
IN PARTNERSHIP WITH:
**Ecole des Ponts ParisTech**

# Activity Report 2017

# Project-Team MATHERIALS

## MATHematics for MatERIALS

IN COLLABORATION WITH: Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique (CERMICS)

RESEARCH CENTER
**Paris**

THEME
**Numerical schemes and simulations**

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*Creation of the Team: 2014 January 01, updated into Project-Team: 2015 April 01*

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# 1. Personnel

**Research Scientists**

Claude Le Bris [Team leader, École Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Sébastien Boyaval [École Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Éric Cancès [École Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Virginie Ehrlacher [École Nationale des Ponts et Chaussées, Researcher]
Frédéric Legoll [École Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Tony Lelièvre [École Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Antoine Levitt [Inria, Researcher]
Gabriel Stoltz [École Nationale des Ponts et Chaussées, Senior Researcher, HDR]

**Post-Doctoral Fellows**

Dena Kazerani [Inria, from Oct 2017]
Pierre Monmarché [Inria, until Aug 2017]

**PhD Students**

Grégoire Ferré [École Nationale des Ponts et Chaussées]
Marc Josien [Ministère de la Transition écologique et solidaire]
Adrien Lesage [École Nationale des Ponts et Chaussées, from Oct 2017]

Boris Nectoux [École Nationale des Ponts et Chaussées and Inria, until Nov 2017]
Mouad Ramil [École Nationale des Ponts et Chaussées, from Oct 2017]
Pierre-Loïk Rothé [École Nationale des Ponts et Chaussées]
Julien Roussel [École Nationale des Ponts et Chaussées]
Laura Silva Lopes [École Nationale des Ponts et Chaussées]
Sami Siraj-Dine [Université Paris-Est, from Oct 2017]
Pierre Terrier [Ministère de la Transition écologique et solidaire]

**Interns**

Adrien Lesage [Inria, from May 2017 until Sep 2017]
Sami Siraj-Dine [Inria, from Apr 2017 until Jul 2017]

**Administrative Assistants**

Kevin Bonny [Inria, from Jun 2017 until Sep 2017]
Sabrine Boumizy [Inria, from Oct 2017]
Sarah Le [Inria, from Jan 2017 until May 2017]

# 2. Overall Objectives

## 2.1. Overall Objectives

The MATHERIALS project-team has been created jointly by the École des Ponts ParisTech (ENPC) and Inria in 2015. It is the follow-up and an extension of the former project-team MICMAC originally created in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques et Calcul Scientifique) at École des Ponts. The permanent research scientists of the project-team have positions at CERMICS and at two other laboratories of École des Ponts: Institut Navier and Laboratoire Saint-Venant. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulation of computational chemistry at the microscopic level and to create simulations coupling this microscopic scale with meso- or macroscopic scales (possibly using parallel algorithms). Over the years, the project-team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the project-team is to have created a corpus of literature, authoring books and research monographs on the subject [1], [2], [3], [5], [6] that other scientists may consult in order to enter the field.

# 3. Research Program

## 3.1. Research Program

Quantum Chemistry aims at understanding the properties of matter through the modelling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström ($10^{-10}$ meters), and the size of the nucleus embedded in it is $10^{-15}$ meters; the typical vibration period of a molecular bond is the femtosecond ($10^{-15}$ seconds), and the characteristic

relaxation time for an electron is $10^{-18}$ seconds. Consequently, Quantum Chemistry calculations concern very short time (say $10^{-12}$ seconds) behaviors of very small size (say $10^{-27}$ m$^3$) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability of minerals to naturally split along crystal surfaces (e.g. mica yields to thin flakes), is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time-dependent form or in its time-independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its $L^2$ norm is set to one.

The time-dependent equation is a first-order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of $L^2(\mathbb{R}^d)$, with $d = 3(M + N)$, $M$ and $N$ respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter $d$ is already 39 for a single water molecule and rapidly reaches $10^6$ for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is $10^4$ times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on $L^2(\mathbb{R}^3)$. The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the

focus has progressively shifted to problems at other scales. Such problems are described in the following sections.

# 4. Application Domains

## 4.1. Electronic structure of large systems

As the size of the systems one wants to study increases, more efficient numerical techniques need to be resorted to. In computational chemistry, the typical scaling law for the complexity of computations with respect to the size of the system under study is $N^3$, $N$ being for instance the number of electrons. The Holy Grail in this respect is to reach a linear scaling, so as to make possible simulations of systems of practical interest in biology or material science. Efforts in this direction must address a large variety of questions such as

- how can one improve the nonlinear iterations that are the basis of any *ab initio* models for computational chemistry?
- how can one more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?
- how can one design a sufficiently small variational space, whose dimension is kept limited while the size of the system increases?

An alternative strategy to reduce the complexity of *ab initio* computations is to try to couple different models at different scales. Such a mixed strategy can be either a sequential one or a parallel one, in the sense that

- in the former, the results of the model at the lower scale are simply used to evaluate some parameters that are inserted in the model for the larger scale: one example is the parameterized classical molecular dynamics, which makes use of force fields that are fitted to calculations at the quantum level;
- while in the latter, the model at the lower scale is concurrently coupled to the model at the larger scale: an instance of such a strategy is the so called QM/MM coupling (standing for Quantum Mechanics/Molecular Mechanics coupling) where some part of the system (typically the reactive site of a protein) is modeled with quantum models, that therefore accounts for the change in the electronic structure and for the modification of chemical bonds, while the rest of the system (typically the inert part of a protein) is coarse grained and more crudely modeled by classical mechanics.

The coupling of different scales can even go up to the macroscopic scale, with methods that couple a microscopic representation of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

## 4.2. Computational Statistical Mechanics

The orders of magnitude used in the microscopic representation of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 6 \times 10^{23}$, the typical distances are expressed in Å ($10^{-10}$ m), the energies are of the order of $k_{\mathrm{B}}T \simeq 4 \times 10^{-21}$ J at room temperature, and the typical times are of the order of $10^{-15}$ s.

To give some insight into such a large number of particles contained in a macroscopic sample, it is helpful to compute the number of moles of water on earth. Recall that one mole of water corresponds to 18 mL, so that a standard glass of water contains roughly 10 moles, and a typical bathtub contains $10^5$ mol. On the other hand, there are approximately $10^{18}$ m$^3$ of water in the oceans, *i.e.* $7 \times 10^{22}$ mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating $\mathcal{N}_A$ atoms and performing $\mathrm{O}(10^{15})$ time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of a few microseconds.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of $N$ particles correctly approximate the macroscopic property, formally obtained in the thermodynamic limit $N \to +\infty$ (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

Despite its intrinsic limitations on spatial and timescales, molecular simulation has been used and developed over the past 50 years, and its number of users keeps increasing. As we understand it, it has two major aims nowadays.

First, it can be used as a *numerical microscope*, which allows us to perform "computer" experiments. This was the initial motivation for simulations at the microscopic level: physical theories were tested on computers. This use of molecular simulation is particularly clear in its historic development, which was triggered and sustained by the physics of simple liquids. Indeed, there was no good analytical theory for these systems, and the observation of computer trajectories was very helpful to guide the physicists' intuition about what was happening in the system, for instance the mechanisms leading to molecular diffusion. In particular, the pioneering works on Monte-Carlo methods by Metropolis *et al.*, and the first molecular dynamics simulation of Alder and Wainwright were performed because of such motivations. Today, understanding the behavior of matter at the microscopic level can still be difficult from an experimental viewpoint (because of the high resolution required, both in time and in space), or because we simply do not know what to look for! Numerical simulations are then a valuable tool to test some ideas or obtain some data to process and analyze in order to help assessing experimental setups. This is particularly true for current nanoscale systems.

Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative answers. Sometimes, these properties are accessible through experiments, but in some cases only numerical computations are possible since experiments may be unfeasible or too costly (for instance, when high pressure or large temperature regimes are considered, or when studying materials not yet synthesized). More generally, molecular simulation is a tool to explore the links between the microscopic and macroscopic properties of a material, allowing one to address modelling questions such as "Which microscopic ingredients are necessary (and which are not) to observe a given macroscopic behavior?"

## 4.3. Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on how to couple models written at the atomistic scale with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

The following observation motivates the idea of coupling atomistic and continuum representation of materials. In many situations of interest (crack propagation, presence of defects in the atomistic lattice, ...), using a model based on continuum mechanics is difficult. Indeed, such a model is based on a macroscopic constitutive law, the derivation of which requires a deep qualitative and quantitative understanding of the physical and mechanical properties of the solid under consideration. For many solids, reaching such an understanding is a challenge, as loads they are subjected to become larger and more diverse, and as experimental observations

helping designing such models are not always possible (think of materials used in the nuclear industry). Using an atomistic model in the whole domain is not possible either, due to its prohibitive computational cost. Recall indeed that a macroscopic sample of matter contains a number of atoms on the order of $10^{23}$. However, it turns out that, in many situations of interest, the deformation that we are looking for is not smooth in *only a small part* of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them, in a domain decomposition spirit. In most of the domain, the deformation is expected to be smooth, and reliable continuum mechanics models are then available. In the rest of the domain, the expected deformation is singular, so that one needs an atomistic model to describe it properly, the cost of which remains however limited as this region is small.

From a mathematical viewpoint, the question is to couple a discrete model with a model described by PDEs. This raises many questions, both from the theoretical and numerical viewpoints:

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to provide a good description of the materials;
- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

More generally, the presence of numerous length scales in material science problems represents a challenge for numerical simulation, especially when some *randomness* is assumed on the materials. It can take various forms, and includes defects in crystals, thermal fluctuations, and impurities or heterogeneities in continuous media. Standard methods available in the literature to handle such problems often lead to very costly computations. Our goal is to develop numerical methods that are more affordable. Because we cannot embrace all difficulties at once, we focus on a simple case, where the fine scale and the coarse-scale models can be written similarly, in the form of a simple elliptic partial differential equation in divergence form. The fine scale model includes heterogeneities at a small scale, a situation which is formalized by the fact that the coefficients in the fine scale model vary on a small length scale. After homogenization, this model yields an effective, macroscopic model, which includes no small scale. In many cases, a sound theoretical groundwork exists for such homogenization results. The difficulty stems from the fact that the models generally lead to prohibitively costly computations. For such a case, simple from the theoretical viewpoint, our aim is to focus on different practical computational approaches to speed-up the computations. One possibility, among others, is to look for specific random materials, relevant from the practical viewpoint, and for which a dedicated approach can be proposed, that is less expensive than the general approach.

# 5. Highlights of the Year

## 5.1. Highlights of the Year

### *5.1.1. Awards*

E. Cancès was awarded the 2017 Dargelos Prize from the Alumni of Ecole Polytechnique.

# 6. New Software and Platforms

## 6.1. simol

KEYWORDS: Molecular simulation - Quantum chemistry - Statistical physics - C++ - OpenMP
FUNCTIONAL DESCRIPTION: Molecular simulation software written in C++

- Contact: Gabriel Stoltz

# 7. New Results

## 7.1. Electronic structure calculations

**Participants:** Éric Cancès, Virginie Ehrlacher, Antoine Levitt, Sami Siraj-Dine, Gabriel Stoltz.

In electronic structure calculation as in most of our scientific endeavors, we pursue a twofold goal: placing the models on a sound mathematical grounding by an appropriate mathematical analysis, and improving the numerical approaches by a dedicated numerical analysis. We also insist on rigorously studying current materials of technological interest.

### *7.1.1. Mathematical analysis*

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

### *7.1.2. Numerical analysis*

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

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

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

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

### *7.1.3. New materials*

As an external collaborator of the MURI project on 2D materials (PI: M. Luskin), E. Cancès has collaborated with P. Cazeaux (Kansas) and M. Luskin (University of Minnesota) on the computation of the electronic and optical properties of multilayer 2D materials. In particular, they have adapted the $C^*$-algebra framework for aperiodic solids introduced by J. Bellissard and collaborators, to the case of tight-binding models of incommensurate (and possibly disordered) multilayer systems [13].

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

## 7.2. Computational Statistical Physics

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

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

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

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

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

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

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

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

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

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

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

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

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

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

### 7.2.4. Coarse-graining

In [25], F. Legoll and T. Lelièvre, in collaboration with S. Olla (Dauphine), analyzed the error introduced when deriving an effective dynamics for a stochastic process in large dimension on a few degrees of freedom using a projection approach *à la Zwanzig*. More precisely, a pathwise error estimate was obtained, which is an improvement compared to a previous result by F. Legoll and T. Lelièvre where only the marginal in times were considered. This analysis is also useful to obtain quantitative estimate for some averaging procedure on two-scale dynamics.

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

In [28], a joint work with Manuel Athènes, Thomas Jourdan (CEA/Saclay SRMP) and Gilles Adjanor (EDF R&D, MMC), G. Stoltz and P. Terrier presented a coupling algorithm for cluster dynamics. Rate equation cluster dynamics (RECD) is a mean field technique where only defect concentrations are considered. It consists in solving a large set of ODEs (one equation per cluster type) governing the evolution of the concentrations. Since clusters might contain up to million of atoms or defects, the number of equations becomes very large. Therefore solving such a system of ODEs becomes computationally prohibitive as the cluster sizes increase. Efficient deterministic simulations propose an approximation of the equations for large clusters by a single Fokker-Planck equations. Nevertheless this approach is still limited by the number of equations to solve in the case of complex materials. Fully stochastic simulations see the RECD as a master equation, hence reducing

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

## 7.3. Homogenization

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

### *7.3.1. Deterministic non-periodic systems*

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

### *7.3.2. Stochastic homogenization*

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

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

### *7.3.3. Multiscale Finite Element approaches*

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

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

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

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

### *7.3.4. Dislocations*

In the context of the PhD thesis of M. Josien, some results have been obtained regarding the modeling and numerical simulation of dislocations. Plastic properties of crystals are due to dislocations, which are thus objects of paramount importance in materials science. The geometrical shape of dislocations may be described by (possibly time-dependent) nonlinear integro-differential equations (e.g. the Weertman equation and the dynamical Peierls-Nabarro equation), involving non-local operators.

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

## 7.4. Complex fluids

**Participants:** Sébastien Boyaval, Dena Kazerani.

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

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

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

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

## 7.5. Various topics

**Participant:** Virginie Ehrlacher.

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

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

# 8. Bilateral Contracts and Grants with Industry

## 8.1. Contracts and grants with Industry

Many research activities of the project-team are conducted in close collaboration with private or public companies: CEA, SANOFI, IRDEP, EDF, IFPEN. The project-team is also supported by the Office of Naval Research and the European Office of Aerospace Research and Development, for multiscale simulations of random materials. All these contracts are operated at and administrated by the École des Ponts.

# 9. Partnerships and Cooperations

## 9.1. National Initiatives

The project-team is involved in several ANR projects:

- S. Boyaval is the PI of the ANR JCJC project SEDIFLO (2016-2020) to investigate new numerical models of solid transport in rivers.
- G. Stoltz is the PI of the ANR project COSMOS (2014-2018) which focuses on the development of efficient numerical techniques to simulate high-dimensional systems in molecular dynamics and computational statistics. It includes research teams from Institut Mines-Telecom, Inria Rennes and IBPC Paris.
- E. Cancès is a member of the ANR project BECASIM (2013-2017), PI: I. Danaila (Université de Rouen). This project is concerned with the numerical simulation of Bose-Einstein condensates.
- F. Legoll is a member of the ANR project CINE-PARA (2015-2019), PI: Y. Maday, UPMC. This project is concerned with parallel-in-time algorithms.

Members of the project-team are participating in the following GdR:

- CORREL (correlated methods in electronic structure computations),
- EGRIN (gravity flows),
- MANU (MAthematics for NUclear applications)
- MASCOT-NUM (stochastic methods for the analysis of numerical codes),
- MEPHY (multiphase flows)
- DYNQUA (time evolution of quantum systems, with applications to transport problems, nonequilibrium systems, etc.),
- REST (theoretical spectroscopy),
- CHOCOLAS (experimental and numerical study of shock waves).

The project-team is involved in two Labex, namely the Labex Bezout (started in 2011) and the Labex MMCD (started in 2012).

## 9.2. European Initiatives

The ERC consolidator Grant MSMATH (ERC Grant Agreement number 614492, PI T. Lelièvre) is running (it started in June 2014).

## 9.3. International Initiatives

The *Germaine de Staël* grant awarded to S. Boyaval (from CampusFrance Hubert-Curien program) has been used in 2017 to pursue the collaboration with A. Caboussat (Lausanne) about 3D numerical simulations of free-surface flows.

T. Lelièvre, G. Stoltz and F. Legoll participate in the Laboratoire International Associé (LIA) CNRS / University of Illinois at Urbana-Champaign on complex biological systems and their simulation by high performance computers. This LIA involves French research teams from Université de Nancy, Université de Lyon and Université Aix-Marseille. The LIA is renewed for 4 years, starting January 1st, 2018.

# 10. Dissemination

## 10.1. Promoting Scientific Activities

E. Cancès

- is the director of CERMICS, the Applied Mathematics department at École des Ponts,
- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-), SIAM Journal of Scientific Computing (2008-), Communications in Mathematical Sciences (2011-), SIAM Multiscale Modeling and Simulation (2012-), and the Journal of Computational Mathematics (2017-),
- was a member of the executive committee of the CEA-EDF-Inria schools in applied mathematics and computer science (2010-July 2017),
- is co-organizing the IMA Long Program on Multiscale Mathematics and Computing in Science and Engineering, 2017-2018.

V. Ehrlacher

- is a member of the "Conseil d'Enseignement et de Recherche" of Ecole des Ponts,
- has co-organized the Oberwolfach workshop on "Applications of Optimal Transportation in the Natural Sciences", January 2017 (with J.-D. Benamou and D. Matthes),
- has co-organized a minisymposium on "Numerical methods for electronic structure calculations" at the SIAM CSE conference, February 2017 (with B. Stamm, L. Lin and C. Yang),
- has co-organized the IPAM workshop on "Uncertainty Quantification for Stochastic Systems and Applications", November 2017 (with M. Katsoulakis, T. Lelièvre, P. Plechac, A. Stuart and D. Trinkle).

G. Ferré and J. Roussel co-organize the working group J-PSI (Jeunes chercheurs en physique statistique et interactions) at IHP, which aims at stimulating interactions between PhD students and post-docs coming from different institutions in Paris and working on the analysis of models in statistical physics.

C. Le Bris is editor-in-chief of Applied Mathematics Research Express (2003-2017). He is a managing editor of Networks and Heterogeneous Media. He is a member of the editorial boards of Annales mathématiques du Québec (2013-), Archive for Rational Mechanics and Analysis (2004-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Nonlinearity (2005-) and Journal de Mathématiques Pures et Appliquées (2009-).

He is a member of the editorial boards of the monograph series Mathématiques & Applications, Series, Springer (2008-), Modelling, Simulations and Applications, Series, Springer (2009-), Springer Monographs in Mathematics, Springer (2016-).

He is a member of

- the Cabinet of the High Commissioner for Atomic Energy,
- the "Comité d'experts" for the Fondation de Recherche pour l'Aéronautique et l'Espace,
- the "International Scientific Advisory Committee" of the Centre de Recherche Mathématique, Université de Montréal,
- the "Advisory Board" of the DFG Cluster of Excellence Engineering of Advanced Materials, Erlangen,
- the "International Scientific Advisory Board" of the DFG research center Matheon, Berlin,
- the "Conseil scientifique de la SMAI" (Scientific Council of the French Applied Maths Society),
- the International Mathematical Union Circle.

He is the president of the strategic committee of the Institut des Sciences du calcul et des données, Sorbonne Universités.

He has held a regular position of Visiting Professor at the University of Chicago.

F. Legoll is a member of the editorial board of SIAM MMS (2012-) and of ESAIM: Proceedings and Surveys (2012-).

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings and Surveys (with D. Chafai, C. Imbert and P. Lafitte),
- is a member of the "Conseil d'Administration" of SMAI and École des Ponts,
- has co-organized the Journées EDP-Probas at Institut Henri Poincaré (with F. Malrieu),
- has co-organized the IPAM Long Program on "Complex High-Dimensional Energy Landscapes", September 11th - December 15th 2017 (with C. Clementi, G. Henkelman, R. Hennig, M. Luskin, N. Marom, P. Plechac and C. Schuette),
- has co-organized the ICTS program on "Large deviation theory in statistical physics: Recent advances and future challenges", August 14th - October 13th 2017 (with A. Ayyer, F. den Hollander, A. Dhar, J.P. Garrahan, C. Jarzynski, M. Krishnapur, S. Sabhapandit and H. Touchette),
- has co-organized with Florent Malrieu and Pierre-André Zitt the workshop "Piecewise Deterministic Markov Processes and sampling", January 25-27th, 2017,
- has co-organized with C. Chipot and G. Stoltz the "Rencontre Math-Industrie simulation moléculaire dans l'industrie pharmaceutique", at IHP on 28th April 2017,
- has co-organized with A. Jentzen the Stochastic Computation Workshop at FoCM 2017, Barcelona, July 10th-12th, 2017.

G. Stoltz

- is a member of the scientific council of UNIT (Université Numérique Ingénierie et Technologie),
- has co-organized the IHP trimester "Stochastic Dynamics Out of Equilibrium", Spring 2017 (with G. Giacomin, S. Olla, E. Saada and H. Spohn).

## 10.2. Teaching - Supervision - Juries

The members of the project-team have taught the following courses:

- Licence: Outils mathématiques pour l'ingénieur, 15h, L3, École des Ponts (E. Cancès, V. Ehrlacher, M. Josien, F. Legoll, T. Lelièvre),
- Licence: Analyse et calcul scientifique, 30h, L3, École des Ponts (G. Ferré, A. Levitt, M. Josien, G. Stoltz),
- Licence: Projet de 1ère Année, 6h, L3, École des Ponts (J. Roussel, P. Terrier),
- Licence: Mathématiques, 36h, L1, Université Paris Dauphine (G. Ferré, J. Roussel),
- Licence: Optimisation, 15h, L3, École des Ponts (A. Levitt),
- Licence: Équations aux dérivées partielles et éléments finis, 15h, L3, École des Ponts (F. Legoll, A. Levitt),
- Licence: Méthodes numériques pour les problèmes en grande dimension, 17h30, L3, École des Ponts (V. Ehrlacher, S. Boyaval),
- Licence: Maths 1 et 2, 9h, L3, École des Mines (G. Stoltz),
- Licence: méthodes pour la grande dimension, L3, École des Ponts (V. Ehrlacher 10h, S. Boyaval 5h),
- Licence: hydraulique numérique, 15h, L3, École des Ponts (S. Boyaval),
- Master: Modéliser Programmer Simuler, 28 h, M1, École des Ponts (T. Lelièvre),
- Master: Analyse variationnelle des équations aux dérivées partielles, 32h, École Polytechnique (T. Lelièvre),
- Master: Aléatoire, 32h, École Polytechnique (T. Lelièvre),
- Master: Simulation moléculaire, 6h, UVSQ (T. Lelièvre, G. Stoltz),
- Master: Analyse de Fourier, 15h, M1, École des Ponts (V. Ehrlacher, A. Levitt, G. Stoltz),
- Master: Partial differential equations, 21h, M1, École des Ponts (E. Cancès),
- Master: Control of dynamical systems, 16h, M1, École Polytechnique (E. Cancès),
- Master: Projet du département IMI, 12h, M1, École des Ponts (J. Roussel, G. Ferré),
- Master: Analyse spectrale et application aux Équations aux dérivées partielles, 36h, M1, École des Ponts (F. Legoll, V. Ehrlacher),
- Master: Spectral theory and variational methods, 10h, M2, UPMC (E. Cancès),
- Master: Méthodes de quantification des incertitudes en ingénierie, 18h, M2, École des Ponts (V. Ehrlacher),
- Master: Simulation moléculaire en sciences des matériaux, 6h, M1, École des Ponts (V. Ehrlacher),
- Master: Introduction to computational statistical physics, 20h, M2, UPMC (G. Stoltz),
- Master: Méthodes numériques probabilistes, 36 h, M2, UPMC (T. Lelièvre),
- Master: Problèmes multiéchelles, aspects théoriques et numériques , 20h, M2, UPMC (F. Legoll).

The following Habilitation thesis has been defended in the group at École des Ponts:

- Sébastien Boyaval, Topics in the numerical modelling of flows, Université Paris-Est, defended on December 21 2017.

The following PhD theses have been defended in the group at École des Ponts:

- Athmane Bakhta, Modélisation and simulation for photovoltaic applications, Université Paris-Est, École des Ponts, defended on December 19th, 2017, supervised by E. Cancès and T. Lelièvre, co-supervised by V. Ehrlacher,
- Gérôme Faure, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, École des Ponts and CEA/DAM, defended on November 29th 2017, supervised by G. Stoltz and J.-B. Maillet (CEA/DAM),
- Alessandra Iacobucci, Nonequilibrium steady-states of rotor and oscillator chains, defended on October 20th 2017, University Paris Dauphine, supervised by S. Olla (Dauphine) and G. Stoltz,
- Henri Louvin, Development of adaptive variance reduction methods for Monte Carlo particle transport, Ecole Doctorale PHENIICS, defended on October 12th, supervised by Check Diop (CEA) and T. Lelièvre,
- Boris Nectoux, Spectral analysis and semi-classical analysis for metastability in molecular dynamics, Université Paris-Est, École des Ponts, defended on November 20th, supervised by T. Lelièvre and E. Cancès.

The following PhD theses are ongoing in the group at École des Ponts:

- Amina Benaceur, Thèse CIFRE EDF, started January 1st, 2016, supervised by A. Ern, co-supervised by V. Ehrlacher, in collaboration with G. Blatman (EDF) and S. Meunier (EDF),
- Lingling Cao, Mathematical analysis of models of thermo-electronic transport, Université Paris-Est, École des Ponts, started November 1st, 2016, supervised by E. Cancès and G. Stoltz,
- Rafaël Coyaud, Méthodes numériques déterministes et stochastiques pour le transport optimal, Université Paris-Est, École des Ponts, started October 1st, 2017, supervised by A. Alfonsi and co-supervised by V. Ehrlacher,
- Qiming Du, Mathematical analysis of splitting methods, École Doctorale Sciences Mathématiques de Paris Centre, started September 1st, 2016, supervised by A. Guyader (UPMC) and T. Lelièvre,
- Grégoire Ferré, Efficient sampling methods for nonequilibrium systems, Université Paris-Est, École des Ponts started October 1st, 2016, supervised by G. Stoltz,
- Marc Josien, Multiscale approaches for materials science, started September 1st, 2015, supervised by C. Le Bris,
- Sofiane Martel, Modélisation de la turbulence par mesures invariantes d'EDPS, Université Paris-Est, École des Ponts, started January 1st, 2017, supervised by S. Boyaval and co-supervised by J. Reygner (CERMICS),
- Julien Roussel, Variance reduction techniques for nonequilibrium systems, Université Paris-Est, École des Ponts, started September 1st, 2015, supervised by G. Stoltz,
- Pierre-Loïk Rothé, Numerical methods for the estimation of fluctuations in multi-scale materials and related problems, started October 1st, 2016, supervised by F. Legoll,
- Mouad Ramil, Metastability for interacting particle systems, started October 1st 2017, supervised by T. Lelièvre and J. Reygner (CERMICS),
- Laura Silva Lopes, Rare event simulation and applications to biological systems, started October 1st, 2016, supervised by J. Hénin (IBPC) and T. Lelièvre,
- Sami Siraj-Dine, Modélisation mathématique des matériaux 2D, École des Ponts, started October 2017, supervised by E. Cancès, C. Fermanian and co-supervised by A. Levitt,
- Pierre Terrier, Reduced models for defect migration in metals, Université Paris-Est, École des Ponts and CEA Saclay, started September 1st, 2015, supervised by G. Stoltz and M. Athènes (CEA).

Project-team members have participated in the following PhD juries:

- S. Boyaval, PhD of Riad Sanchez (“Application des techniques de bases réduites à la simulation des écoulements poreux”), defended at IFPEN in December 2017,
- E. Cancès, PhD of Geneviève Dusson, defended at UPMC in October 2017,
- E. Cancès, PhD of Chaoyu Quan, defended at UPMC in November 2017,
- V. Ehrlacher, PhD of Xianglong Duang (“Transport optimal et diffusion de courants”), defended at Université Paris-Saclay in September 2017,
- V. Ehrlacher, PhD of Eleonora Musharbash (“Dynamical Low Rank approximation for PDEs with random parameters”), defended at EPFL in May 2017,
- V. Ehrlacher, PhD of Julien Ricaud (“Symétrie et brisure de symétrie pour certains problèmes non linéaires”), defended at Université de Cergy-Pontoise in June 2017,
- V. Ehrlacher, PhD of Pierre-Éric Allier (“Contrôle d’erreur pour et par les modèles réduits PGD”), defended at ENS Paris-Saclay in November 2017,
- V. Ehrlacher, PhD of Quentin Ayoul-Guilmard (“Méthodes numériques pour la prise en compte de défauts aléatoires en mise en forme de composites quasi-périodiques”), defended at Ecole Centrale Nantes in December 2017,
- T. Lelièvre, referee for the PhD of Arthur Talpaert (“Simulation numérique directe de bulles sur maillage adaptatif avec algorithmes distribuées”, defended at Ecole Polytechnique in February 2017,
- T. Lelièvre, PhD of Romain Poncet (“Méthodes numériques pour la simulation d’équations aux dérivées partielles stochastiques non-linéaires en condensation de Bose-Einstein”, defended at Ecole Polytechnique in October 2017,
- T. Lelièvre, president of the jury for the PhD of Manon Baudel (“Théorie spectrale pour des applications de Poincaré aléatoires”), defended at Université d’Orléans in December 2017,
- T. Lelièvre, referee for the PhD of Riad Sanchez (“Application des techniques de bases réduites à la simulation des écoulements en milieux poreux”), defended at Université Paris Saclay in December 2017,
- G. Stoltz, referee for the PhD of Romain Poncet (“Méthodes numériques pour la simulation d’éequations aux dérivées partielles stochastiques non-linéaires en condensation de Bose-Einstein”), defended at École Polytechnique in October 2017,
- G. Stoltz, referee for the PhD of Viviana Letizia (“Modèles microscopiques pour la loi de Fourier”), defended at Université Paris Dauphine in December 2017.

Project-team members have participated in the following habilitation jury:

- T. Lelièvre, HDR of Fabio Pietrucci (“Inventing general simulation methods to study the transformations of matter”), defended at UPMC on December 1st 2017.

## 10.3. Conference participation

Members of the project-team have delivered lectures in the following seminars, workshops and international conferences:

- S. Boyaval, Finite-Element for Flows, Roma, April 2017,
- S. Boyaval, RWTH AICS colloquim, Aachen, November 2017,
- S. Boyaval, weekly seminar of Collège de France, Paris, December 2017,
- E. Cancès, workshop on New trends in Mathematical Physics at the interface of Analysis and Probability, University College London, England, February 2017,
- E. Cancès, SIAM conference on Scientific Computing, Atlanta, Georgia, February 2017,
- E. Cancès, Mathematical Physics seminar, Université Paris Dauphine, March 2017,

- E. Cancès, weekly seminar of the Mathematics department, University of Metz, March 2017,
- E. Cancès, workshop on Wavelet and Tensor Methods for Partial Differential Equations, Berlin, May 2017,
- E. Cancès, IMA workshop on Mathematical Modeling of 2D Materials, Minneapolis, Minnesota, May 2017,
- E. Cancès, weekly seminar of the Mathematics department, Peking University, Beijing, China, June 2017,
- E. Cancès, workshop on Focus activity on quantum and kinetic problems, Beijing, China, June 2017,
- E. Cancès, BIRS workshop on Mathematical and Numerical Methods for Time-Dependent Quantum Mechanics from Dynamics to Quantum Information, Oaxaca, Mexico, August 2017,
- E. Cancès, workshop on Advances in mathematical modelling and numerical simulation of superfluids, University of Rouen, August 2017,
- E. Cancès, Colloquium lecture, University of Kansas, Lawrence, Kansas, September 2017,
- E. Cancès, workshop on Multiscale Theory and Computation, Minneapolis, Minnesota, September 2017,
- E. Cancès, MOANSI workshop, Aachen, Germany, October 2017,
- V. Ehrlacher, Demi-journée d'échange Labex Bézout/EADS, Marne-la-Vallée, October 2017,
- V. Ehrlacher, Seminar Institut für Numerische Simulation, Bonn, Allemagne, November 2017,
- V. Ehrlacher, IPAM workshop on "Uncertainty Quantification for Stochastic Systems and Applications", Los Angeles, California, November 2017,
- V. Ehrlacher, MORTECH 2017 (keynote lecture), Sevilla, Spain, November 2017,
- V. Ehrlacher, Oberwolfach workshop on "Multiscale and High-Dimensional Problems", Oberwolfach, Germany, April 2017,
- V. Ehrlacher, Conference in honor of Y. Maday's 60th birthday, Roscoff, May 2017,
- V. Ehrlacher, SIAM CSE conference, Atlanta, Georgia, February 2017,
- G. Ferré, Young researchers' seminar, IHP semester, "Stochastic dynamics out of equilibrium", Paris, June 2017,
- G. Ferré, Large deviation theory in statistical physics, ICTS, Bengalore, September 2017,
- M. Josien, CAMP Seminar, University of Chicago, April 2017,
- M. Josien, SciCADE Conference, Bath, September 2017,
- M. Josien, Séminaire de Physique Mathématique-EDP, Institut de Mathématiques de Bordeaux, December 2017,
- D. Kazerani, weekly seminar, Orléans, October 2017,
- D. Kazerani, Post-doc days of IHES, Orsay, October 2017,
- D. Kazerani, weekly seminar IRD, Paris, October 2017,
- C. Le Bris, Conference in honor of Yvon Maday's 60th birthday, May 2017,
- C. Le Bris, Conference in honor of Patrick Joly's 60th birthday, August 2017,
- C. Le Bris, Workshop HPC, Institut d'Etudes Scientifiques de Cargèse, September 2017,
- C. Le Bris, Multiscale Modeling, Theory, and Computation, Conference in honor of Mitchell Luskin's 65th birthday, Minneapolis, September 2017,
- C. Le Bris, Homogenization Theory and Applications, Weierstrass Institute Berlin, October 2017,
- C. Le Bris, BIRS Workshop on "Computational Uncertainty Quantification", Banff International Research Station (BIRS), Canada, October 2017,
- C. Le Bris, Séminaire d'Automatique du plateau de Saclay, June 2017,

- C. Le Bris, Forum Teratec, July 2017,
- F. Legoll, Workshop stochastic homogenization, Bonn, February 2017,
- F. Legoll, UNECECOMP Conference, Rhodes, June 2017,
- F. Legoll, ADMOS Conference, Verbania, June 2017,
- F. Legoll, CIMPA Summer school on multiscale methods, Lucknow, India, July 2017,
- F. Legoll, USNCCM Conference, Montreal, July 2017,
- F. Legoll, COMPLAS 2017 Conference, Barcelona, September 2017,
- F. Legoll, Scicade conference, Bath, September 2017,
- F. Legoll, IMA program on multiscale mathematics, Minneapolis, September 2017,
- F. Legoll, séminaire Université de Genève, October 2017,
- F. Legoll, MORTECH 2017 conference, Sevilla, November 2017,
- F. Legoll, IPAM Program, Los Angeles, November, 2017,
- T. Lelièvre, workshop on Multiscale methods for stochastic dynamics, Geneva, February 2017,
- T. Lelièvre, Séminaire du Laboratoire de Chimie Physique, Université Paris-Sud, March 2017,
- T. Lelièvre, CECAM workshop "Exploiting finite-size effects in simulations", UPMC, April 2017,
- T. Lelièvre, CIRM workshop "interactions EDP/probabilités - équations cinétiques, temps long et propagation du chaos", Marseille, April 2017,
- T. Lelièvre, Colloquium Lorrain de Mathématiques, Université de Nancy, April 2017,
- T. Lelièvre, IHP trimester on Stochastic Dynamics Out of Equilibrium, Paris, April 2017,
- T. Lelièvre, CECAM workshop "Beyond Kd's: New computational methods to address challenges in drug discovery", EPFL, Lausanne June 2017,
- T. Lelièvre, Séminaire de probabilités, ENS Lyon, June 2017,
- T. Lelièvre, "Multiscale Theory and Computation Conference", University of Minneapolis, September 2017,
- T. Lelièvre, "Quasistationary Distributions: Analysis and Simulation", University of Paderborn, September 2017,
- T. Lelièvre, Colloquium du laboratoire Dieudonné, Université Nice Sophia Antipolis, October 2017,
- T. Lelièvre, "Workshop Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces", IPAM, Los Angeles, October 2017,
- T. Lelièvre, Workshop "Bridging Scales in Molecular Biology", Mathematics & Physical Sciences conference of the Simons Foundation, New York, November 2017,
- T. Lelièvre, workshop "Mathématiques pour la neutronique", GDR MANU, Paris, November 2017,
- T. Lelièvre, Mathematisches Kolloquium RWTH Aachen University, Aachen, December 2017,
- A. Levitt, Young researchers working group, UPMC, January 2017,
- A. Levitt, Chemistry colloquium, Cornell, New York, February 2017,
- A. Levitt, THEOS seminar, Cornell, New York, February 2017,
- A. Levitt, SIAM CSE conference, Atlanta, Georgia, February 2017,
- A. Levitt, Conference in honor of Y. Maday's 60th birthday, Roscoff, May 2017,
- A. Levitt, Scalable solvers group seminar, Lawrence Berkeley National Lab, California, June 2017,
- A. Levitt, CCP17, Paris, July 2017,
- A. Levitt, Density Functional Theory and Beyond, Warwick, July 2017,
- A. Levitt, Mathematical physics summer school, Zurich, July 2017,
- A. Levitt, ICJ seminar, Lyon, November 2017,

- P. Monmarché, Groupe de travail Prob., Théo. Erg. et Systèmes Dynamiques, LMRS, Rouen, January 2017,
- P. Monmarché, Workshop PDMP et sampling, ENPC, Marne-la-Vallée, January 2017,
- P. Monmarché, Conférence PDE/Probability Interactions: Kinetic Equations, CIRM, Marseille, April 2017,
- P. Monmarché, Seminar of the Department of Statistics, University of Oxford, May 2017,
- P. Monmarché, Groupe de travail de probabilités, Université Paris 5, May 2017,
- P. Monmarché, Trimestre IHP dynamiques hors équilibre, Institut Henri Poincaré, Paris, June 2017,
- B. Nectoux, Worskhop "Interactions EDP/probabilités : équations cinétiques, temps long et propagation du chaos", CIRM, April 2017,
- B. Nectoux, SciCADE, university of Bath, UK, Septembre 11-15, 2017,
- B. Nectoux, Workshop "Quasi-stationary distribution: analysis and simulation", Paderborn, September 2017,
- P.-L. Rothé, SciCADE 2017 Conference, Bath, UK, September 2017,
- P.-L. Rothé, USNCCM14, 14th U.S. National Congress on Computational Mechanics, Montreal, Canada, July 2017,
- P.-L. Rothé, Congrès SMAI 2017, La Tremblade, June 2017,
- J. Roussel, Young researchers' seminar, IHP semester "Stochastic dynamics out of equilibrium", Paris, June 2017,
- J. Roussel, ICL Seminar, London, November 2017,
- L. Silva Lopes, "Hands-on" Workshop on Enhanced Sampling and Free-Energy Calculation, Urbana-Champaign, Illinois, September 2017,
- G. Stoltz, seminar at Army Research Laboratory, Aberdeen Proving Grounds, February 2017,
- G. Stoltz, seminar at University of Massachussetts, February 2017,
- G. Stoltz, seminar at University of Geneva, March 2017,
- S. Siraj-Dine, Density Functional Theory and Beyond, Warwick, July 2017,
- P. Terrier, The MRS Spring Meeting & Exhibit, Phoenix, April 2017,
- P. Terrier, Séminaire des doctorants du LAMFA, Amiens, December 2017.

Members of the project-team have delivered the following series of lectures:

- E. Cancès, The mathematics of quantum chemistry, 9h, GDR CORREL winter school, Paris, January 2017,
- E. Cancès, Density Functional Theory: Models and numerical methods, 4h, Beijing, China, June 2017,
- E. Cancès, Mathematical aspects of electronic structure theory, 3h, Aussois, France, June 2017,
- E. Cancès, Mathematical structure of quantum mechanics, 3h, Heidelberg, Germany, October 2017,
- T. Lelièvre, Lectures on "Algorithms for computational statistical physics", 3h, ICTS, Bangalore, August 2017,
- T. Lelièvre, Tutorial on "Sampling efficiently metastable dynamics: algorithms and mathematical analysis", 2h, IPAM, Los Angeles, September 2017,
- A. Levitt, Numerical analysis of periodic quantum systems, 2h, Aalborg, Denmark, June 2017,
- G. Stoltz, From a microscopic description of matter to a macroscopic one on a computer: computational statistical physics, 6h, CIMPA Summer School on Multiscale Computational Methods and Error Control, IIT Kanpur, India, July 2017,
- Random homogenization, theoretical and numerical aspects, 6h, CIMPA Summer School on Multiscale Computational Methods and Error Control, IIT Kanpur, India, July 2017.

Members of the project-team have presented posters in the following seminars, workshops and international conferences:

- G. Ferré, Complex high-dimensional energy landscapes, UCLA, Los Angeles, October 2017,
- G. Ferré, Numerical Aspects of Nonequilibrium dynamics, IHP semester "Stochastic dynamics out of equilibrium", Paris, April 2017,
- G. Ferré, Trends and Advances in Monte Carlo Sampling Algorithms, Duke University, Durham (North Carolina), December 2017,
- D. Kazerani, colloque EDP Normandie, Caen, October 2017,
- B. Nectoux, Workshop "Dynamiques stochastiques hors d'équilibre", CIRM, April 2017,
- P.-L. Rothé, colloque EDP Normandie, Caen, October 2017,
- J. Roussel, workshop "Trends and Advances in Monte Carlo Sampling Algorithms", SAMSI (Duke University), December 2017,
- J. Roussel, Numerical Aspects of Nonequilibrium dynamics, IHP semester "Stochastic dynamics out of equilibrium", Paris, April 2017,
- L. Silva Lopes, Beyond Kd's: New computational methods to address challenges in drug discovery, Lausanne, Switzerland, June 2017,
- L. Silva Lopes, CEMRACS 2017: Numerical methods for stochastic models: control, uncertainty quantification, mean-field, Marseille, July, 2017,
- L. Silva Lopes, 11th Triennial Congress of the World Association of Theoretical and Computational Chemistry, Munich, Germany, August 2017,
- L. Silva Lopes, Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, Los Angeles, California, October 2017,
- P. Terrier, SMAI 2017, La Tremblade, June 2017.

Pierre Terrier has won the best poster award at SMAI 2017.

Members of the project-team have participated (without giving talks nor presenting posters) in the following seminars, workshops and international conferences:

- M. Josien, colloque EDP Normandie, Caen, October 2017,
- Mouad Ramil, PDE/Probability Interactions: Kinetic Equations, Long time and Propagation of Chaos at CIRM, Marseille, April 2017
- Mouad Ramil, Workshop on Quasi-Stationary distributions, Paderborn, September 2017
- P.-L. Rothé, Winter School on Numerical Analysis of Multiscale Problems, Hausdorff Research Institute for Mathematics, Bonn, Germany, January 2017,
- J. Roussel, CEMRACS, CIRM, July 2017,
- L. Silva Lopes, IPAM Long Program on "Complex High-Dimensional Energy Landscapes", Los Angeles, California, September-November 2017.

## 10.4. Software development and contributions

- A. Levitt has added methods for optimization on Riemannian manifolds to the Optim.jl optimization library, see https://github.com/JuliaNLSolvers/Optim.jl.
- A. Levitt has published an implementation of the method developed in [16] to construct Wannier functions, see https://github.com/antoine-levitt/wannier.
- In the framework of the PhD of Laura Silva Lopes, L. Silva Lopes and T. Lelièvre have implemented a new tutorial on the NAMD code in order to popularize the Adaptive Multilevel Splitting method among the practitioners, see http://www.ks.uiuc.edu/Training/Tutorials/namd/ams-tutorial/tutorial-AMS.pdf.

- J. Roussel and G. Stoltz have added new features to the Simol code, in particular concerning the use of control variates.

## 10.5. Popularization

- G. Ferré gave a talk about statistical physics and its applications to undergraduate students at Lycée Pierre Corneille, Rouen, in November 2017.
- A. Levitt is a member of the editorial board of Interstices, Inria's popularization website.
- P. Monmarché gave a talk about mathematics and music to high school students at lycée Pablo Picasso, Avion, in May 2017.
- P. Monmarché participated to Les Matinales de la Recherche de l'ENPC and presented a poster about his work to the students of ENPC in April 2017.
- G. Stoltz participated to Les Matinales de la Recherche de l'ENPC and gave a talk about his work to the staff of ENPC in April 2017.
- G. Stoltz, together with Gilles Buisson (Ecole des Ponts), published a contribution to the proceedings of QPES 2017 (Questions de Pédagogie dans l'Enseignement Supérieur), on his teaching experience involving flipped classrooms organized at the level of a complete class of first year students at Ecole des Ponts. See G. Buisson and G. Stoltz, La classe inversée à grande échelle en école d'ingénieur, Actes du colloque QPES 2017, 633-640.

# 11. Bibliography

## Major publications by the team in recent years

[1] E. CANCÈS, M. DEFRANCESCHI, W. KUTZELNIGG, C. LE BRIS, Y. MADAY. *Computational Quantum Chemistry: A Primer*, 2003, Le Bris, Claude (ed.), Special Volume: Computational Chemistry. Amsterdam: North-Holland. Handb. Numer. Anal. 10, 3-270 (2003)

[2] E. CANCÈS, C. LE BRIS, Y. MADAY. *Mathematical Methods in Quantum Chemistry. An Introduction. (Méthodes mathématiques en chimie quantique. Une introduction.)*, Mathématiques et Applications (Berlin) 53. Berlin: Springer. xvi, 409 p. , 2006

[3] I. CATTO, C. LE BRIS, P.-L. LIONS. *The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models*, Oxford Mathematical Monographs. Oxford: Clarendon Press. xiii, 277 p., 1998

[4] J.-F. GERBEAU, C. LE BRIS, T. LELIÈVRE. *Mathematical Methods for the Magnetohydrodynamics of Liquid Metals*, Numerical Mathematics and Scientific Computation. Oxford: Oxford University Press., 324 p., 2006

[5] C. LE BRIS. *Multi-scale Analysis. Modeling and Simulation. (Systèmes multi-échelles. Modélisation et simulation.)*, Mathématiques et Applications (Berlin) 47. Berlin: Springer. xi, 212 p., 2005

[6] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Free Energy Computations: A Mathematical Perspective*, Imperial College Press, 458 p., 2010

# Publications of the year

## Articles in International Peer-Reviewed Journals

[7] X. ANTOINE, A. LEVITT, Q. TANG. *Efficient spectral computation of the stationary states of rotating Bose-Einstein condensates by the preconditioned nonlinear conjugate gradient method*, in "Journal of Computational Physics", August 2017, vol. 343, pp. 92-109, https://arxiv.org/abs/1611.02045 [*DOI :* 10.1016/J.JCP.2017.04.040], https://hal.archives-ouvertes.fr/hal-01393094

[8] R. ASSARAF, B. JOURDAIN, T. LELIÈVRE, R. ROUX. *Computation of sensitivities for the invariant measure of a parameter dependent diffusion*, in "Stochastics and Partial Differential Equations: Analysis and Computations", October 2017, https://arxiv.org/abs/1509.01348 [*DOI :* 10.1007/S40072-017-0105-6], https://hal.archives-ouvertes.fr/hal-01192862

[9] F. AVIAT, A. LEVITT, B. STAMM, Y. MADAY, P. REN, J. W. PONDER, L. LAGARDERE, J.-P. PIQUEMAL. *Truncated Conjugate Gradient (TCG): an optimal strategy for the analytical evaluation of the many-body polarization energy and forces in molecular simulations*, in "Journal of Chemical Theory and Computation", January 2017, vol. 13, n$^{o}$ 1, pp. 180–190 [*DOI :* 10.1021/ACS.JCTC.6B00981], https://hal.archives-ouvertes.fr/hal-01395833

[10] A. BAKHTA, V. EHRLACHER. *Global existence of bounded weak solutions to degenerate cross-diffusion equations in moving domain*, in "ESAIM: Mathematical Modelling and Numerical Analysis", 2017, forthcoming, https://hal.archives-ouvertes.fr/hal-01238636

[11] N. BERGLUND, G. DI GESÙ, H. WEBER. *An Eyring–Kramers law for the stochastic Allen–Cahn equation in dimension two*, in "Electronic Journal of Probability", April 2017, vol. 22, n$^{o}$ 41, pp. 1-27 [*DOI :* 10.1214/17-EJP60], https://hal.archives-ouvertes.fr/hal-01304559

[12] X. BLANC, M. JOSIEN. *From the Newton equation to the wave equation : the case of shock waves*, in "AMRX", February 2017, https://arxiv.org/abs/1605.00974v1 [*DOI :* 10.1093/AMRX/ABX001], https://hal.archives-ouvertes.fr/hal-01314690

[13] E. CANCÈS, P. CAZEAUX, M. LUSKIN. *Generalized Kubo Formulas for the Transport Properties of Incommensurate 2D Atomic Heterostructures*, in "Journal of Mathematical Physics", May 2017, vol. 58, n$^{o}$ 6, pp. 1-29 [*DOI :* 10.1063/1.4984041], https://hal.inria.fr/hal-01403588

[14] E. CANCÈS, G. DUSSON. *Discretization error cancellation in electronic structure calculation: toward a quantitative study*, in "ESAIM: Mathematical Modelling and Numerical Analysis", September 2017, vol. 51, n$^{o}$ 5, pp. 1617 - 1636 [*DOI :* 10.1051/M2AN/2017035], http://hal.upmc.fr/hal-01435054

[15] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: conforming approximations*, in "SIAM Journal on Numerical Analysis", September 2017, vol. 55, n$^{o}$ 5, pp. 2228-2254 [*DOI :* 10.1137/15M1038633], https://hal.inria.fr/hal-01194364

[16] É. CANCÈS, A. LEVITT, G. PANATI, G. STOLTZ. *Robust determination of maximally-localized Wannier functions*, in "Physical Review B : Condensed matter and materials physics", February 2017, vol. 95, https://arxiv.org/abs/1605.07201 [*DOI :* 10.1103/PHYSREVB.95.075114], https://hal.archives-ouvertes.fr/hal-01323700

[17] V. EHRLACHER, D. LOMBARDI. *A dynamical adaptive tensor method for the Vlasov-Poisson system*, in "Journal of Computational Physics", 2017, vol. 319, pp. 285-306, https://hal.archives-ouvertes.fr/hal-01335507

[18] G. FAURE, G. STOLTZ. *Stable and accurate schemes for smoothed dissipative particle dynamics*, in "Applied Mathematics and Mechanics", January 2018, vol. 39, n$^{o}$ 1, pp. 83-102, https://arxiv.org/abs/1707.04232 [*DOI :* 10.1007/s10483-018-2256-8], https://hal.archives-ouvertes.fr/hal-01562490

[19] G. FORT, B. JOURDAIN, T. LELIÈVRE, G. STOLTZ. *Self-Healing Umbrella Sampling: Convergence and efficiency*, in "Statistics and Computing", January 2017, vol. 27, n$^{o}$ 1, pp. 147–168, https://arxiv.org/abs/1410.2109 [*DOI :* 10.1007/s11222-015-9613-2], https://hal.archives-ouvertes.fr/hal-01073201

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[22] C. LE BRIS, F. LEGOLL. *Examples of computational approaches for elliptic, possibly multiscale PDEs with random inputs*, in "Journal of Computational Physics", 2017, vol. 328, pp. 455-473, https://arxiv.org/abs/1604.05061 , https://hal.archives-ouvertes.fr/hal-01304040

[23] C. LE BRIS, F. LEGOLL, S. LEMAIRE. *On the best constant matrix approximating an oscillatory matrix-valued coefficient in divergence-form operators*, in "ESAIM: Control, Optimisation and Calculus of Variations", 2018, https://arxiv.org/abs/1612.05807 , https://hal.archives-ouvertes.fr/hal-01420187

[24] C. LE BRIS, F. LEGOLL, F. MADIOT. *A numerical comparison of some Multiscale Finite Element approaches for advection-dominated problems in heterogeneous media*, in "ESAIM: Mathematical Modelling and Numerical Analysis", 2017, vol. 51, n$^{o}$ 3, pp. 851-888, https://arxiv.org/abs/1511.08453 - DOI: http://dx.doi.org/10.1051/m2an/2016057, https://hal.archives-ouvertes.fr/hal-01235642

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cember 2017, vol. 350, pp. 280-295, https://arxiv.org/abs/1610.02949 [*DOI :* 10.1016/J.JCP.2017.08.015], https://hal.archives-ouvertes.fr/hal-01378916

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### International Conferences with Proceedings

[30] Q. H. TRAN, G. ENCHÉRY, R. SANCHEZ, S. BOYAVAL. *A Reduced-Basis Approach to Two-Phase Flow in Porous Media*, in "FVCA 2017", Lille, France, Finite Volumes for Complex Applications VIII - Hyperbolic, Elliptic and Parabolic Problems, June 2017 [*DOI :* 10.1007/978-3-319-57394-6_50], https://hal-enpc.archives-ouvertes.fr/hal-01587116

### Conferences without Proceedings

[31] L. CHAMOIN, F. LEGOLL. *Certified computations with PGD model reduction in the MsFEM framework*, in "14th National Congress on Computational Mechanics - USNCCM14", Montréal, Canada, July 2017, https://hal.archives-ouvertes.fr/hal-01581791

[32] F. LEGOLL, L. CHAMOIN. *A posteriori error estimation for multiscale computations based on MsFEM*, in "14th National Congress on Computational Mechanics - USNCCM14", Montréal, Canada, July 2017, https://hal.archives-ouvertes.fr/hal-01581797

[33] F. LEGOLL, L. CHAMOIN. *Multiscale computations based on MsFEM: model reduction and goal-oriented a posteriori error estimation*, in "8th International Conference on Adaptive Modeling and Simulation - ADMOS 2017", Verbania, Italy, June 2017, https://hal.archives-ouvertes.fr/hal-01583144

### Scientific Books (or Scientific Book chapters)

[34] S. BOYAVAL. *A Finite-Volume discretization of viscoelastic Saint-Venant equations for FENE-P fluids*, in "Finite Volumes for Complex Applications VIII - Hyperbolic, Elliptic and Parabolic Problems. FVCA 2017. Springer Proceedings in Mathematics & Statistics", C. CANCÈS, P. OMNES (editors), Springer, 2017, vol. 200, pp. 163-170, https://arxiv.org/abs/1701.04639 [*DOI :* 10.1007/978-3-319-57394-6_18], https://hal-enpc.archives-ouvertes.fr/hal-01433712

### Other Publications

[35] A. BENACEUR, V. EHRLACHER, A. ERN, S. MEUNIER. *A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems* , November 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01599304

[36] A. BAKHTA, V. EHRLACHER. *Cross-diffusion systems with non-zero flux and moving boundary conditions*, September 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01397682

[37] A. BAKHTA, V. EHRLACHER, D. GONTIER. *Numerical reconstruction of the first band(s) in an inverse Hill's problem*, September 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01591133

[38] J. W. BARRETT, S. BOYAVAL. *Finite Element Approximation of the FENE-P Model*, April 2017, working paper or preprint, https://hal-enpc.archives-ouvertes.fr/hal-01501197

[39] T. BOIVEAU, V. EHRLACHER, A. ERN, A. NOUY. *Low-rank approximation of linear parabolic equations by space-time tensor Galerkin methods*, December 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01668316

[40] S. BOYAVAL. *Derivation and numerical approximation of hyperbolic viscoelastic flow systems: Saint-Venant 2D equations for Maxwell fluids*, December 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01661269

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