovering the domain vocabulary for a new topic using a directed crawler we created. We are currently creating hundreds of taxonomy for personal themes (hobbies, illnesses) that can be integrated into our Personal Semantics platform PTraces. The challenges for the coming year will be deploying and evaluating the taxonomies, and introducing newer machine learning methods, such as Latent Dirichlet Allocation, for better recognizing domain vocabularies.

- **Distributed system observation** The work on distributed system automated analaysis and description [59][60], has been persued thru the continued development of the GAMA multi-agent framework https://github.com/gama-platform/gama/wiki. The simulation framework has been applied to the study of a new anytime reverse auctions protocol [53]. Philippe Caillou is associated to the young researcher ANR ACTEUR, coordinated by Patrick Taillandier (IDEES, Rouen university). With this project, a new BDI cognitive agent model, designed to be easy to use for non computer scientist, has been proposed [29] and applied to Rouen traffic simulation [57]. Finaly, agent behavior has been extracted from human player logs to study the perception of emotive behaviors in board games [37].
- **Digital humanities** Amiqap and Cartolabe projects both start in 2016. The Cartolabe project applies machine learning techniques to determine comprehensible structures in unstructured data. The goal is to use raw textual data, and underspecified ontologies, to provide intuitive access to pertinent research activities in a large research organisation. Amiqap studies the relation between worker well-being and company performance, in collaboration with Mines ParisTech sociology department and La Fabrique de l'Industrie for research, Secafi and DARES for the data.
  These activities will benefit from Paola Tubaro's arrival (researcher CNRS in sociology and economy) in 2016.

7.4. Designing criteria

- **Criterion design and optimization methods for computer vision** On the topic of large-scale image segmentation with multiple object detection, targetting as an application the analysis of high-resolution multispectral satellite images covering the Earth, challenges are numerous: scalable complexity, finding good features to distinguish objects, designing shape statistics as well as an optimization method able to incorporate them. We propose a solution [42], [43] based on the construction of binary partition trees and on their optimization, whose cost is alleviated thanks to theoretical results reducing the search space. Concerning video segmentation, we have extended previous work, on the inclusion of shape growth constraints into classical MRF settings (graph cuts with globally optimal segmentation), to the case of multimodal sequences of medical 3D scans [19]. We also studied a new family of metrics in [9], together with a redefinition of the associated gradient and practical ways to compute it. This allows the consideration of new types of priors on planar curve evolution, such as piecewise-rigid motions. Surprisingly, the problem of finding the best piecewise-rigid approximation of a motion turns out to be convex, and to be linked to sparsity approaches.
- **Algorithm selection and configuration** Two PhD theses are still related to the former *Crossing the Chasm* SIG: Nacim Belkhir has worked on inline parameter tuning for the CMA-ES algorithm in the context of a large number of cores [21], and is now using surrogate models to compute the features of expensive continuous optimization (submitted). François Gonard's PhD is dedicated to algorithm selection. The original application domain is that of expensive car industry simulations (within the IRT-ROM project). Initial results concern combinatorial optimization, and François obtained a "Honorable mention from the jury" for his submission to the ICON Challenge (http://iconchallenge.insight-centre.org/), for its original approach coupling a pre-scheduler and an algorithm selector. A paper describing the algorithms and analyzing the results has been submitted.
- **A statistical physics perspective** In the topic of MRF design, with motivating applications in large scale inference problems like traffic congestions, we have finalized in [13] an approach based on the disordered Ising model relying on approximate solutions to the Inverse Ising problem. To this specific problem we also propose new approximate solutions, compliant with the generalized belief-propagation algorithm in the static [63] and a new l_0 regularized method based on a maximum likelihood maximization for the dynamical case[11]. In fact in [63] we have developped a method adapted to the generalized belief propagation framework, aiming at adressing directly and systematically the loop corrections without loss of scalability, offering new possibilities in the context of inference by MRF models. In parallel, a better understanding of the so-called mean-field approximation when the phase space is clustered has been derived [68] giving a direct method to solve static inverse problem

in the weak coupling limit. Apart from the method point of view, some consideration over what can be said on the data has been considered, still in the topic of MRF design. In this sense, it is shown in [69] that the reconstruction of the MRF model depends strongly on how the data are gathered, and how to remove redundant data and keep a good reconstruction.

- **Multi-objective AI Planning** This activity had almost stopped since the end of the DESCARWIN ANR project. However, a productive intership resulted in some new benchmarks in the ZenoTravel domain together with an exact solver ensuring the knowledge of the true Pareto front [48], [47].

7.5. Deep Learning and Information Theory

- **Natural Gradients for Deep Learning** Deep learning is now established as a state-of-the-art technology for performing different tasks such as image or sequence processing. Nevertheless, much of the computational burden is spent on tuning the hyper-parameters. On-going work, started during the TIMCO project, is proposing, in the framework of Riemannian gradient descents, invariant algorithms for training neural networks that effectively reduce the number of arbitrary choices, e.g., affine transformations of the activation functions or shuffling of the inputs. Moreover, the Riemannian gradient descent algorithms perform as well as the state-of-the-art optimizers for neural networks, and are even faster for training complex models. The proposed approach is based on Amari's theory of information geometry and consists in practical and well-grounded approximations for computing the Fisher metric. The scope of this framework is larger than Deep Learning and encompasses any class of statistical models.
- **Training dynamical systems online without backtracking** with application to recurrent neural networks [73]. We propose an algorithm to learn the parameters of a dynamical system in an online, memoryless setting, thus requiring no backpropagation through time, and consequently scalable, avoiding the large computational and memory cost of maintaining the full gradient of the current state with respect to the parameters. The algorithm essentially maintains, at each time, a single search direction in parameter space. The evolution of this search direction is partly stochastic and is constructed in such a way to provide, at every time, an unbiased random estimate of the gradient of the loss function with respect to the parameters.
- **Approximating Bayesian predictors thanks to Laplace's rule of succesion** Laplace's "add-one" rule of succession modifies the observed frequencies in a sequence of heads and tails by adding one to the observed counts. This improves prediction by avoiding zero probabilities and corresponds to a uniform Bayesian prior on the parameter. We prove that, for any exponential family of distributions, arbitrary Bayesian predictors can be approximated by taking the average of the maximum likelihood predictor and the sequential normalized maximum likelihood predictor from information theory, which generalizes Laplace's rule. The proof heavily involves the geometry provided by the Fisher information matrix. Thus it is possible to approximate Bayesian predictors without the cost of integrating or sampling in parameter space[46].

ASPI Project-Team

5. New Results

5.1. Adaptive multilevel splitting

Participants: Frédéric Cérou, Arnaud Guyader.

We have show last year that an adaptive version of multilevel splitting for rare events is strongly consistent and that the estimates satisfy a CLT (central limit theorem), with the same asymptotic variance as the non–adaptive algorithm with the optimal choice of the parameters. This year we have generalized these results to include Markov kernels used to move the particles (or *shakers*) are of Metropolis–Hastings type. This is a non–trivial generalization to a very important case.

5.2. Adaptive multilevel splitting as a Fleming–Viot system

Participants: Frédéric Cérou, Arnaud Guyader.

This is a collaboration with Bernard Delyon (université de Rennes 1) and Mathias Rousset (EPI MATHERIALS, Inria Paris Rocquencourt).

By considering the adaptive multilevel splitting algorithm as a Fleming–Viot particle system for a stochastic wave, in the sense of [42], we have shown the mean square convergence using a general result [67] about the convergence of Fleming–Viot (Villemonais, 2013). We are currently working on the proof of a central limit theorem, but the proof is not yet complete. We have nevertheless identified the expression of the asymptotic variance.

5.3. Bias and variance reduction in rare event simulation

Participant: François Le Gland.

This is a collaboration with Damien Jacquemart (ONERA, Palaiseau) and Jérôme Morio (ONERA, Toulouse).

In [17], we highlight a bias induced by the discretization of the sampled Markov paths in the splitting algorithm, and we propose to correct this bias using a deformation of the intermediate regions, as proposed in [48]. Moreover, we propose two numerical methods to design intermediate regions in the splitting algorithm that minimise the variance. One is connected with a partial differential equation approach, the other one is based on the discretization of the state space of the process.

5.4. Simulation–based algorithms for the optimization of sensor deployment

Participant: François Le Gland.

This is a collaboration with Christian Musso (ONERA, Palaiseau) and with Sébastien Paris (LSIS, université du Sud Toulon Var).

The problem considered here can be described as follows: a limited number of sensors should be deployed by a carrier in a given area, and should be activated at a limited number of time instants within a given time period, so as to maximize the probability of detecting a target (present in the given area during the given time period). There is an information dissymmetry in the problem: if the target is sufficiently close to a sensor position when it is activated, then the target can learn about the presence and exact position of the sensor, and can temporarily modify its trajectory so as to escape away before it is detected. This is referred to as the target intelligence. Two different simulation–based algorithms have been designed in [23] to solve separately or jointly this optimization problem, with different and complementary features. One is fast, and sequential: it proceeds by running a population of targets and by dropping and activating a new sensor (or re–activating a sensor already available) where and when this action seems appropriate. The other is slow, iterative, and non–sequential: it proceeds by updating a population of deployment plans with guaranteed and increasing criterion value at each iteration, and for each given deployment plan, there is a population of targets running to evaluate the criterion. Finally, the two algorithms can cooperate in many different ways, to try and get the best of both approaches. A simple and efficient way is to use the deployment plans provided by the sequential algorithm as the initial population for the iterative algorithm.

5.5. Kalman Laplace filtering

Participant: François Le Gland.

This is a collaboration with Paul Bui Quang (CEA, Bruyères–le–Châtel) and Christian Musso (ONERA, Palaiseau).

We propose in [21] a new nonlinear Bayesian filtering algorithm where the prediction step is performed like in the extended Kalman filter, and the update step is done thanks to the Laplace method for integral approximation. This algorithm is called the Kalman Laplace filter (KLF). The KLF provides a closed–form non–Gaussian approximation of the posterior density. The hidden state is estimated by the maximum a posteriori. We describe a way to alleviate the computation cost of this maximization, when the likelihood is a function of a vector whose dimension is smaller than the state space dimension. The KLF is tested on three simulated nonlinear filtering problems: target tracking with angle measurements, population dynamics monitoring, motion reconstruction by neural decoding. It exhibits a good performance, especially when the observation noise is small.

5.6. Combining analog method and ensemble data assimilation

Participants: François Le Gland, Valérie Monbet, Chau Thi Tuyet Trang.

This is a collaboration with Pierre Ailliot (université de Bretagne Occidentale), Ronan Fablet and Pierre Tandéo (Télécom Bretagne), Anne Cuzol (université de Bretagne Sud) and Bernard Chapron (IFREMER, Brest).

Nowadays, ocean and atmosphere sciences face a deluge of data from spatial observations, in situ monitoring as well as numerical simulations. The availability of these different data sources offer new opportunities, still largely underexploited, to improve the understanding, modeling and reconstruction of geophysical dynamics. The classical way to reconstruct the space–time variations of a geophysical system from observations relies on data assimilation methods using multiple runs of the known dynamical model. This classical framework may have severe limitations including its computational cost, the lack of adequacy of the model with observed data, modeling uncertainties. In [24], we explore an alternative approach and develop a fully data–driven framework, which combines machine learning and statistical sampling to simulate the dynamics of complex system. As a proof concept, we address the assimilation of the chaotic Lorenz–63 model. We demonstrate that a nonparametric sampler from a catalog of historical datasets, namely a nearest neighbor or analog sampler, combined with a classical stochastic data assimilation scheme, the ensemble Kalman filter and smoother, reach state–of–the–art performances, without online evaluations of the physical model.

5.7. Markov–switching vector autoregressive models

Participant: Valérie Monbet.

This is a collaboration with Pierre Ailliot (université de Bretagne Occidentale), Julie Bessac (Argonne National Laboratory, Chicago) and Julien Cattiaux (Météo–France, Toulouse).

Multivariate time series are of interest in many fields including economics and environment. The most popular tools for studying multivariate time series are the vector autoregressive (VAR) models because of their simple specification and the existence of efficient methods to fit these models. However, the VAR models do not allow to describe time series mixing different dynamics. For instance, when meteorological variables are observed, the resulting time series exhibit an alternance of different temporal dynamics corresponding to weather regimes. The regime is often not observed directly and is thus introduced as a latent process in time series models in the spirit of hidden Markov models. Markov switching vector autoregressive (MSVAR) models have been introduced as a generalization of autoregressive models and hidden Markov models. They lead to flexible and interpretable models. In this mutivariate context, several questions occur.

- The discrete hidden variable also called regime has to be correctly defined. Indeed the regime can be local (e.g. link to a subset of the variables) or global (e.g. the same for all the variables). It can also be observed and inferred a priori or hidden. In the second case, it has to be estimated at the same time as the model parameters.
  The question of the definition of the regime is investigated in [26] for the specific problem of multi site wind modeling.
- Markov Switching VAR models (MSVAR) suffer of the same dimensionality problem as VAR models. For large (and even moderate) dimensions, the number of autoregressive coefficients in each regime can be prohibitively large which results in noisy estimates. When the variables are correlated, which is the standard situation in multivariate time series, over–learning is frequent. The estimated parameters contains spurious non–zero coefficients and are then difficult to interpret. The predictions associated to the model are usually unstable. Collinearity causes also ill–conditioning of the innovation covariance. In [29], we propose a likelihood penalization method with hard thresholding for MSVAR models leading to sparse MSVAR. Both autoregressive matrices and precision matrices are penalized using smoothly clipped absolute deviation (SCAD) penalties.

5.8. Dependent time changed processes

Participant: Valérie Monbet.

This is a collaboration with Pierre Ailliot (université de Bretagne Occidentale), Bernard Delyon (université de Rennes 1) and Marc Prevosto (IFREMER, Brest).

Many records in environmental sciences exhibit asymmetric trajectories and there is a need for simple and tractable models which can reproduce such feature. In [25] we explore an approach based on applying both a time change and a marginal transformation on Gaussian processes. The main originality of the proposed model is that the time change depends on the observed trajectory. We first show that the proposed model is stationary and ergodic and provide an explicit characterization of the stationary distribution. This result is then used to build both parametric and non–parametric estimate of the time change function whereas the estimation of the marginal transformation is based on up–crossings. Simulation results are provided to assess the quality of the estimates. The model is applied to wave data and it is shown that the fitted model is able to reproduce important statistics of the data such as its spectrum and marginal distribution which are important quantities for practical applications. An important benefit of the proposed model is its ability to reproduce the observed asymmetries between the crest and the troughs and between the front and the back of the waves by accelerating the chronometer in the crests and in the front of the waves.

5.9. An efficient algorithm for video super–resolution based on a sequential model

Participant: Patrick Héas.

This is a collaboration with Angélique Drémeau (ENSTA Bretagne, Brest) and Cédric Herzet (EPI FLUMINANCE, Inria Rennes–Bretagne Atlantique)

In the work [27], we propose a novel procedure for video super–resolution, that is the recovery of a sequence of high–resolution images from its low–resolution counterpart. Our approach is based on a *sequential* model (i.e. each high–resolution frame is supposed to be a displaced version of the preceding one) and considers the use of sparsity–enforcing priors. Both the recovery of the high–resolution images and the motion fields relating them is tackled. This leads to a large–dimensional, non–convex and non–smooth problem. We propose an algorithmic framework to address the latter. Our approach relies on fast gradient evaluation methods and modern optimization techniques for non–differentiable/non–convex problems. Unlike some other previous works, we show that there exists a provably–convergent method with a complexity linear in the problem dimensions. We assess the proposed optimization method on several video benchmarks and emphasize its good performance with respect to the state of the art.

5.10. Reduced–order modeling of hidden dynamics

Participant: Patrick Héas.

This is a collaboration with Cédric Herzet (EPI FLUMINANCE, Inria Rennes–Bretagne Atlantique).

The objective of the paper [28] is to investigate how noisy and incomplete observations can be integrated in the process of building a reduced–order model. This problematic arises in many scientific domains where there exists a need for accurate low–order descriptions of highly–complex phenomena, which can not be directly and/or deterministically observed. Within this context, the paper proposes a probabilistic framework for the construction of POD–Galerkin reduced–order models. Assuming a hidden Markov chain, the inference integrates the uncertainty of the hidden states relying on their posterior distribution. Simulations show the benefits obtained by exploiting the proposed framework.

CQFD Project-Team

7. New Results

7.1. Control of parallel non-observable queues: asymptotic equivalence and optimality of periodic policies

The following result has been obtained by J. Anselmi (Inria CQFD), T. Nesti and B. Gaujal.

We consider a queueing system composed of a dispatcher that routes deterministically jobs to a set of non-observable queues working in parallel. In this setting, the fundamental problem is which policy should the dispatcher implement to minimize the stationary mean waiting time of the incoming jobs. We present a structural property that holds in the classic scaling of the system where the network demand (arrival rate of jobs) grows proportionally with the number of queues. Assume that each queue of type r is replicated k times and consider the set of policies that are periodic with period $k\sum_r p_r$ and such that exactly p_r jobs are sent in a period to each queue of type r. When $k \to \infty$, our main result shows that all the policies in this set are equivalent, in the sense that they yield the same mean stationary waiting time, and optimal, in the sense that no other policy having the same aggregate arrival rate to all queues of a given type can do better in minimizing the stationary mean waiting time. This property holds in a strong probabilistic sense. Furthermore, the limiting mean waiting time achieved by our policies is a convex function of the arrival rate in each queue, which facilitates the development of a further optimization aimed at solving the fundamental problem above for large systems.

7.2. Decentralized Proportional Load Balancing

The following result has been obtained by J. Anselmi (Inria CQFD), and N. Walton.

Load balancing is a powerful technique commonly used in communication and computer networks to improve system performance, robustness and fairness. In this paper, we consider a general model capturing the performance of communication and computer networks, and on top of it we propose a decentralized algorithm for balancing load among multiple network paths. The proposed algorithm is inspired by the modus operandi of the processor-sharing queue and on each network entry point operates as follows: every time a unit of load completes its service on a path, it increases by one unit the load of that path and decreases by one unit the load of a path selected at random with probability proportional to the amount of load on each of the available paths. We develop a dynamical system to argue that our load-balancer achieves a desirable network-wide utility optimization.

A paper has been accepted for publication in the SIAM Journal of Applied Mathematics.

7.3. Conditional quantile estimation through optimal quantization

The following result has been obtained by Isabelle Charlier (CQFD member), Davy Paindaveine, and Jérôme Saracco (CQFD member)

We use quantization to construct a nonparametric estimator of conditional quantiles of a scalar response Y given a d-dimensional vector of covariates X. First we focus on the population level and show how optimal quantization of X, which consists in discretizing X by projecting it on an appropriate grid of N points, allows to approximate conditional quantiles of Y given X. We show that this approximation is arbitrarily good as N goes to infinity and provide a rate of convergence for the approximation error. Then we turn to the sample case and define an estimator of conditional quantiles based on quantization ideas. We prove that this estimator is consistent for its fixed-N population counterpart. The results are illustrated on a numerical example. Dominance of our estimators over local constant/linear ones and nearest neighbor ones is demonstrated through extensive simulations in the companion paper Charlier et al. (2014).

7.4. A linear programming formulation for constrained discounted continuous control for piecewise deterministic Markov processes

The following result has been obtained by Oswaldo Costa and François Dufour (CQFD member).

This work deals with the constrained discounted control of piecewise deterministic Markov process (PDMPs) in general Borel spaces. The control variable acts on the jump rate and transition measure, and the goal is to minimize the total expected discounted cost, composed of positive running and boundary costs, while satisfying some constraints also in this form. The basic idea is, by using the special features of the PDMPs, to re-write the problem via an embedded discrete-time Markov chain associated to the PDMP and re-formulate the problem as an infinite dimensional linear programming (LP) problem, via the occupation measures associated to the discrete-time process. It is important to stress however that our new discrete-time problem is not in the same framework of a general constrained discrete-time Markov Decision Process and, due to that, some conditions are required to get the equivalence between the continuous-time problem and the LP formulation. We provide in the sequel sufficient conditions for the solvability of the associated LP problem. We provide some examples to illustrate the obtained results.

7.5. Impulsive control for continuous-time Markov decision processes

The following result has been obtained by Alexey Piunovskiy and François Dufour (CQFD member).

The objective of this work is to study continuous-time Markov decision processes on a general Borel state space with both impulsive and continuous controls for the infinite-time horizon discounted cost. The continuous-time controlled process is shown to be non explosive under appropriate hypotheses. The so-called Bellman equation associated to this control problem is studied. Sufficient conditions ensuring the existence and the uniqueness of a bounded measurable solution to this optimality equation are provided. Moreover, it is shown that the value function of the optimization problem under consideration satisfies this optimality equation. Sufficient conditions are also presented to ensure on one hand the existence of an optimal control strategy and on the other hand the existence of an ε-optimal control strategy. The decomposition of the state space in two disjoint subsets is exhibited where roughly speaking, one should apply a gradual action or an impulsive action correspondingly to get an optimal or ε-optimal strategy. An interesting consequence of our previous results is as follows: the set of strategies that allow interventions at time $t = 0$ and only immediately after natural jumps is a sufficient set for the control problem under consideration.

7.6. Impulsive control for continuous-time Markov decision processes: A Linear Programming Approach

The following result has been obtained by Alexey Piunovskiy and François Dufour (CQFD member).

The objective of this work is to investigate an optimization problem for continuous-time Markov decision processes with both impulsive and continuous controls. We consider the so-called constrained problem where the objective of the controller is to minimize a total expected discounted optimality criterion associated with a cost rate function while keeping other performance criteria of the same form, but associated with different cost rate functions, below some given bounds. Our model allows multiple impulses at the same time moment. The main objective of this work is to study the associated linear program defined on a space of measures including the occupation measures of the controlled process and to provide sufficient conditions to ensure the existence of an optimal control.

7.7. Conditions for the Solvability of the Linear Programming Formulation for Constrained Discounted Markov Decision Processes

The following result has been obtained by François Dufour (CQFD member) and T. Prieto-Rumeau.

This result concerns discrete-time constrained discounted Markov decision processes (MDP) with Borel state and action spaces, compact action sets, and lower semi-continuous cost functions. We introduce a set of hypotheses related to a positive weight function which allow us to consider cost functions that might not be bounded below by a constant, and which imply the solvability of the linear programming formulation of the constrained MDP. In particular, we establish the existence of a constrained optimal stationary policy. Our results are illustrated with an application to a fishery management problem.

7.8. Comparison of Kernel Density Estimators with Assumption on Number of Modes

The following result has been obtained by Gilles Durrieu, Raphaël Coudret and Jérôme Saracco (CQFD member).

A data-driven bandwidth choice for a kernel density estimator called critical bandwidth is investigated. This procedure allows the estimation to have as many modes as assumed for the density to estimate. Both Gaussian and uniform kernels are considered. For the Gaussian kernel, asymptotic results are given. For the uniform kernel, an argument against these properties is mentioned. These theoretical results are illustrated with a simulation study that compares the kernel estimators that rely on critical bandwidth with another one that uses a plug-in method to select its bandwidth. An estimator that consists in estimates of density contour clusters and takes assumptions on number of modes into account is also considered. Finally, the methodology is illustrated using environment monitoring data.

7.9. EEG classification for the detection of mental states

The following result has been obtained by Laurent Vezard, Pierrick Legrand (CQFD member), Marie Chavent (CQFD member), Frederique Faita-Ainseba and Trujillo Leonardo

The objective of the present work is to develop a method that is able to automatically determine mental states of vigilance; i.e., a person's state of alertness. Such a task is relevant to diverse domains, where a person is expected or required to be in a particular state of mind. For instance, pilots and medical staff are expected to be in a highly alert state and the proposed method could help to detect possible deviations from this expected state. This work poses a binary classification problem where the goal is to distinguish between a "relaxed" state and a baseline state ("normal") from the study of electroencephalographic signals (EEG) collected with a small number of electrodes. The EEG of 58 subjects in the two alertness states (116 records) were collected via a cap with 58 electrodes. After a data validation step, 19 subjects were retained for further analysis. A genetic algorithm was used to select a subset of electrodes. Common spatial pattern (CSP) coupled to linear discriminant analysis (LDA) was used to build a decision rule and thus predict the alertness of the subjects. Different subset sizes were investigated and the best compromise between the number of selected electrodes and the quality of the solution was obtained by considering 9 electrodes. Even if the present approach is costly in computation time (GA search), it allows to construct a decision rule that provides an accurate and fast prediction of the alertness state of an unseen individual.

7.10. Modeling and optimization of a launcher integration process

The following result has been obtained by Christophe Nivot (CQFD member), Benoîte De Saporta, François Dufour (CQFD member), Jacques Béhar, Damien Bérard-Bergery and Charles Elegbede.

We deal with the modeling and the optimization of a launcher integration process. The subassemblies go through various types of operations which are split up into workshops. Their operating time is supposed random due to possible breakdowns or staff issues. Storage capacity of output products is limited and costly. Launches have to be performed according to a predetermined schedule, and lateness also costs money. The rate of production of the subassemblies must be decided every year. Therefore, the system can be modeled with a Markov decision process which is suitable for decision optimization and cost minimization. Indeed, one must find a balance between slow production (thus low storage levels and high probability to be late), and fast production (high storage levels but respected schedule).

We propose a model of this integration process based on Markov decision models. We present the simulation we have performed so far and discuss the difficulties of the optimization.

7.11. ClustGeo: Ascendant Hierarchical Clustering (AHC) with geographical constraints

The following result has been obtained by Marie Chavent (CQFD member), Vanessa Kuentz-Simonet, Amaury Labenne and Jerome Saracco (CQFD member).

Hierarchical Ascendant Clustering (HAC) is a well-known method of individual clustering. This method aims to bring together individuals who are similar regarding to variables which describe them. But when individuals are geographical units, the user may wish geographically close individuals to be put in same clusters and that, without too much deteriorating the quality of the partition. The proposed ClustGeo method allows geographical constraints of proximity to be taken into account within the HAC. For that purpose, a new Ward homogeneity criterion based on two different matrices of distances is proposed.

7.12. Approche bayésienne non paramétrique pour la factorisation de matrice binaire à faible rang avec loi de puissance

The following result has been obtained by Adrien Todeschini (CQFD member) and François Caron.

We introduce a low-rank Bayesian nonparametric (BNP) model for bipartite graphs. Recently, Caron (2012) proposed a BNP model where each node is given its own sociability parameter allowing to capture the power-law behavior of real world bipartite graphs. This model can be considered as a rank one nonnegative factorization of the adjacency matrix. Building on the compound random measures recently introduced by Griffin and Leisen (2014), we derive a rank p generalization of this model where each node is associated with a p-dimensional vector of sociability parameters accounting for several latent dimensions. While preserving the desired properties of interpretability, scalability and power-law behavior, our model is more flexible and provides better predictive performance as illustrated on several datasets.

7.13. Compétitions d'apprentissage automatique avec le package R rchallenge

The following result has been obtained by Adrien Todeschini (CQFD member) Robin Genuer.

In machine learning, empirical performance on real data are crucial in the success of a method. Recent years have seen the emergence of a large number of machine learning competitions. These challenges are motivated by industrial (Netflix prize) or academic (HiggsML challenge) applications and put in competition researchers and data scientists to obtain the best performance. We wanted to expose students to this reality by submitting a challenge in the context of the machine learning course. The leaderboard is displayed on an automatically updated web page allowing emulation among students. The history of the results also allows them to visualize their progress through the submissions. In addition, the challenge can continue outside of the supervised sessions promoting independence and exploration of new learning techniques and computer tools. The system we have implemented is available as an R package for reuse by other teachers. Building on the R Markdown and Dropbox tools, it requires no network configuration and can be deployed very easily on a personal computer.

7.14. Novelty Search

The following result has been obtained by Enrique Naredo, Leonardo Trujillo and Pierrick Legrand (CQFD member).

Novelty Search (NS) is a unique approach towards search and optimization, where an explicit objective function is replaced by a measure of solution novelty. However, NS has been mostly used in evolutionary robotics while its usefulness in classic machine learning problems has been unexplored. This work presents a NS-based Genetic Programming (GP) algorithm for supervised classification. Results show that NS can solve real-world classification tasks, validated on real-world benchmarks for binary and multiclass problems. These results are made possible by using a domain-specific behavior descriptor. Two new versions of the NS algorithm are proposed, Probabilistic NS (PNS) and a variant of Minimum Criterion NS (MCNS). The former models the behavior of each solution as a random vector and eliminates all of the original NS parameters while reducing the computational overhead of the NS algorithm. The latter uses a standard objective function to constrain and bias the search towards high performance solutions. The paper also discusses the effects of NS on GP search dynamics and code growth. Results show that NS can be used as a realistic alternative for supervised classi?cation, and for binary problems the NS algorithm exhibits an implicit bloat control ability.

Keywords: Novelty Search, Behavior-based Search, Supervised Classification, Bloat

7.15. Classification of Epileptic states

The following result has been obtained by Emigdio Z. FLores, Leonardo Trujillo and Pierrick Legrand (CQFD member).

The neurological disorder known as Epilepsy is characterized by involuntary recurrent seizures that diminish a patient's quality of life. Automatic seizure detection can help improve a patient's interaction with her/his environment, and while many approaches have been proposed the problem is still not trivially solved. In this work, we present a novel methodology for feature extraction on EEG signals that allows us to perform a highly accurate classification of epileptic states. Specifically, Hölderian regularity and Matching Pursuit are used as the main feature extraction techniques, and are combined with basic statistics to construct the final feature sets. These sets are then delivered to a Random Forests classification algorithm. Furthermore, several versions of the basic problem are tested and statistically validated producing perfect accuracy in most problems and 92% accuracy on the most difficult case. A comparison with recent results in relevant literature using a well known database reveals that our proposal achieves state-of-the-art performance.

Keywords: Epilepsy detection, Hölderian regularity, Matching Pursuit, EEG Classification

7.16. Prediction of expected performance

The following result has been obtained by Yuliana Martinez, Leonardo Trujillo and Pierrick Legrand (CQFD member).

The study of problem difficulty is an open issue in Genetic Programming (GP). The goal of this work is to generate models that predict the expected performance of a GP-based classifier when it is applied to an unseen task. Classification problems are described using domain-specific features, some of which are proposed in this work, and these features are given as input to the predictive models. These models are referred to as predictors of expected performance (PEPs). We extend this approach by using an ensemble of specialized predictors (SPEPs), dividing classification problems into specified groups and choosing the corresponding SPEP. The proposed predictors are trained using 2D synthetic classification problems with balanced datasets. The models are then used to predict the performance of the GP classifier on unseen real-world datasets that are multidimensional and imbalanced. Moreover, as we know, this work is the first to provide a performance prediction of the GP classifier on test data, while previous works focused on predicting training performance. Accurate predictive models are generated by posing a symbolic regression task and solving it with GP. These results are achieved by using highly descriptive features and including a dimensionality reduction stage that simplifies the learning and testing process. The proposed approach could be extended to other classification algorithms and used as the basis of an expert system for algorithm selection.

7.17. Simulation of SPDEs for Excitable Media Using Finite Elements

The following result has been obtained by

M. Boulakia, A. Genadot (CQFD member) and M. Thieullen.

This result concerns the question of the discretization of Stochastic Partial Differential Equations (SPDE's) for excitable media. Working with SPDE's driven by colored noise, we consider a numerical scheme based on finite differences in time (Euler-Maruyama) and finite elements in space. Motivated by biological considerations, we study numerically the emergence of reentrant patterns in excitable systems such as the Barkley or Mitchell-Schaeffer models.

7.18. Conditional quantile estimation through optimal quantization: theoretical aspects

The following result has been obtained by J. Saracco (Inria CQFD) and I. Charlier (Inria CQFD), D. Paindaveine (ULB).

In this work, we use quantization to construct a nonparametric estimator of conditional quantiles of a scalar response Y given a d-dimensional vector of covariates X. First we focus on the population level and show how optimal quantization of X, which consists in discretizing X by projecting it on an appropriate grid of N points, allows to approximate conditional quantiles of Y given X. We show that this approximation is arbitrarily good as N goes to infinity and provide a rate of convergence for the approximation error. Then we turn to the sample case and define an estimator of conditional quantiles based on quantization ideas. We prove that this estimator is consistent for its fixed-N population counterpart. The results are illustrated on a numerical example.

7.19. Conditional quantile estimation based on optimal quantization: From theory to practice

The following result has been obtained by J. Saracco (Inria CQFD) and I. Charlier (Inria CQFD), D. Paindaveine (ULB).

In this work, small-sample properties of a nonparametric estimator of conditional quantiles based on optimal quantization, that was recently introduced(Charlier et al., JSPI, 2015),are investigated. More precisely, (i) the practical implementation of this estimator is discussed (by proposing in particular a method to properly select the corresponding smoothing parameter, namely the number of quantizers) and (ii) its finite-sample performances are compared to those of classical competitors. Monte Carlo studies reveal that the quantization-based estimator competes well in all cases and sometimes dominates its competitors, particularly when the regression function is quite complex. A real data set is also treated.While the main focus is on the case of a univariate covariate, simulations are also conducted in the bivariate case.

7.20. QuantifQuantile: An R Package for Performing Quantile Regression Through Optimal Quantization

The following result has been obtained by J. Saracco (Inria CQFD) and I. Charlier (Inria CQFD), D. Paindaveine (ULB).

In this work, we describe an R package, called QuantifQuantile, that allows to perform quantization-based quantile regression. In quantile regression, various quantiles of a response variable Y are modelled as functions of covariates (rather than its mean). An important application is the construction of reference curves/surfaces and conditional prediction intervals for Y. Recently, a nonparametric quantile regression method based on the concept of optimal quantization was proposed. This method competes very well with k-nearest neighbor, kernel, and spline methods. We describe also the various functions of the package and provide examples.

7.21. Numerical methods for simulation and optimization of piecewise deterministic Markov processes

This book is focused on theoretical and numerical aspects of simulation and optimization for piecewise deterministic Markov processes (PDMP's). PDMP's have been introduced in the literature by M. Davis as a general class of stochastic hybrid models. They form a family of Markov processes involving deterministic motion punctuated by random jumps. The motion of a PDMP includes both continuous and discrete variables. The continuous state variable represents the physical parameters of the system under consideration. The discrete mode characterizes the regimes of operation of the physical system and/or the environment. The process is defined through three local characteristics, namely the flow describing the deterministic trajectory between two consecutive jumps, the intensity function giving the jump rate and the Markov kernel specifying the post-jump location. A suitable choice of the state space and these local characteristics provides stochastic models covering a large number of problems such as engineering systems, operation research, economics, management science, biology, internet traffic, networks and reliability. The class of PDMP's is thus considered and recognized as a powerful modeling tool for complex systems.

However, surprisingly few works are devoted to the development of numerical methods for PDMP's to solve problems of practical importance such as evaluation and optimization of functionals of the process. The main objective of this book consists in presenting mathematical tools recently developed by the authors to address such problems. This book is not only focused on theoretical aspects such as proof of convergence of the approximation procedures but is also concerned with its applicability to practical problems. The approach we are proposing is general enough to be applied to several application domains. In particular, our results are illustrated by examples from the field of reliability.

Our approximation technique is based on the discretization using quantization of the underlying discrete-time Markov chain given by the post-jump locations and jump times of the PDMP. This strategy enables us to address a large class of numerical problems. In particular, in this book we focus, on the one hand, on the computation of expectation of functionals of PDMP's with applications to the evaluation of service times. On the other hand, we are interested in solving optimal control problems with applications to maintenance optimization.

MATHRISK Project-Team

7. New Results

7.1. Liquidity risk

Participants: Aurélien Alfonsi, Pierre Blanc.

A. Alfonsi and P. Blanc are working on the optimal execution problem when many large traders who modify the market prices. In a previous study, they have developed a price impact model that takes into account an exogeneous flow of market orders, in which the optimal execution strategy is known explicitly. This year,they have worked on the practical implementation of this model. Namely, they have proposed an estimation procedure to estimate the model parameters (decay kernel of the price impact and Hawkes kernel for the self excitation of the order flow). They have run this estimation on market data and backtested the optimal execution strategy.

7.2. Backward stochastic (partial) differential equations with jumps, optimal stopping and stochastic control with nonlinear expectation, risk minimization

Participants: Roxana Dumitrescu, Marie-Claire Quenez [(Univ Paris 7)], Arnaud Lionnet, Agnès Sulem.

R. Dumitrescu, M.C. Quenez and A. Sulem have provided a weak dynamic principle for Combined Optimal Stopping/Stochastic Control with $\mathcal{E}^f-$conditional Expectation . They have investigated the links between generalized Dynkin games and double barriers reflected BSDEs with jumps and also studied mixed generalized Dynkin games in a Markovian framework and associated nonlinear HJB equations with barriers .

In the recent paper [43], they study game options in an imperfect market with default. They extend the results obtained by Kifer [68] in a perfect market model to the case of imperfections taken into account via the nonlinearity of the wealth dynamics. In this framework, the pricing system is expressed as a nonlinear g-expectation/evaluation induced by a nonlinear BSDE with jump. They prove that the superhedging price of a game option coincides with the value function of a corresponding *generalized* Dynkin game expressed in terms of the g-evaluation. They also address the case of ambiguity on the model, - for example an ambiguity on the default probability -, and characterize the superhedging price of a game option as the value function of a *mixed generalized* Dynkin game. They prove the existence of a cancellation time and a trading strategy which allows the seller to be super-hedged, whatever the model is. This study is introduced by the analysis of the simpler case of American options.

In collaboration with Jane Bielagt (Humbold Univ.) and Gonąlo Dos Reis (Univ. of Edimburgh), Arnaud Lionnet investigates in the effects of the social interactions of a finite set of agents on an equilibrium pricing mechanism. They consider an incomplete market where agents invest so as to minimize their risk measure. Here, agents assess risk using convex dynamic risk measures expressed by Backward Stochastic Differential Equations (BSDE). Beside the risk associated with their own economic activity, the agents compare their trading gains to that of the others, and factor this relative performance in the evaluation of their risk/satisfaction. When a derivative product is introduced to complete the market and allow agents to trade a non-financial risk factor (such as temperature), the risk of each agent is lowered, as expected. However, agents then find it in their interest to be more concerned with their relative performance. This leads them to behave more like a herd and this destabilizes the previously stable, purely financial market.

7.3. Systemic risk

Participants: Hamed Amini [EPFL], Andreea Minca [Cornell University)], Agnès Sulem, Rui Chen, Romuald Elie.

We study the issue of control of systemic risk in the framework of random graph models. The paper [16] by H. Amini, A. Minca and A. Sulem, provides important insight on the relation between the value of a financial system, connectivity and optimal intervention. More precisely, we consider a core-periphery random financial network in which links lead to the creation of projects in the outside economy but make banks prone to contagion risk. The controller seeks to maximize, under budget constraints, the value of the financial system, defined as the total value of the projects funded. Under partial information on interbank links, revealed in conjunction with the spread of contagion, the optimal control problem is shown to become a Markov decision problem. Our results show that up to a certain connectivity, the value of the financial system increases with connectivity. However, this is no longer the case if connectivity becomes too large. This insight shows that it is far from obvious that connectivity of a core bank should always be brought forward as an argument for priority intervention and it may be sometimes preferable to invest in non-core banks that lend directly to the economy. The natural question remains how to create incentives for the banks to attain an optimal level of connectivity and how to design a guarantee fund that would represent an intervention fund that can be used to maximize the benefits of connectivity. This is under study with the PhD student Rui Chen.

Moreover R. Elie obtained a CVRS PEPS grant on systemic risk modeling with graphs in collaboration with the Inria team COATI and the economic department of Université de Nice.

7.4. Dependence modeling

7.4.1. Estimation of the parameters of a Wishart process

A.Alfonsi with A. Kebaier and C. Rey have studied the Maximum Likelihood Estimator for the Wishart processes and in particular its convergence in the ergodic and in some non ergodic cases. In the non ergodic cases, their analysis rely on refined results on the Laplace transform for Wishart processes. This work also extends a recent paper by Ben Alaya and Kebaier on the maximum likelihood estimation for the CIR process.

7.5. Interest rate modeling

A. Alfonsi, E. Palidda and A. Ahdida extend the Linear Gaussian Model (LGM) by replacing the constant convariation matrix by some Wishart dynamics. This extension allows them to generate smile while keeping the affine structure of the model. They have obtained a price expansion around the LGM for Caplet and Swaption prices. They also present a second order discretization scheme that allow them to compute exotic prices within this model.

7.6. Numerical Probability

A. Alfonsi with A. Kohatsu-Higa and M. Hayashi are investigating how to apply the parametric method recently proposed by V. Bally and A. Kohatsu-Higa for reflected SDEs. This method allows them to obtain an unbiased estimator for expectations of general functions of the process.

7.7. Optimal transport

Participant: Benjamin Jourdain.

With J. Corbetta (postdoc financed by the chair financial risks), A. Alfonsi and B. Jourdain study a general formula for the time-derivative of the wasserstein distance between the time-marginals of two Markov processes. They have checked the validity of this formula for pure-jump Markov processes with a bounded intensity of jumps. They now study the extension to piecewise deterministic Markov processes.

7.8. Multitype sticky particle systems

Participant: Benjamin Jourdain.

B. Jourdain and J. Reygner study multitype sticky particle systems which can be obtained as vanishing noise limits of multitype rank-based diffusions. Rank-based diffusion processes and their multitype generalization permit to reproduce empirical features of stock markets. B. Jourdain and J. Reygner have obtained the optimal rate of convergence as the number of particles grows to infinity of the approximate solution to a diagonal system of hyperbolic conservation laws based on multitype sticky particles.

7.9. Numerical Probability

7.9.1. American option pricing.

Damien Lamberton with M. Pistorius has worked on the approximation of American options by Canadian options, which originated from the work of Peter Carr. This lead them to revise old results on the binomial approximation of the American put. D. Lamberton is also working with M. Zervos on American options involving the maximum of the underlying.

7.9.2. Convergence in total variation of approximation schemes for Markov processes

(V. Bally and PhD student C. Rey [40])

The main issue was to consider very general approximation schemes and to estimate the approximation error for test functions which are just measurable and bounded. It is worth to mention that the input of noise in the approximation schemes is allowed to be quite general, while in the standard approximation schemes for diffusion processes one considers Gaussian input only. In some sense this means that we treat invariance principles as well. We also considered approximation schemes of higher order, as the Victoir Nynomia scheme for example. An important ingredient is an abstract Malliavin calculus for general random variables (which has been settled in previous papers of V. Bally and Lucia Caramellino.

7.9.3. Approximation schemes for Piecewise Deterministic Markov Processes

(V. Bally and PhD student V.Rabiet [39]).

PDMP processes are very popular in many practical fields as biology, chemistry or fiability theory. The main idea is that such a model may present different scales: slow ones and rapid onces. And from a numerical point of view it is extremely difficult to implement algorithms which take care of rapid scales in details. Then the idea is to average the rapid scales (in the spirit of the Central Limit Theorem) and consequently to replace small (and rapid) jumps by a Brownien component. This procedure is already widely used by practitioners. Our work was to derive estimates of the error which is done by this procedure.

7.9.4. Convergence in distribution norms in the Central Limit Theorem

(V. Bally with Lucia Caramellino and Guillaume Poly)

In the classical theory, the convergence which has already been studied is the convergence in total variation (measurable test functions). The main result is the theorem of Prohorov, in the fifties. We have proved that under similar hypothesis (with more finite moments however) one may obtain a much more accurate estimate of the error, in some norms which are close to distribution norms. As a remarkable consequence, we obtained a CLT for the zeros of trigonometric polynomials with random coefficients.

TOSCA Project-Team

7. New Results

7.1. Probabilistic numerical methods, stochastic modelling and applications

Participants: Mireille Bossy, Nicolas Champagnat, Madalina Deaconu, Coralie Fritsch, Benoît Henry, James Inglis, Antoine Lejay, Oana-Valeria Lupascu, Sylvain Maire, Paolo Pigato, Alexandre Richard, Denis Talay, Etienne Tanré, Denis Villemonais.

7.1.1. Published works and preprints

- M. Bossy with H. Quinteros (UChile) submitted a paper [36] on the strong convergence of the symmetrized Milstein scheme for some CEV-like SDEs.
- M. Bossy and J.-F. Jabir (University of Valparaíso) submitted a paper [35] on the particle approximation for Lagrangian stochastic models with specular boundary condition.
- M. Bossy with N. Maizi (Mines ParisTech) and O. Pourtallier (Inria) published a book chapter [31] on game theory analysis for carbon auction market through electricity market coupling hypothesis.
- M. Bossy, O. Faugeras (Inria Sophia, EPI NEUROMATHCOMP), and D. Talay published a clarification on the well-posedness of the limit equations to the mean-field N-neuron models proposed in [58] and proven the associated propagation of chaos property. They also have completed the modeling issue in [58] by discussing the well-posedness of the stochastic differential equations which govern the behavior of the ion channels and the amount of available neurotransmitters. See [15].
- M. Bossy, N. Champagnat, S. Maire and L. Violeau worked with H. Leman (CMAP, Ecole Polytechnique) and M. Yvinec (Inria Sophia, GEOMETRICA team) on Monte Carlo methods for the linear and non-linear Poisson-Boltzmann equations [14]. These methods are based on walk on spheres algorithm, simulation of diffusion processes driven by their local time, and branching Brownian motion to deal with the nonlinear case.
- Together with M. Baar and A. Bovier (Univ. Bonn), N. Champagnat studied the adaptive dynamics of populations under the assumptions of large population, rare and small mutations [34]. In this work, the three limits are taken simultaneously, contrary to the classical approach, where the limits of large population and rare mutations are taken first, and next the limit of small mutations [59]. We therefore obtain the precise range of assumptions under which these limits can be taken, and provide explicit biological conditions for which our approximation is valid.
- N. Champagnat and C. Fritsch worked with F. Campillo (Inria Sophia-Antipolis, LEMON team) on the links between a branching process and an integro-differential equation of a growth-fragmentation-death model [37]. They proved that the two representations of the model lead to the same criteria of invasion of a population in a given environment.
- Using a new method to compute the expectation of an integral with respect to a random measure, N. Champagnat and B. Henry obtained explicit formulas for the moments of the frequency spectrum in the general branching processes known as Splitting Trees, with neutral mutations and under the infinitely-many alleles model [40]. This allows them to obtain a law of large numbers for the frequency spectrum in the limit of large time.
- N. Champagnat and P.-E. Jabin (Univ. Maryland) improved significantly the description of the functional spaces in the preprint [41], devoted to the study of strong existence and pathwise uniqueness for stochastic differential equations (SDE) with rough coefficients, typically in Sobolev spaces.

- N. Champagnat and D. Villemonais obtained criteria for existence and uniqueness of quasi-stationary distributions (QSD) and Q-processes for general absorbed Markov processes [17]. A QSD is a stationary distribution conditionally on non-absorbtion, and the Q-process is defined as the original Markov process conditioned to never be absorbed. The criteria ensure exponential convergence of the t-marginal of the process conditioned not to be absorbed at time t, to the QSD and also the exponential ergodicity of the Q-process.
- N. Champagnat and D. Villemonais obtained criteria for existence, uniqueness and exponential convergence in total variation to QSD for general absorbed and killed diffusion processes [43], [42]. For diffusions without killing [43], the criterion obtained is equivalent to the property that a diffusion on natural scale coming down from infinity has uniformly (w.r.t. the initial condition) bounded expectation at a fixed time t. The criteria obtained for diffusion processes with killing on $[0,\infty)$ [42] combine the last criteria and conditions on the killing time only close to 0, provided ∞ is an entrance boundary.
- N. Champagnat and D. Villemonais obtained criteria for existence, uniqueness and exponential convergence in total variation to QSD for general multi-dimensional birth and death processes in $\mathbb{Z}_+^d$ absorbed at the boundary $\mathbb{Z}_+^d \setminus \mathbb{N}^d$ [44]. These birth and death models are motivated by population dynamics and the criteria obtained assume stronger intra-spectific competition than inter-specific competition. These resuls are the first one for such processes, except for the particular case of branching processes, which can be studied using very specific methods.
- M. Deaconu, S. Herrmann and S. Maire introduced a new method for the simulation of the exit time and position of a δ-dimensional Brownian motion from a domain. This method is based on the connexion between the δ-dimensional Bessel process and the δ-dimensional Brownian motion thanks to an explicit Bessel hitting time distribution associated with a particular curved boundary. This allows to build a fast and accurate numerical scheme for approximating the brownian hitting time [19].
- M. Deaconu and O. Lupaşcu worked with L. Beznea (Bucharest, Romania) on the probabilistic interpretation of fragmentation phenomena. They constructed a continuous time branching process and characterized its behavior by using new potential theoretical tools [12].
- M. Deaconu, O. Lupaşcu and L. Beznea (Bucharest, Romania) started a new challenging work on the description of rupture phenomena like avalanches, by using fragmentation models. The physical properties of the model are deeply involved in this study. The first results concern a stochastic equation of fragmentation and branching processes related to avalanches [13].
- M. Deaconu, B. Dumortier and E. Vincent are working with the Venathec SAS on the acoustic control of wind farms. They constructed a new approach to control wind farms with a control model based on real-time source separation. They first designed a deterministic algorithm in order to maximize the electric production of the wind farms under the legal acoustic constraints. They showed that it is a non linear knapsack optimization problem and they proposed an efficient solution in that context using a branch and bound algorithm based on continuous relaxation. This work was published at the EWEA 2015 [30].
- In [49], B. Henry showed a central limit theorem for the population counting process of a supercritical Splitting Tree in the limit of large time. Thanks to the results of [40], he also obtained a central limit theorem for the frequency spectrum of Splitting Trees with neutral mutations and under the infinitely-many alleles model.
- S. Herrmann and E. Tanré have proposed a new very efficient algorithm to simulate the first-passage-time of a one-dimensional Brownian motion over a continuous curved boundary [23].
- J. Inglis and E. Tanré together with F. Delarue and S. Rubenthaler (Univ. Nice – Sophia Antipolis) completed their study of the mean-field convergence of a highly discontinuous particle system modeling the behavior of a spiking network of neurons [21].

- In collaboration with J. Maclaurin (Inria Sophia, EPI NEUROMATHCOMP) J. Inglis has presented a general framework to rigorously study the effect of spatio-temporal noise on traveling waves and stationary patterns. In particular the framework can incorporate versions of the stochastic neural field equation that may exhibit traveling fronts, pulses or stationary patterns. They have formulated a local SDE that describes the position of the stochastic wave up until a discontinuity time, at which point the position of the wave may jump and studied the local stability of this stochastic front and the long-time behavior of the stochastic wave [50].
- A. Lejay has continued his work on the Snapping Out Brownian motion, especially with regard to the simulation issues, with potential application to brain imaging techniques [33], [53].
- A. Lejay has continued his work on the simulation of processes with either discontinuous drift (with Arturo Kohatsu-Higa, Ritsumeikan Universitey and Kazuhiro Yasuda, Hosei University, Japan) [52] or with discontinuous coefficients (with Lionel Lenêtre and Géraldine Pichot, EPI SAGE, Irisa) [54].
- A. Lejay has continued his work on the theory of rough paths, notably with the sensitivity aspects with Laure Coutin (Univ. Toulouse III) [47].
- In collaboration with Ivan Dimov and Jean-Michel Sellier (BAS), S. Maire developed a new Monte Carlo method, called the walk on equations, to solve linear systems of equations [22].
- In collaboration with Xuan Vu, Caroline Chaux-Moulin and Nadege Thirion-Moreau, S. Maire developed a stochastic algorithm to decompose large non-negative tensors with applications in spectroscopy [28].
- In collaboration with Martin Simon, Sylvain Maire developed a variant of the walk on spheres method to deal with diffusion equations appearing in electrical impedance tomography.
- With Giang Nguyen, Sylvain Maire worked on finite differences techniques to deal with many kinds of boundary conditions that are met during the Monte Carlo simulation of diffusions [25].
- A. Richard submitted a paper [56] on the spectral representation of L^2-indexed increment-stationary processes. The main result states that any random field (i.e. process indexed by a multidimensional parameter of a function in L^2) with stationary increments can be written as an integral against a random measure satisfying certain properties. Applications to sample path properties of a multiparameter fractional Brownian motion are exhibited.
- D. Villemonais worked with P. Del Moral (Univ. Sydney) on the conditional ergodicity of time inhomogeneous diffusion processes [48]. They proved that, conditionally on non extinction, an elliptic time-inhomogeneous diffusion process forgets its initial distribution exponentially fast. An interacting particle scheme to numerically approximate the conditional distribution is also provided.
- D. Villemonais proved a Foster-Lyapunov type criterion which ensures the α-positive recurrence of birth and death processes. This criterion also provides a non-trivial subset of the domain of attraction for quasi-stationary distributions. Finally, this study leads to a Foster-Lyapunov type criterion which ensures the exponential ergodicity of a Fleming-Viot type particle system whose particles evolve as birth and death processes. The criterion also ensures the tightness of the sequence of empirical stationary distributions considered as a family of random measures. A numerical study of the speed of convergence of the particle system is also obtained under various settings [29].
- J. Inglis and D. Talay ended their work on mean-field limits of a stochastic particle system smoothly interacting through threshold hitting-times and applications to neural networks with dendritic component [51].

7.1.2. Other works in progress

- Together with M. Andrade (Univ. Paris 7) and R. Ferrière (ENS Paris and Univ. Arizona), N. Champagnat is working on the phenomenon of clustering in populations structured by space and traits for which local adaptation favors different trait values at different spatial locations. Two methods are used and numerically validated: a Turing instablity method and a Hamilton-Jacobi approximation of the population density. This work is currently being written.

- N. Champagnat and J. Claisse (Ecole Polytechnique) are currently working on the ergodic and infinite horizon controls of discrete population dynamics with almost sure extinction in finite time. This can either correspond to control problems in favor of survival or of extinction, depending on the cost function. They have proved that these two problems are related to the QSD of the processes controled by Markov controls. This work is currently being written.
- N. Champagnat and C. Fritsch worked with F. Campillo (Inria Sophia-Antipolis, LEMON team) on the variations of the principal eigenvalue (resp. the survival probability) of an integro-differential equation (resp. branching process) of growth-fragmentation-death models with respect to an environmental parameter. This work is currently being written.
- N. Champagnat, K. Coulibaly-Pasquier (Univ. Lorraine) and D. Villemonais are currently working on general criteria for existence, uniqueness and exponential convergence in total variation to QSD for multi-dimensional diffusions in a domain absorbed at its boundary. These results both improve and simplify the existing results and methods. This work is currently being written.
- N. Champagnat and D. Villemonais are currently working on extensions of their work [17] to general penalized processes, including time-inhomogeneous Markov processes with absorption. Their method allows to improve significantly the former results of [60], [61]. This work is currently being written.
- N. Champagnat and D. Villemonais are also working on extensions of the criteria of [17] in the form of Foster-Lyapunov criteria allowing to deal with cases where the convergence of conditional distribution to the QSD is not uniform with respect to the initial distribution. This work is currently being written.
- M. Deaconu and S. Herrmann are working on the numerical approach of the time-space Dirichlet problem.
- M. Deaconu, O. Lupaşcu and L. Beznea (Bucharest, Romania) worked on the numerical scheme for the simulation of an avalanche by using the fragmentation model. This work is currently being written.
- M. Deaconu, B. Dumortier and E. Vincent are working with the Venathec SAS on the acoustic control of wind farms. They plan to submit another article to IEEE transaction on sustainable energy soon. Currently they work on handling uncertainties in the model in order to design a stochastic algorithm.
- C. Fritsch worked with F. Campillo (Inria Sophia-Antipolis, LEMON team) and O. Ovaskainen (Univ. Helsinki) about the numerical analysis of the invasion of mutant populations in a chemostat, using branching processes and integro-differential models.
- C. Fritsch started a collaboration with B. Cloez (INRA, Montpellier) on a central limit theorem of mass-structured individual-based chemostat model.
- With P. Pigato, A. Lejay has continued his work on the estimation of parameters of skew diffusions.
- Within the ANESTOC Associate Team, R. Rebolledo (Pontificia Universidad Católica de Chile) and A. Richard initiated a work on the long-term behavior of a class of non-Markovian stochastic differential equations. These equations of Volterra type can be used to model the motion of a particle subject to friction forces in a heat bath, which could also be interesting in neuroscience for ion channels.
- A. Richard and E. Tanré are working with P. Orio (CINV, Chile) on the measurement of long-range dependence in series of neuronal spikes, and are providing a leaky integrate-and-fire model with fractional noise to include this effect. So far, we produced numerical experiments that confirm the existence of memory in our model, and A. Richard and E. Tanré now work on the convergence of the statistical estimator that measures this phenomenon.

- A. Richard, E. Tanré and S. Torres (Universidad de Valparaíso, Chile) are working on the definition of a skew fractional Brownian motion. The skew Brownian motion (sBm) is a process which is partly reflected when it reaches the horizontal line, making it a natural model for the motion of a particle crossing media with different diffusion properties. The fractional sBm is a modification of this process to incorporate long-range dependences. So far, we constructed a reflected fractional Brownian motion, and we are now investigating its approximation by a discrete-time process.
- During her internship supervised by E. Tanré and Romain Veltz (NEUROMATHCOMP team), Roberta Evangelista worked on "A stochastic model of gamma phase modulated orientation selectivity". Neurons in primary visual cortex (V1) are known to be highly selective for stimulus orientation. Recent experimental evidence has shown that, in awake monkeys, the orientation selectivity of V1 neurons is modulated by gamma oscillations. In particular, neurons' firing rate in response to the preferred orientation changes as a function of the gamma phase of spiking. The effect is drastically reduced for non-preferred orientations. We have introduced a stochastic model of a network of orientation-dependent excitatory and inhibitory spiking neurons. We have found conditions on the parameters such that the solutions of the mathematical model reproduce the experimental behavior.
- During his internship supervised by E. Tanré and Romain Veltz (NEUROMATHCOMP team), Quentin Cormier studies numerically and theoretically a model of spiking neuron in interaction with plasticity. The synaptic weights evolve according to biological law of plasticity. We study the existence of separable time scales. During his internship, Quentin Cormier also develop a numerical code to simulate large networks of neurons evolving according to this dynamics.
- C. Graham (Ecole Polytechnique) and D. Talay have written a large part of the second volume of their series on Mathematical Foundation of Stochastic Simulation.

7.2. Financial Mathematics

Participants: Mireille Bossy, Madalina Deaconu, Antoine Lejay, Sylvain Maire, Khaled Salhi, Denis Talay, Etienne Tanré.

7.2.1. Published works and preprints

- In collaboration with Jerome Lelong and Christophe Deluigi, Sylvain Maire built a new algorithm for the automatic integration and approximation of irregular functions [18]. This algorithm is tested numerically on the pricing of multidimensional exotic options.
- In collaboration with V. Reutenauer and C. Michel (CA-CIB), D. Talay and E. Tanré worked on a model in financial mathematics including bid-ask spread cost. They study the optimal strategy to hedge an interest rate swap that pays a fixed rate against a floating rate. They present a methodology using a stochastic gradient algorithm to optimize strategies. A paper is in revision [55].

7.2.2. Other works in progress

- K. Salhi works on partial hedging of options in an incomplete market, under constraints on the initial capital of the investor and assuming that the stock price is described by a Lévy process. In this case, perfect hedging is no more possible and we talk about partial hedging and minimization of risk. K. Salhi focuses on the Conditional Value-at-Risk minimization. He tries to give a numerical approximation to the solution in this context.
- In collaboration with J. Bion-Nadal (Ecole Polytechnique and CNRS), D. Talay pursued the study of a new calibration methodology based on dynamical risk measures and stochastic control PDEs.