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Ecole des Ponts ParisTech

Activity Report 2016

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. Members

Research Scientists

Claude Le Bris [Team leader, ENPC, HDR]
Antoine Levitt [Inria, Researcher]
Mathias Rousset [Inria, Researcher, until Aug 2016, HDR]
Sébastien Boyaval [ENPC]
Éric Cancès [ENPC, HDR]
Virginie Ehrlacher [ENPC]
Frédéric Legoll [ENPC, HDR]
Tony Lelièvre [ENPC, HDR]
Gabriel Stoltz [ENPC, HDR]

Faculty Members

Ludovic Chamoin [ENS Cachan, Associate Professor, *en délégation*, until Aug 2016, HDR]
Dorian Le Peutrec [Univ. Paris XI, Faculty Member, Associate Professor, *en délégation*, until Jul 2016]
Pierre-André Zitt [Univ. Paris Est, Associate Professor, *en délégation*, until Aug 2016, HDR]

Engineer

Cédric Doucet [Inria SED, Part-time, until March 2016]

PhD Students

Grégoire Ferré [ENPC, from Oct 2016]
Marc Josien [Min. Ecologie]
Boris Nectoux [ENPC]
Pierre-Loïk Rothé [ENPC, from Oct 2016]
Julien Roussel [ENPC]
Laura Silva Lopes [ENPC, from Oct 2016]
Pierre Terrier [Min. Ecologie]
François Madiot [ENPC, until Dec 2016]

Post-Doctoral Fellows

Michaël Bertin [Univ. Paris Est, until Feb 2016]
Giacomo Di Gesù [ENPC, until Aug 2016]
Pierre Monmarché [Inria, from Oct 2016]
Thomas Hudson [Inria, until Aug 2016]

Administrative Assistants

David Dinis [Inria, until Apr 2016]
Sarah Le [Inria, from Jul 2016]

Other

Frédérique Noël [Intern Inria, from May to Sep 2016]

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. 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.

4.2. 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.

4.3. 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 when the proton mass is the reference mass.

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.* 7×10^{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 0.1 μs.

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?"

5. New Software and Platforms

5.1. SIMOL

KEYWORDS: C++ - Statistical physics - Quantum chemistry - Molecular simulation
FUNCTIONAL DESCRIPTION

SIMOL (SIMulation of MOLecular systems) is a software written in C++. It is a research code aimed at testing new ideas and algorithms, and provides a unified development platform for the members of the project-team. It is composed of three parts: a common core of input/output functions, linear algebra, random number generators, etc; and two specific applicative branches: one for computational statistical physics and one for quantum chemistry. The methods implemented for computational statistical physics are based on discretizations of ergodic stochastic differential equations such as the Langevin dynamics and its overdamped limit. The systems that can be simulated range from a single isolated particle to Lennard-Jones fluids. For quantum chemistry, the building block is the Hartree-Fock model, solved via fixed-point iterations; and various refinements including greedy methods.

- Contact: Gabriel Stoltz
- URL: https://gitlab.inria.fr/matherials/simol

6. New Results

6.1. Electronic structure calculations

Participants: Éric Cancès, Virginie Ehrlacher, Claude Le Bris, Antoine Levitt, 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.

6.1.1. Molecular systems

The work of the project-team on molecular systems has focused on advanced approaches for the computation of the electronic state of molecular systems, including the effects of electronic correlation and of the environment.

In [12], E. Cancès, D. Gontier (former PhD student of the project-team, now at Université Paris Dauphine) and G. Stoltz have analyzed the GW method for finite electronic systems. This method enables the computation of 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.

Implicit solvation models aim at computing the properties of a molecule in solution (most chemical reactions indeed take place in the liquid phase) by replacing all the solvent molecules except the 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 (UPMC), 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 has pursued his collaboration with Pierre Rouchon (Ecole des Mines de Paris) on the study of high dimensional Lindblad type equations at play in the modelling of open quantum systems. In order to complement and better understand the numerical approaches developed in the past couple of years, some theoretical aspects are now under study, in particular regarding the well-posedness of the equations and their convergence in the long time limit.

6.1.2. Crystals and solids

Periodic systems are mathematically treated using Bloch theory, raising specific theoretical and numerical issues.

A. Bakhta (CERMICS) and V. Ehrlacher are 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.

As an external collaborator of the MURI project on 2D materials (PI: M. Luskin), E. Cancès has started a collaboration with P. Cazeaux and M. Luskin (University of Minnesota) on the computation of the electronic and optical properties of multilayer 2D materials. Together with E. Kaxiras (Harvard) and members of his group, they have developped a perturbation method for computing the Kohn-Sham density of states of incommensurate bilayer systems. They have also 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 [36].

É. Cancès, A. Levitt and G. Stoltz, in collaboration with G. Panati (Rome) have proposed a new method for the computation of Wannier functions, a standard post-processing of density functional theory computations [38]. Compared to previous approaches, it does not require an initial guess for the shape of the Wannier functions, and is therefore more robust.

6.1.3. Numerical analysis

Members of the project-team have worked on the numerical analysis of partial differential equations arising from electronic structure theory.

E. Cancès and N. Mourad (CERMICS) 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.

E. Cancès has pursued his long-term collaboration with Y. Maday (UPMC) on the numerical analysis of electronic structure models. Together with G. Dusson (UMPC), B. Stamm (UMPC), and M. Vohralík (Inria), they have designed a new post processing 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 homogeneous Dirichlet boundary conditions [37]. In particular, upper and lower bounds for any simple eigenvalue are established. These bounds are guaranteed, fully computable, and converge with the optimal rate to the exact eigenvalue.

A. Levitt, in collaboration with X. Antoine and Q. Tang (Nancy), has proposed a new numerical method to compute the ground state of rotating Bose-Einstein condensates [31]. This method combines a nonlinear conjugate gradient method with efficient preconditionners. Compared to the state of the art (implicit timestepping on the imaginary-time equation), gains of one to two orders of magnitude are achieved.

6.2. Complex fluids

Participant: Sébastien Boyaval.

The aim of the research performed in the project-team about complex fluids is to guide the mathematical modelling of gravity flows with a free-surface for application to the hydraulic engineering context, and to account for non-Newtonian rheologies in particular (like in mudflows for instance). On the one hand, thin-layer (reduced) models have long been favored, and one current trend aims at incorporating non-Newtonian effects [10]. This has stimulated some research about a new hyperbolic PDE system [35]. On the other hand, there is currently a strong need to perform full 3D numerical simulations using new non-Newtonian models in complex geometries with a view to comparing them with physical observations ; this is an ongoing work, in the framework of the ANR project SEDIFLO with E. Audusse (Paris 13), A. Caboussat (Genève), A. Lemaitre (ENPC), M.Parisot (Inria).

6.3. Homogenization

Participants: Michaël Bertin, Ludovic Chamoin, Virginie Ehrlacher, Thomas Hudson, Marc Josien, Claude Le Bris, Frédéric Legoll, François Madiot, Pierre-Loïk Rothé.

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 non-periodic systems. In former publications, several theoretical aspects have been considered, for the case of linear elliptic equations in divergence form. In the context of the PhD thesis of M. Josien, new issues are being explored, including the rate of convergence of the approximation, along with the convergence of the Green functions associated to the problems under consideration. The studies are motivated by several practically relevant problems, in particular the problem of defects in periodic structures and the "twin boundaries" problem in materials science. Also, some other equations than linear elliptic equations in divergence form have been considered lately. The case of advection-diffusion equations is currently examined. In addition, one ongoing work, in collaboration with P. Souganidis (University of Chicago) and P. Cardaliaguet (Université Paris-Dauphine), considers the non-periodic setting for Hamilton-Jacobi type equations.

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 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.

Over the past years, the project-team has proposed several variance reduction techniques, which have been reviewed and compared to one another in [9], [20]. In particular, in [23], 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. The efficiency of the approach has been demonstrated for various types of random materials, including composite materials with randomly located inclusions.

Besides the (averaged) behavior of the oscillatory solution u_ε on large space scales (which is given by the homogenized limit u_* of u_ε), another question of interest is to understand how much u_ε fluctuates around its coarse approximation u_*. This question will be explored in the PhD thesis of P.-L. Rothé, which started in October 2016.

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, because not all the information on the microscopic medium is available. Following an interaction with A. Cohen (Paris 6), C. Le Bris, F. Legoll and S. Lemaire (post-doc in the project-team until 2015), have shown that the constant matrix that “best” (in a sense made precise in [44]) represents the oscillatory matrix describing the medium converges to the homogenized matrix in the limit of infinitely rapidly oscillatory coefficients. Furthermore, the corresponding optimization problem can be efficiently solved using standard algorithms and yield accurate approximation of the homogenized matrix. It has also been 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. The details are now available in [44].

6.3.3. Multiscale Finite Element approaches

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

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.

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 stems here from the geometry of the domain. On the boundary of the perforations, we set either homogeneous Dirichlet or homogeneous Neumann conditions. In the spirit of the work [21], the purpose of our ongoing work is to investigate, on perforated domains, the behavior of several variants of the Multiscale Finite Element method, 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. All the variants considered are based upon local functions satisfying weak continuity conditions in the Crouzeix-Raviart sense on the boundary of mesh elements. 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. The type of boundary conditions on the perforations (either homogeneous Dirichlet or homogeneous Neumann boundary conditions) drastically affects the nature of the flow, and therefore the conclusions regarding which numerical approach is best to adopt. In short, homogeneous Dirichlet boundary conditions on the perforations damp the effect of advection, making the flow more stable than it would be in the absence of perforations, while this is not the case for homogeneous Neumann boundary conditions. This intuitive fact is investigated thoroughly at the numerical level, and particularly well exemplified, at the theoretical level, by the comparison of the respective homogenization limits.

Advection-diffusion equations that are both non-coercive and advection-dominated have also been considered (in a single-scale framework). Many numerical approaches have been proposed in the literature to address such difficult cases. C. Le Bris, F. Legoll and F. Madiot have proposed an approach based on the invariant measure associated to the original equation. The approach has been summarized in [22], and extensively described, analyzed and numerically tested in [45]. It is shown there that this approach allows for an unconditionally well-posed finite element approximation, and that it can be stable, as accurate as, and more robust than classical stabilization approaches.

Most of the numerical analysis studies of the MsFEM are focused on obtaining *a priori* error bounds. In collaboration with L. Chamoin, who was on leave in the project-team (from ENS Cachan, from September 2014 to August 2016), members of the project-team have been working on *a posteriori* error analysis for MsFEM approaches, with the aim of developing error estimation and adaptation tools. They have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution u_h has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux $k\nabla u$. In the context of the MsFEM, it is important to be able to perform all expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach thus needs to be adapted to that context. The proposed approach yields very interesting results, and provides an accurate and robust estimation of the global error. The approach has also been adapted towards the design of adaptive algorithms for specific quantities of interest (in the so-called "goal-oriented" setting), and towards the design of model reduction approaches (such as the Proper Generalized Decomposition (PGD)) in the specific context of multiscale problems. The work will be reported on in a forthcoming publication in preparation.

6.3.4. Discrete systems and their thermodynamic limit

In collaboration with X. Blanc (Paris 7), M. Josien has studied the macroscopic limit of a chain of atoms governed by Newton's equations. It is known from the works of X. Blanc (Paris 7), C. Le Bris and P.-L. Lions (Collège de France) that this limit is the solution of a nonlinear wave equation, as long as the solution remains smooth. For a large class of interaction potentials, X. Blanc and M. Josien have shown in [34], theoretically and numerically, that, if the distance between particles remains bounded, the above description in terms of a non-linear wave equation equation no longer holds when there are shocks. Indeed, the system of particles produces dispersive waves that are not predicted by the nonlinear wave equation.

6.3.5. 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. Weertman's equation and the dynamical Peierls-Nabarro equation), involving non-local operators. In collaboration with Y.-P. Pellegrini (CEA), M. Josien has first focused on the steady state regime (where the equation of interest is the Weertman equation), and has designed an efficient numerical method for approximating its solution. The approach is based on a splitting strategy between the nonlinear local terms (which are integrated in real space) and the linear nonlocal terms (which are integrated in Fourier space). Current efforts are devoted to the simulation of physically relevant test-cases, with the aim of comparing the obtained numerical results with results of the physics literature. The work will be reported on in a forthcoming publication in preparation.

6.4. Computational Statistical Physics

Participants: Grégoire Ferré, Giacomo Di Gesù, Thomas Hudson, Dorian Le Peutrec, Frédéric Legoll, Tony Lelièvre, Pierre Monmarché, Boris Nectoux, Julien Roussel, Mathias Rousset, Laura Silva Lopes, Gabriel Stoltz, Pierre Terrier, Pierre-André Zitt.

In [24], T. Lelièvre and G. Stoltz have given an overview of state-of-the art mathematical techniques which are useful to analyze and quantify the efficiency of the algorithms used in molecular dynamics, both for sampling thermodynamic quantities (canonical averages and free energies) and dynamical quantities (transition rates, reactive paths and transport coefficients).

6.4.1. Improved sampling methods

This section is devoted to recent methods which have been proposed in order to improve the sampling of the canonical distribution by modifying the Langevin or overdamped Langevin dynamics, or its discretization. Two general strategies have been pursued by the project-team along these lines: (i) constructing dynamics with better convergence rate and hence smaller statistical errors; (ii) the stabilization of discretization schemes by Metropolis procedures in order to allow for larger timesteps while maintaining acceptable rejection rates.

A first approach to obtaining better convergence rates consists in modifying the drift term in the overdamped-Langevin dynamics, in order to improve the rate of converge to equilibrium. This method was considered by T. Lelièvre with A. Duncan and G.A. Pavliotis (Imperial College) in [14]. It is shown that nonreversible dynamics always result in a smaller asymptotic variance (statistical error). The efficiency of the whole algorithm crucially depends on the time discretization, which may induce some bias (deterministic error). It is shown on some examples how to balance the two errors (bias and statistical errors) in order to obtain an efficient algorithm.

The discretization of overdamped Langevin dynamics, using schemes such as the Euler-Maruyama method, may lead to numerical methods that 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 (Toulouse) present in [15] 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 reduce the bias in the estimation of transport coefficients characterizing the effective dynamical behavior of the dynamics.

The sampling properties of Langevin dynamics can be improved by considering more general non-quadratic kinetic energies. This was accomplished in [26], where G. Stoltz, with S. Redon and Z. Trstanova (Inria Grenoble), have studied the properties of Langevin dynamics with general, non-quadratic kinetic energies $U(p)$, showing in particular the ergodicity of the dynamics even when the kinetic force ∇U vanishes on open sets and proving linear response results for the variance of the process for kinetic energies which correspond to the so-called adaptively restrained particle simulations. This work has been complemented by [51], where G. Stoltz and Z. Trstanova provide accurate numerical schemes to integrate the modified Langevin dynamics with general kinetic energies, with possibly non globally Lipschitz momenta.

6.4.2. Adaptive methods

When direct sampling methods fail, it is worth considering importance sampling strategies, where the slowest direction is described by a reaction coordinate ξ, and the invariant measure is biased by (a fraction of) the free energy associated with ξ.

The first group of results along these lines concerns the study of adaptive biasing methods to compute free energy differences:

- The result obtained by H. Al Rachid (CERMICS) in collaboration with T. Lelièvre and R. Talhouk (Beirut) on the existence of a solution to the non linear Fokker Planck equation associated to the ABF process has been published, see [7].
- T. Lelièvre and G. Stoltz, together with G. Fort (Toulouse) and B. Jourdain (CERMICS), have studied the well-tempered metadynamics and many variants of this method in [41]. This dynamics can be seen as some extension of the so-called self-healing umbrella sampling method, with a partial biasing of the dynamics only. In particular, the authors propose a version which leads to much shorter exit times from metastable states (accelerated well-tempered metadynamics).

The project-team also works on adaptive splitting techniques, which forces the exploration in the direction of increasing values of the reaction coordinate. In [29], T. Lelièvre, together with C. Mayne, K. Schulten and I. Teo (Univ. Illinois), has reported on the calculation of the unbinding rate of the benzamidine-trypsin system using the Adaptive Multilevel Splitting algorithm. This is the first "real-life" test case for the adaptive multilevel splitting. In [11], T. Lelièvre and M. Rousset, in collaboration with C.E. Bréhier (Lyon), M. Gazeau (Créteil) and L. Goudenège (Centrale), propose a generalization of the Adaptive Multilevel Splitting method for discrete-in-time processes. It is shown how to make the estimator unbiased. Numerical experiments illustrate the performance of the method.

6.4.3. Coarse-graining and reduced descriptions

A fully atomistic description of physical systems leads to problems with a very large of unknowns, which raises challenges both on the simulation of the system and the interpretation of the results. Coarse-grained approaches, where complex molecular systems are described by a simplified model, offer an appealing alternative.

F. Legoll and T. Lelièvre, together with S. Olla (Dauphine), have proposed an analysis of 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 [48]. More precisely, a pathwise error estimate is obtained, which is an improvement compared to a previous result by F. Legoll and T. Lelièvre where only the marginal in times were considered.

Another line of research concerns dissipative particle dynamics, where a complex molecule is replaced by an effective mesoparticle. The work [17] by G. Stoltz, together with A.-A. Homman and J.-B. Maillet (CEA), on new parallelizable numerical schemes for the integration of Dissipative Particle Dynamics with Energy conservation, has been published. Together with G. Faure and J.-B. Maillet, G. Stoltz has proposed in [16] a new formulation of smoothed dissipative particle dynamics, which can be seen as some meshless discretization of the Navier–Stokes equation perturbed by some random forcing arising from finite size effects of the underlying mesoparticles. The reformulation, in terms of internal energies rather than internal entropies, allows for a simpler and more efficient simulation, and also opens the way for a coupling with standard dissipative particle dynamics models.

G. Stoltz also suggested in [50] a new numerical integrator for DPDE which is more stable than all the previous integrators. The key point is to reduce the stochastic part of the dynamics to elementary one-dimensional dynamics, for which some Metropolis procedure can be used to prevent the appearance of negative energies at the origin of the instability of the numerical methods.

During the post-doctoral stay of I.G. Tejada (ENPC), G. Stoltz, F. Legoll and E. Cancès studied in collaboration with L. Brochard (ENPC) the derivation of a concurrent coupling technique to model fractures at the atomistic level by combining a reactive potential with a reduced harmonic approximation. The results have appeared in [28].

G. Stoltz and P. Terrier, in a joint work with M. Athènes, T. Jourdan (CEA) and G. Adjanor (EDF), have presented a coupling algorithm for cluster dynamics [52]. 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 equation. The proposed coupling algorithm is based on a splitting of the dynamics and combines deterministic and stochastic approaches. In addition, F. Legoll and G. Stoltz have proposed in [19], with T. Jourdan (CEA) and L. Monasse (CERMICS), a new method for numerically integrating the Fokker–Planck approximation of large cluster dynamics.

6.4.4. Eyring–Kramers formula and quasi-stationary distributions

G. Di Gesù, T. Lelièvre and B. Nectoux, together with D. Le Peutrec, have explored the interest of using the quasi-stationary distribution approach in order to justify kinetic Monte Carlo models, and more precisely their parameterizations using the Eyring-Kramers formulas, which provide a simple rule to compute transition rates from one state to another [13]. The paper is essentially a summary of the results which have been obtained during the first two years of the PhD of B. Nectoux. A preprint with detailed proofs of these results is in preparation.

In [33], G. Di Gesù has studied with N. Berglund (Orléans) and H. Weber (Warwick) the spectral Galerkin approximations of an Allen-Cahn equation over the two-dimensional torus perturbed by weak space-time white noise. They show sharp upper and lower bounds on the transition times from a neighborhood of the stable configuration -1 to the stable configuration 1 in the small noise regime. These estimates are uniform in the discretization parameter, suggesting an Eyring-Kramers formula for the limiting renormalized stochastic PDE.

6.4.5. Functional inequalities and theoretical aspects

The interplay between probability theory and analysis in statistical physics is best exemplified by the functional analysis study of the semigroups associated with the generator of the stochastic processes under consideration. These generators are elliptic or hyperbolic operators. Several functional-analytic results were obtained by the team on problems of statistical physics.

D. Le Peutrec has derived Brascamp-Lieb type inequalities for general differential forms on compact Riemannian manifolds with boundary from the supersymmetry of the semiclassical Witten Laplacian [47]. These results imply the usual Brascamp-Lieb inequality and its generalization to compact Riemannian manifolds without boundary.

T. Hudson has considered with C. Hall (Oxford) and P. van Meurs (Univ. Kanazawa, Japan) the minimization of the potential energy of N particles mutually interacting under a repulsive interaction potential with a certain algebraic decay assumption [42]. A major novelty of the approach is that it does not assume a finite range of interaction. The main focus of the work is on characterizing the boundary behavior of minimizers in the limit where the number of particles N tends to infinity with a constant density of particles per unit volume.

G. Di Gesù has studied with M. Mariani (Rome) the small temperature limit of the Fisher information of a given probability measure with respect to the canonical measure with density proportional to $\exp(-\beta V)$ [39]. The expansion reveals a hierarchy of multiple scales reflecting the metastable behavior of the underlying overdamped Langevin dynamics: distinct scales emerge and become relevant depending on whether one considers probability measures concentrated on local minima of V, probability measures concentrated on critical points of V, or generic probability measures on $\mathbb{R}^d$.

6.5. Various topics

Participants: Virginie Ehrlacher, Tony Lelièvre, Antoine Levitt.

In [18], T. Lelièvre has explored with J. Infante Acevedo (CERMICS) the interest of using the greedy algorithm (also known as the Proper Generalized Decomposition) for the pricing of basket options.

V. Ehrlacher and D. Lombardi have developped a new tensor-based numerical method for the resolution of kinetic equations [40] in a fully Eulerian framework.This theory enables to describe a large system of particles by a distribution function $f(x, v, t)$ that encodes the probability of finding a particle at time t, position $x \in \mathbb{R}^3$ and velocity $v \in \mathbb{R}^3$. These systems are used to model the behavior of plasma of the transport of electrons in semiconductors for instance. However, simulating such systems involves the resolutions of problems defined on $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+$, which leads to very high-dimensional systems. The new approach developped in [40] circumvents the curse of dimensionality for these systems, by efficiently adapting the rank of the decomposition of the solution through time. Encouraging preliminary numerical results have been obtained on $3D \times 3D$ systems.

A system of cross-diffusion equations has been proposed in [32] by A. Bakhta and V. Ehrlacher for the modelling of a Physical Vapor Deposition (PVD) process used for the manufacturing of thin film solar cells. This process works as follows: a substrate wafer is introduced in a hot chamber where different chemical species are injected under gaseous form. These different species deposit on the surface of the substrate, so that a thin film layer grows upon the surface of the substrate. Two phenomena have to be taken into account in the modelling: 1) the evolution of the thickness of the thin film layer; 2) the diffusion of the various species inside the bulk. The existence of a weak solution to the system proposed in [32] has been proved, along with the existence of optimal fluxes to be injected in the chamber in order to obtain target concentration profiles at the end of the process. The long-time behavior of solutions has been studied in the case when the injected fluxes are constant. Moreover, numerical results on the simulation of this system have been compared with experimental data given by IRDEP on CIGS (Copper, Indium, Gallium, Selenium) solar cells. The project is a collaboration with IRDEP.

A. Levitt, in collaboration with F. Aviat, L. Lagardère, Y. Maday, J.-P. Piquemal (UPMC), B. Stamm (Aachen), P. Ren (Texas) and J. Ponder (Saint Louis), has proposed a new method for the solution of the equations of polarizable force fields [8]. Previous methods had to solve a linear system to high accuracy in order for the energy to be preserved in simulations. The method presented, based on an explicit differentiation of the energy produced by the truncated iterative method, is able to conserve the energy even with loose convergence criteria, thus allowing stable and fast simulations at degraded accuracy.

7. Bilateral Contracts and Grants with Industry

7.1. 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.

8. Partnerships and Cooperations

8.1. National Initiatives

The project-team is involved in several ANR projects:

- S. Boyaval's SEDIFLO project, funded by ANR as a JCJC (Jeunes Chercheuses Jeunes Chercheurs) grant, has started investigating new numerical models of solid transport in rivers that include new non-Newtonian terms.
- E. Cancès is involved in the ANR BECASIM, which is concerned with the numerical simulation of Bose-Einstein condensates. This ANR has been accepted in June 2012, and is coordinated by I. Danaila (Université de Rouen).
- T. Lelièvre is member of the ANR-project "STAB" (PI: I. Gentil, Université de Lyon).
- F. Legoll is a member of the ANR project CINE-PARA (PI: Y. Maday, Paris 6)
- The ANR COSMOS (PI: G. Stoltz) 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.

In addition, the project-team is participating in

- the GdR CORREL (correlated methods in electronic structure computations),
- the GdR EGRIN (gravity flows),
- the GdR MASCOT-NUM (stochastic methods for the analysis of numerical codes),
- the GdR Maths-entreprise (math/industry collaboration),
- the GdR DYNQUA (time evolution of quantum systems, with applications to transport problems, nonequilibrium systems, etc.),
- the GdR REST (theoretical spectroscopy),
- the GdR 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).

8.2. European Initiatives

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

8.3. International Initiatives

The *Germaine de Staël* grant to S. Boyaval (from CampusFrance Hubert-Curien program) has been renewed for 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 Inria Rennes.

9. Dissemination

9.1. Promoting Scientific Activities

E. Cancès

- 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-), and SIAM MMS (2012-),

- is a member of the executive committee of the CEA-EDF-Inria schools in applied mathematics and computer science.

He has organized or co-organized:

- a CECAM workshop on the mathematical and numerical analysis of electronic structure models, Roscoff, Jul. 8-12, 2016,
- the MMM 2016 conference (Multiscale Modelling of Materials), Dijon, Oct. 10-14, 2016,
- an IPAM workshop on collective variables in quantum mechanics, Los Angeles, Nov. 14-18, 2016.

L. Chamoin has organized the mini-symposium "Verification of reduced models in computational mechanics" within the ECCOMAS 2016 conference, Greece, June 2016.

V. Ehrlacher has co-organized with A. Cousin the semester on "Uncertainty Quantification" in the framework of the IHP thematic semester on "Monte-Carlo methods" organized by B. Bouchard, E. Gobet and B. Jourdain.

C. Le Bris is editor-in-chief of Applied Mathematics Research Express (2003-). 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 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 Proc (2012-),
- has co-organized the mini-symposium "Mathematical theory and computational techniques for multiscale materials modelling" within the MMM 2016 conference, Dijon, October 10-14, 2016 (with W. Curtin, C. Garcia-Cervera, J. Kermode, X. Li, A. Lozinski, M. Luskin and C. Ortner).

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings (with D. Chafai, P. Lafitte and C. Mouhot),
- is a member of the "Conseil d’Administration" of SMAI and Ecole des Ponts,
- has been a member of the ANR committee CES-40 "mathématiques et informatique",
- has co-organized the Journées EDP-Probas at Institut Henri Poincaré (with F. Malrieu),
- has co-organized the workshop "COmputational Statistics and MOlecular Simulation" in Paris, February 2-5th, 2016 (with A. Guyader and G. Stoltz),

- has co-organized the IHP conference on "Recent developments in numerical methods for model reduction", November 7-10th 2016. (with S. Perotto and G. Rozza),
- will co-organize 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),
- will co-organize 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).

G. Stoltz

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

9.2. 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: Équations aux dérivées partielles et éléments finis, 15h, L3, École des Ponts (T. Hudson, F. Legoll, A. Levitt),
- Licence: Hydrodynamique numérique, 15h, L3, École des Ponts (S. Boyaval),
- Licence: Maths 1 et 2, 9h, L3, École des Mines (G. Stoltz),
- Licence: Mathématiques pour l'économie, 36h, L1, Dauphine (J. Roussel),
- Licence: Analyse et calcul scientifique, 30h, L3, Ecole des Ponts (T. Hudson, M. Josien, B. Nectoux, G. Stoltz),
- Master: Mécanique des milieux continus - partie solides, 14h, M1, ENS Cachan (L. Chamoin),
- Master: Ondes et chocs dans les structures, 8h, M1, ENS Cachan (L. Chamoin),
- Master: Mathématiques des modèles multiéchelles, 39h, M1, École des Ponts (F. Legoll),
- Master: Analyse et équations aux dérivées partielles, 36 h, M1, École des Ponts (T. Lelièvre),
- Master: Projet de département IMI, 12h, M1, École des Ponts (J. Roussel),
- Master: Projets de physique, 10h, M1, École des Ponts, France (A. Levitt, G. Stoltz),
- Master: Modélisation mathématique des vagues, 3h, École des Ponts (S. Boyaval),
- Master: Analyse de Fourier et applications, 16h, M1, École des Ponts (V. Ehrlacher, A. Levitt, G. Stoltz),
- Master: Approximation numérique et optimisation, 32h, École Polytechnique (E. Cancès, T. Lelièvre) ,
- Master: Analyse variationnelle des équations aux dérivées partielles, 32h, École Polytechnique (E. Cancès),
- Master: Contrôle des modèles et dualité, 24h, M2 Mathématiques et Applications, ENS Cachan (L. Chamoin),
- Master: Problèmes multi-échelles, 24h, M2 Mathématiques et Applications, Paris 6 (F. Legoll),
- Master: Méthodes variationnelles et théorie spectrale, 10h, M2 Mathématiques et Applications, Paris 6 (E. Cancès),
- Master: Méthodes numériques probabilistes, 24 h, M2 Mathématiques et Applications, Paris 6 (T. Lelièvre),
- Master: Introduction to computational statistical physics, 20h, M2 Mathématiques et Applications, Paris 6 (G. Stoltz).

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

- Eddy Bernard, Université Paris-Est, defended on Nov. 25, 2016, supervised by G. Chambaud (Université Paris-Est) and E. Cancès,
- Jean-Léopold Vié, Université Paris-Est, École des Ponts and Ecole Polytechnique, defended on Dec. 16, 2016, supervised by G. Allaire (Polytechnique) and E. Cancès,
- Ahmed-Amine Homman, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, École des Ponts and CEA/DAM, defended on June 16, 2016, supervised by G. Stoltz and J.-B. Maillet (CEA),
- François Madiot, Multiscale finite element methods for advection diffusion problems, Université Paris-Est, Ecole des Ponts ParisTech, defended on December 8, 2016, supervised by C. Le Bris and F. Legoll,
- Rémi Sainct, Study of instabilities in traffic models, defended on September 22, 2016, supervised by T. Lelièvre and X. Louis (IFSTTAR),

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

- Athmane Bakhta, Modélisation and simulation for photovoltaic applications, Université Paris-Est, École des Ponts, started October 1st, 2014, supervised by E. Cancès and T. Lelièvre, co-supervised by V. Ehrlacher,
- 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,
- 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,
- Gérôme Faure, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, École des Ponts and CEA/DAM, started November 1st 2014, supervised by G. Stoltz and J.-B. Maillet (CEA),
- 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,
- Henri Louvin, Splitting methods and radioprotection, Ecole Doctorale PHENIICS, started September 1st, 2014, supervised by Check Diop (CEA) and T. Lelièvre,
- Boris Nectoux, Metastability and quasi stationary distribution, started November 1st, 2014, supervised by T. Lelièvre and E. Cancès,
- Julien Roussel, Variance reduction techniques for nonequilibrium systems, Université Paris-Est, École des Ponts, started September 1st, 2015, supervised by G. Stoltz,
- Pierre-Loik Rothé, Numerical methods for the estimation of fluctuations in multi-scale materials and related problems, started October 1st, 2016, supervised by F. Legoll,
- Laura Silva Lopes, Rare event simulation and applications to biological systems, started October 1st, 2016, supervised by J. Hénin (IBPC) and T. Lelièvre,
- 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 was in the jury for the PhD of Viljami Laurmaa ("An octree-based adaptive semi-Lagrangian free surface flow solver"), defended at EPFL in May 2016.
- S. Boyaval was in the jury for the PhD of Joubine Aghili ("Méthodes de discrétisation et de réduction de modèle pour des EDP à coefficients variables"), defended in Montpellier in December 2016.
- E. Cancès was a referee of the PhD of Maxime Morinière ("États résonants en théorie de perturbation à plusieurs corps"), defended in Grenoble in December 2016.
- V. Ehrlacher was in the jury for the PhD of Luca Nenna ("Numerical methods for Multi-Marginal Optimal Transport"), defended at Paris Dauphine in December 2016.
- V. Ehrlacher was in the jury for the PhD of Jean-Léopold Vié ("Second-order derivatives for shape optimization with a level-set method"), defended at CERMICS in December 2016.
- V. Ehrlacher was in the jury for the PhD of Faizan Nazar ("Electronic Structure of Defects in the Thomas-Fermi-von Weiszäcker Model"), defended at Warwick in December 2016.
- F. Legoll was in the jury for the PhD of Dena Kazerani ("Études mathématiques de fluides à frontières libres en dynamique incompressible"), defended at UPMC in November 2016.
- T. Lelièvre was a referee for the PhD of Tomasz Badowski on "Adaptive importance sampling via minimization of estimators of cross-entropy, mean square and inefficiency constants" defended at Freie Universität Berlin.
- T. Lelièvre was a referee for the PhD of Arthur Talpaert on "Direct Numerical Simulation of bubbles with Adaptive Mesh Refinement with distributed algorithms" defended at École Polytechnique.
- T. Lelièvre was in the jury for the PhD of Ahmed-Amine Homman ("Développement de schémas numériques d'intégration de méthodes multi-échelles"), defended at CERMICS in June 2016.
- T. Lelièvre was in the jury for the PhD of Gang Liu on "Rare event simulation by shaking transformation and Non-intrusive stratified resampling method for dynamic programming", defended at École Polytechnique in November 2016.

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

- E. Cancès was a referee of Stéphane Redon's HdR, defended in Grenoble in May 2016.
- E. Cancès participated in the HdR jury of Nicolas Rougerie, defended in Grenoble in November 2016.
- T. Lelièvre was a referee of Pierre Etoré's HDR ("Quelques contributions à l'étude et à la simulation des diffusions asymétriques"), defended in Grenoble in December 2016.

9.3. Conference participation

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

- S. Boyaval, Atelier Sillage et ondes de surface, Orsay, April 2016,
- S. Boyaval, Séminaire Modélisation mathématique et calcul scientifique, ENS Lyon and Institut Camille Jordan, May 2016,
- S. Boyaval, Workshop on Stochastic Partial Differential Equations, Pau, June 2016,
- S. Boyaval, Symposium on shallow-water flows at HYP 2016, Aachen, August 2016,
- S. Boyaval, Symposium on network models in PDEs at SIMAI 2016, Milan, September 2016,
- E. Cancès, seminar, Groupe de travail numérique, Laboratoire Jacques-Louis Lions, UPMC, January 2016,
- E. Cancès, workshop on computation of quantum systems in cold-matter physics and chemistry, Fields Institute, Toronto, February 2016,

- E. Cancès, Colloquium, University of Delaware, May 2016,
- E. Cancès, SIAM MS conference (invited lecture), May 2016,
- E. Cancès, KiNet workshop on mathematical and computational methods in quantum chemistry, Yale, New Haven, May 2016,
- E. Cancès, Solid Math workshop, Aalborg, May 2016,
- E. Cancès, KiNet workshop on quantum and kinetic transport, Jiatong University, Shanghai, June 2016,
- E. Cancès, workshop on coupled mathematical models for physical and nanoscale systems and their applications, Banff, Canada, August 2016,
- E. Cancès, Multiscale Modelling of Materials (MMM 2016) conference (invited lecture), Dijon, October 2016,
- L. Chamoin, Séminaire de l'équipe MISES, UPMC, Paris, April 2016,
- L. Chamoin, SIAM Conference on Uncertainty Quantification, Lausanne, April 2016,
- L. Chamoin, Workshop "New Challenges in Computational Mechanics", Cachan, May 2016,
- L. Chamoin, ECCOMAS conference, Hersonissos, Greece, June 2016,
- G. Di Gesù, IST Austria, Vienne, June 2016,
- G. Di Gesù, Eurandom YEP Workshop on Large Deviations for Interacting Particle Systems and Partial Differential Equations, Eindhoven, March 2016,
- V. Ehrlacher, Workshop on "Challenges in High-Dimensional Analysis and Computation", San Servolo, Italy, May 2016,
- V. Ehrlacher, Séminaire du CEREMADE, Université Paris-Dauphine, September 2016,
- V. Ehrlacher, Institute for Computational and Applied Mathematics seminar, University of Münster, Germany, October 2016,
- V. Ehrlacher, MATHCCES seminar, RWTH Aachen University, Germany, October 2016,
- V. Ehrlacher, EMI 2016 conference, Metz, France, October 2016,
- V. Ehrlacher, MMM 2016 conference, Dijon, France, October 2016,
- V. Ehrlacher, Workshop on "Recent developments in numerical methods for model reduction", Institut Henri Poincaré, France, November 2016,
- V. Ehrlacher, Séminaire "Problèmes spectraux en physique mathématique", December 2016,
- G. Ferré, seminar of the IPAM program 'Understanding Many Particle Systems with Machine Learning, Los Angeles, November 2016,
- G. Ferré, workshop 'Collective Variables in Quantum Mechanics', Los Angeles, November 2016,
- T. Hudson, 7th European Congress of Mathematics, Berlin, July 2016,
- T. Hudson, Applied Math Seminar, UNC Charlotte, May 2016,
- M. Josien, CANUM 2016, Obernai, France, May 2016,
- M. Josien, MMM 2016 conference, Dijon, France, October 2016,
- C. Le Bris, Edinburgh Mathematical Society Lecturer, Dundee, UK, March 18, 2016,
- C. Le Bris, Sissa workshop on Homogenization, SISSA, Trieste, June 6-10, 2016,
- C. Le Bris, PDE Seminar of the University of Chicago, February and November 2016,
- C. Le Bris, Seminar at the Applied Mathematics Department of the University of Washington at Seattle, October 2016,
- F. Legoll, EMI-PMC 2016 conference, Nashville, USA, May 2016,
- F. Legoll, ECCOMAS conference, Hersonissos, Greece, June 2016,
- F. Legoll, Weekly seminar of the LMS laboratory, Ecole Polytechnique, June 2016,

- F. Legoll, AIMS conference, Orlando, USA, July 2016,
- F. Legoll, WCCM conference, Seoul, South Korea, July 2016,
- F. Legoll, ECCM conference, Brussels, Belgium, Sept. 2016,
- F. Legoll, MMM 2016 conference, Dijon, France, October 2016,
- F. Legoll, Workshop on "Recent developments in numerical methods for model reduction", Paris, France, November 2016,
- F. Legoll, CASA weekly seminar, Eindhoven, the Netherlands, November 2016,
- F. Legoll, IFPEn weekly seminar, Paris, France, December 2016,
- T. Lelièvre, Plenary speaker at MCMSKI 2016, Lenzerheide, January 2016,
- T. Lelièvre, Séminaire Laboratoire Jacques-Louis Lions, February 2016,
- T. Lelièvre, Séminaire "Incertitudes" à EDF, March 2016,
- T. Lelièvre, Séminaire Institut de Biologie Physico-Chimique, March 2016,
- T. Lelièvre, Workshop "Particle methods for the management of risks", Paris, April 2016,
- T. Lelièvre, Séminaire équipe Inria ABS, April 2016,
- T. Lelièvre, SIAM Uncertainty Quantification, Lausanne, April 2016,
- T. Lelièvre, Workshop "Challenges in High-Dimensional Analysis and Computation", San Servolo, May 2016,
- T. Lelièvre, CANUM, May 2016,
- T. Lelièvre, Séminaire du laboratoire MICS, Centrale Supélec, June 2016,
- T. Lelièvre, Warwick Mathematics Colloquium, June 2016,
- T. Lelièvre, Workshop "Extreme events in the Earth and planetary sciences", Warwick, July 2016,
- T. Lelièvre, Faraday discussion "Reaction rate theory", Cambridge, September 2016,
- T. Lelièvre, Workshop MMM2016, October 2016,
- A. Levitt, Workshop on computation of quantum systems in cold-matter physics and chemistry, Toronto, Canada, February 2016,
- A. Levitt, Parallel Processing ’16, Paris, April 2016,
- A. Levitt, Remise de prix Bull-Fourier 2015, Paris, April 2016,
- A. Levitt, GDR REST (rencontres de spectroscopie théorique) meeting, Roscoff, May 2016,
- A. Levitt, PASC 2016, Lausanne, May 2016,
- A. Levitt, 2016 ECMI Congress, Santiago de Compostela, May 2016,
- A. Levitt, Mathematical and numerical analysis of electronic structure models, Roscoff, July 2016,
- A. Levitt, Mathematics seminar, Aachen, March 2016,
- A. Levitt, Mathematical physics seminar, Texas A&M, November 2016,
- A. Levitt, Séminaire de mathématiques appliquées, Collège de France, December 2016,
- F. Madiot, CANUM 2016, Obernai, France, May 2016,
- P. Monmarché, Inria junior seminar, September 2016,
- B. Nectoux, groupe de travail "chimie quantique", Université Pierre et Marie Curie, January 2016,
- G. Stoltz, IPAM workshop "Collective Variables in Classical Mechanics", Los Angeles, October 2016,
- G. Stoltz, The 8th Multiscale Materials Modelling international conference, Dijon, November 2016,
- G. Stoltz, SIAM Conference on Mathematical Aspects of Materials Science 2016, Philadelphie, May 2016,
- P. Terrier, The 8th Multiscale Materials Modelling international conference, Dijon, November 2016.

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

- E. Cancès, Optical and electronic excitations in molecules and solids, 3h, Physics department, Harvard University, April 2016,
- E. Cancès, First-principle molecular simulation, 4h, French-Spanish Jacques-Louis Lions Summer School, Gijon, June 2016,
- E. Cancès, Density Functional Theory: models and numerical methods, 4h, KiNet summer school, Santa Barbara, June 2016,
- E. Cancès, Mathematical representations of quantum states, 2h, IPAM tutorial, Los Angeles, September 2016,
- E. Cancès, Mathematical techniques for quantum chemistry, 3h, Modern wavefunction methods in electronic structure theory, Gelsenkirchen, October 2016,
- V. Ehrlacher, Lecture on "Theoretical results on the Progressive Generalized Decomposition algorithm", 2h, cours GdR AMORE, IHP, December 2016,
- C. Le Bris, Series of 6 one-hour lectures on Nonperiodic multiscale problems, Winter school on Calculus of Variations in Physics and Materials Science, Würzburg, Germany, 14 -19 February 2016,
- C. Le Bris, Series of 4 one-hour lectures on Stochastic homogenization, INI Workshop on "From the Grain to the Continuum: Two Phase Dynamics of a Partially Molten, Polycrystalline Aggregate", Cambridge, UK, 14 -15 March 2016,
- T. Lelièvre, Lectures on "Numerical methods in molecular dynamics" (4h30), Winterschool Universität Basel, Engelberg, February 2016,
- T. Lelièvre, Lectures on "Model reduction techniques for stochastic dynamics" (4h), Ecole GDR EGRIN, May 2016,
- T. Lelièvre, Lectures on "Stochastic differential equations in large dimension and numerical methods" (4h), RICAM Winterschool, Linz, December 2016,
- G. Stoltz, "A mathematical introduction to steady-state nonequilibrium systems", Spring school on Molecular Dynamics, Bad Belzig, April 2016.

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

- A. Levitt, COSMOS workshop, Paris, February 2016,
- J. Roussel, NESC, Sheffield, July 2016.

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

- T, Hudson, SIAM Conference on Mathematical Aspects of Materials Science 2016, Philadelphie, May 2016,
- M. Josien, Winterschool on Stochastic Homogenization, Augsburg, Germany, February 2016,
- A. Levitt, IPAM semester “Understanding many-particle systems with machine learning”, Los Angeles, September and November 2016,
- P.-L. Rothé, Workshop on "Recent developments in numerical methods for model reduction", Paris, France, November 2016,
- J. Roussel, MCMSki Conference, Lenzerheide, January 2016,
- J. Roussel, COSMOS Workshop, Paris, February 2016,
- J. Roussel, CEMRACS, CIRM, Marseille, July 2016,
- J. Roussel, IPAM Tutorial, Los Angeles, September 2016,
- P. Terrier, Summer school PISACMS, Paris, September 2016.

9.4. Popularization

- É. Cancès has delivered a conference in Nancy in November 2016, in the framework of the series of lectures “Sciences et société”.
- A. Levitt participated in the “Young doctors” session of the Salon Culture & Jeux Mathématiques in May 2016.

10. 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] H. ALRACHID, T. LELIÈVRE, R. TALHOUK. *Local and global solution for a nonlocal Fokker–Planck equation related to the adaptive biasing force process*, in "Journal of Differential Equations", 2016, vol. 260, n^{o} 9, pp. 7032 - 7058 [*DOI :* 10.1016/J.JDE.2016.01.020], https://hal.archives-ouvertes.fr/hal-01244976

[8] 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", November 2016 [*DOI :* 10.1021/ACS.JCTC.6B00981], https://hal.archives-ouvertes.fr/hal-01395833

[9] X. BLANC, C. LE BRIS, F. LEGOLL. *Some variance reduction methods for numerical stochastic homogenization*, in "Philosophical Transactions of the Royal Society of London. A (1887–1895)", 2016, vol. 374, n^{o} 2066, 20150168 p. , https://hal.archives-ouvertes.fr/hal-01196499

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[11] C.-E. BRÉHIER, M. GAZEAU, L. GOUDENÈGE, T. LELIÈVRE, M. ROUSSET. *Unbiasedness of some generalized adaptive multilevel splitting algorithms*, in "The Annals of Applied Probability : an official journal of the institute of mathematical statistics", 2016, vol. 26, n^{o} 6, pp. 3559 - 3601 [*DOI :* 10.1214/16-AAP1185], https://hal.archives-ouvertes.fr/hal-01142704

[12] E. CANCÈS, D. GONTIER, G. STOLTZ. *A mathematical analysis of the GW0 method for computing electronic excited state energies of molecules*, in "Reviews in Mathematical Physics", June 2016 [*DOI :* 10.1142/S0129055X16500082], https://hal.archives-ouvertes.fr/hal-01160926

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[14] A. B. DUNCAN, T. LELIÈVRE, G. A. PAVLIOTIS. *Variance Reduction Using Nonreversible Langevin Samplers*, in "Journal of Statistical Physics", 2016, vol. 163, n^{o} 3, pp. 457 - 491, 29 pages [*DOI :* 10.1007/s10955-016-1491-2], https://hal.archives-ouvertes.fr/hal-01164466

[15] M. FATHI, G. STOLTZ. *Improving dynamical properties of metropolized discretizations of overdamped Langevin dynamics*, in "Numerische Mathematik", November 2016 [*DOI :* 10.1007/s00211-016-0849-3], https://hal.archives-ouvertes.fr/hal-01153573

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[22] C. LE BRIS, F. LEGOLL, F. MADIOT. *Stabilisation de problèmes non coercifs via une méthode numérique utilisant la mesure invariante (Stabilization of non-coercive problems using the invariant measure)*, in "Comptes Rendus Mathématique", 2016, vol. 354, n^{o} 8, pp. 799-803, https://hal.archives-ouvertes.fr/hal-01348854

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[28] I. G. TEJADA, L. BROCHARD, T. LELIÈVRE, G. STOLTZ, F. LEGOLL, E. CANCÈS. *Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure*, in "Computer Methods in Applied Mechanics and Engineering", 2016, vol. 305, pp. 422 - 440 [*DOI :* 10.1016/J.CMA.2016.03.011], https://hal.archives-ouvertes.fr/hal-01196505

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Other Publications

[31] 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*, November 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01393094

[32] A. BAKHTA, V. EHRLACHER. *Cross-diffusion systems with non-zero flux and moving boundary conditions*, November 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01397682

[33] N. BERGLUND, G. DI GESÙ, H. WEBER. *An Eyring–Kramers law for the stochastic Allen–Cahn equation in dimension two*, April 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01304559

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[35] S. BOYAVAL. *Johnson-Segalman – Saint-Venant equations for viscoelastic shallow flows in the elastic limit*, November 2016, working paper or preprint, https://hal.inria.fr/hal-01402628

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[38] É. CANCÈS, A. LEVITT, G. PANATI, G. STOLTZ. *Robust determination of maximally-localized Wannier functions*, May 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01323700

[39] G. DI GESÙ, M. MARIANI. *Full metastable asymptotic of the fisher information*, November 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01400800

[40] V. EHRLACHER, D. LOMBARDI. *A dynamical adaptive tensor method for the Vlasov-Poisson system*, June 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01335507

[41] G. FORT, B. JOURDAIN, T. LELIEVRE, G. STOLTZ. *Convergence and efficiency of adaptive importance sampling techniques with partial biasing*, October 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01389996

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[43] T. HUDSON. *Upscaling a model for the thermally-driven motion of screw dislocations*, July 2016, Major revision, including overhaul of notation, significant additions to Large Deviations results in Section 6, and resolution of conjecture in original version. 45 pages, 2 figures, 1 table, https://hal.archives-ouvertes.fr/hal-01236494

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[46] A. LE COËNT, L. FRIBOURG, N. MARKEY, F. DE VUYST, L. CHAMOIN. *Distributed Synthesis of State-Dependent Switching Control*, March 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01295738

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