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**Ecole des Ponts ParisTech**

Activity Report 2015

**Project-Team MATHERIALS**

**MATHeMatics for MatERIALS**

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

RESEARCH CENTER  
**Paris - Rocquencourt**

THEME  
**Numerical schemes and simulations**



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# Project-Team MATHERIALS

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## Keywords:

### Computer Science and Digital Science:

- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.1.2. - Stochastic Modeling (SPDE, SDE)
- 6.1.4. - Multiscale modeling
- 6.1.5. - Multiphysics modeling
- 6.2.1. - Numerical analysis of PDE and ODE
- 6.2.2. - Numerical probability
- 6.2.3. - Probabilistic methods
- 6.2.4. - Statistical methods
- 6.2.7. - High performance computing
- 6.3.1. - Inverse problems
- 6.3.4. - Model reduction
- 6.4.1. - Deterministic control
- 7.13. - Quantum algorithms

### Other Research Topics and Application Domains:

- 1.1.2. - Molecular biology
- 4.1.2. - Nuclear energy
- 4.2.4. - Photovoltaics
- 5.3. - Nanotechnology and Biotechnology
- 5.5. - Materials
- 9.4.2. - Mathematics
- 9.4.3. - Physics
- 9.4.4. - Chemistry

## 1. Members

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## 2. Overall Objectives

### 2.1. Overall Objectives

The MATERIALS 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 a former project-team 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 modeling 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<sup>3</sup>) 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 submitted 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. We consider mostly the setting of stochastic homogenization of linear, scalar, second order elliptic PDEs, where analytical formulas for the effective properties are known. The difficulty



stems from the fact that they 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  $N_A \sim 6 \times 10^{23}$ , the typical distances are expressed in Å ( $10^{-10}$  m), the energies are of the order of  $k_B T \simeq 4 \times 10^{-21}$  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<sup>3</sup> 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  $N_A$  atoms and performing  $O(10^{15})$  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  $0.1 \mu\text{s}$ .

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  $N \rightarrow +\infty$  (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 - OpenMP  
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. A first release should be available in Spring 2016.

- Contact: Cédric Doucet

## 6. New Results

### 6.1. Electronic structure calculations

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

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

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

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

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

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

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

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

Implicit solvation models aim at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous medium accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. In collaboration with F. Lipparini (Paris 6), B. Mennucci (Department of Chemistry, University of Pisa) and J.-P. Picquemat (Paris 6), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). E. Cancès, Y. Maday, F. Lipparini and B. Stamm have also extended this approach to the more complex polarizable continuum model (PCM).

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

## 6.2. Complex fluids

**Participant:** Sébastien Boyaval.

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

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

## 6.3. Homogenization

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

### 6.3.1. Deterministic non periodic systems

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

perturbation of the periodic problem and the challenging, practically relevant problem of interfaces between periodic structures of different nature (the celebrated "twin boundaries" problem in materials science). Some related problems will now be addressed in the context of the PhD thesis of M. Josien.

### 6.3.2. Stochastic homogenization

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

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

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

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

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

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

### 6.3.3. Multiscale Finite Element approaches

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

The MsFEM has been introduced more than 10 years ago. However, even in simple deterministic cases, there are still some open questions, for instance concerning multiscale advection-diffusion equations. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interacts with the multiscale character of the equation is an unsolved mathematical question worth considering for numerical purposes. In that spirit, C. Le Bris, F. Legoll and F. Madiot have studied in [46] several variants

of the Multiscale Finite Element Method (MsFEM), specifically designed to address multiscale advection-diffusion problems in the convection-dominated regime. Generally speaking, the idea of the MsFEM is to perform a Galerkin approximation of the problem using specific basis functions, that are precomputed (in an offline stage) and adapted to the problem considered. Several possibilities for the basis functions have been examined (for instance, they may or may not encode the convection field). Depending on how basis functions are defined, stabilization techniques (such as SUPG) may be required. Another option to handle such problems is to use a splitting approach, with two legacy codes, one solving a purely diffusive multiscale equation, the other one solving a single scale, convection-dominated advection-diffusion equation. In [46], these various approaches have been compared in terms of accuracy and computational costs.

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

Most of the numerical analysis studies of the MsFEM are focused on obtaining *a priori* error bounds. In collaboration with L. Chamoin, who is currently in delegation in the project-team for the second year (from ENS Cachan, since September 2014), members of the project-team have been working on *a posteriori* error analysis for MsFEM approaches, with the aim to develop error estimation and adaptation tools. They have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution  $u_h$  has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux  $k\nabla u$ . In the context of the MsFEM, it is important to be able to do all the expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach thus needs to be adapted to that context, in order to keep that feature that makes it adapted to a multiscale, multi-query context. The proposed approach yields very interesting results, and provide an accurate and robust estimation of the global error.

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

#### 6.3.4. Coarse approximation of an elliptic problem with oscillatory coefficients

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

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

possible to construct, in a second stage, approximations to the correctors, in order to recover an approximation of the *gradient* of the solution.

### 6.3.5. Optimization of a material microstructure

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

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

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

### 6.3.6. Discrete systems and their thermodynamic limit

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

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

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

## 6.4. Computational Statistical Physics

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

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

### 6.4.1. Sampling of reactive trajectories

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



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

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

#### **6.4.2. Nonequilibrium systems and non-reversible dynamics**

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

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

#### **6.4.3. Numerical analysis of simulation techniques**

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

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

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

#### **6.4.4. Free energy computations**

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



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

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

#### 6.4.5. Convergence of processes

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

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

#### 6.4.6. Force fields and modeling

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

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

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

### 6.5. Various topics

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

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

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

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

## 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:

- 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).
- S. Boyaval's ANR proposal SEDIFLO, about the improvement of current numerical models of solid transport in rivers operating at large-scale for industrial purposes, by means of new non-Newtonian rheology equations, has been selected for funding as a JCJC (Jeunes Chercheuses Jeunes Chercheurs) grant.
- 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 Quantum dynamics. This interdisciplinary research network is focused on physical and mathematical problems related to the time evolution of quantum systems (transport problems, nonequilibrium systems, etc),
- the GdR Shocks,
- the GdR Maths et entreprise,
- the GdR correl (correlated methods in electronic structure computations),
- the GdR Rest (rencontres de spectroscopie théorique).
- the GdR CoDFT (electronic structure computations using density functional theory).
- the GdR EGRIN
- the GdR MASCOT-NUM (stochastic methods for the analysis of numerical codes),

The MATHERIALS 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) has started in June 2014.

## 8.3. International Initiatives

S. Boyaval has obtained a *Germaine de Staël* grant to pursue his research with A. Caboussat (Lausanne) about 3D numerical simulation 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 on the French side research teams from Université de Nancy, Université de Lyon and Inria Rennes.

# 9. Dissemination

## 9.1. Promoting Scientific Activities

S. Boyaval has coorganized with G. Enchéry (IFPEN) a SMAI 2015 minisymposium about fast numerical simulation techniques for porous-media flows with highly heterogeneous permeabilities, June 2015.

E. Cancès

- is a member of the editorial boards of *Mathematical Modeling 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:

- the ICS summer school on Computational Chemistry and Applied Mathematics, Roscoff, France, Jul. 15-Aug. 14, 2015,
- the MBI Workshop Mathematical Challenges in Drug and Protein Design, Columbus, Ohio, Dec. 7-11, 2015.

L. Chamoin has been a member of the organization committee of the conference "Reduced Basis, POD and PGD Model Reduction Techniques", ENS Cachan, November 2015, and the co-chairman of the "International Conference on Adaptive Modeling and Simulation (ADMOS)", Nantes, June 2015.

He has organized a minisymposium entitled "Applications of error estimation and model adaptation in Computational Mechanics" within the US National Congress of Computational Mechanics, San Diego, July 2015.

V. Ehrlacher has co-organized with Areski 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.

T. Hudson has organized a minisymposium entitled "Modeling microstructure and material instabilities across a range of scales" at the 3rd ECCOMAS Young Investigator's Conference, Aachen, 20-23 July 2015.

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-), and Modeling, Simulations and Applications, Series, Springer (2009-).

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.

He has been a member of the scientific committee of the conference "Dimension reduction: mathematical methods and Applications", Pennsylvania State University, March 21-24, 2015.

He has co-organized

- with G. Hagedorn and C. Lasser, the Oberwolfach Workshop *Mathematical problems in dynamical quantum chemistry*, Oberwolfach, June 1-6 2015,
- with I. Kim, Fang-Hua Lin and P. Souganidis, the Banff Workshop *Developments in the Theory of Homogenization*, BIRS, Banff, July 26-31 2015.

F. Legoll

- is a member of the editorial board of SIAM MMS (2012-) and of ESAIM Proc (2012-),
- has been a member of the Scientific Committee of SciCADE 2015.

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings (with D. Chafai, P. Lafitte and C. Mouhot),
- has co-organized the Workshop "Free-energy calculations: A mathematical perspective" at BIRS, Casa Matemática Oaxaca, Mexico, July 19-24th, 2015 (with C. Chipot and R. Skeel).
- was in the scientific committee of the conference MoRePaS 2015, Trieste, October 2015,

- co-organizes the Journées EDP-Probab at Institut Henri Poincaré (with F. Malrieu),
- is in charge of the Theme 4 (Stochastic modeling, quantification and uncertainty propagation for multiscale mechanical models of materials) of the Labex MMCD,
- is involved in the organization of the IHP trimester on numerical PDEs (PI D.A. Di Pietro, A. Ern and L. Formaggia), September-December 2016.

G. Stoltz co-organizes the IHP trimester "Stochastic Dynamics Out of Equilibrium", Spring 2017 (with G. Giacomini, S. Olla, E. Saada and H. Spohn).

## 9.2. Teaching - Supervision - Juries

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

- Licence: Maths 1 et 2, 9h, L3, École des Mines (G. Stoltz),
- Licence: Outils mathématiques pour l'ingénieur, 15h, L3, École des Ponts (E. Cancès, V. Ehrlacher, T. Hudson, F. Legoll, T. Lelièvre),
- Licence: Analyse et calcul scientifique, 30h, L3, École des Ponts (T. Hudson, 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 multi-échelles, 39h, M1, École des Ponts (F. Legoll),
- Master: Contrôle des modèles et dualité, 24h, M2, ENS Cachan (L. Chamoin),
- Master: Problèmes multi-échelles, 24h, M2, Paris 6 (F. Legoll),
- Master: Approximation numérique et optimisation, 32h, École Polytechnique (E. Cancès),
- Master: Analyse variationnelle des équations aux dérivées partielles, 32h, École Polytechnique (E. Cancès),
- Master: Méthodes variationnelles et théorie spectrale, 10h, M2, Paris 6 (E. Cancès),
- Master: Modélisation mathématique des vagues, 3h, École des Ponts (S. Boyaval),
- Master: Outils Probabilistes pour la Finance, 25h, M1, École des Ponts, France (M. Rousset),
- Master: Analyse Spectrale, 39h, École des Ponts (V. Ehrlacher, A. Levitt),
- Master: Projets de physique, 10h, M1, École des Ponts, France (V. Ehrlacher, G. Stoltz),
- Master: Introduction au calcul Scientifique, 13h, M1, École des Mines, France (G. Stoltz, F. Madiot),
- Master: Introduction to computational statistical physics, 20h, M2, Paris 6 (G. Stoltz),
- Master: Modéliser Programmer Simuler, 28 h, M1, Cours École des Ponts (T. Lelièvre),
- Master: Méthodes numériques probabilistes, 36 h, M2 Mathématiques et Applications, Paris 6 (T. Lelièvre).

The following PhD theses have been defended:

- David Gontier, Contributions mathématiques aux calculs de structures électroniques, Université Paris Est, September 28 2015 (supervised by E. Cancès),
- William Minvielle, Quelques problèmes liés à l'erreur statistique en homogénéisation stochastique, Université Paris-Est, Université Paris Est, September 25 2015 (supervised by C. Le Bris and F. Legoll).

The following PhD theses are ongoing:

- 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,
- Gerome 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,
- Ahmed-Amine Homman, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, École des Ponts and CEA/DAM, started April 1st, 2013, supervised by G. Stoltz and J.-B. Maillet,
- Marc Josien, Multiscale approaches for materials science, started September 1st, 2015, supervised by C. Le Bris,
- François Madiot, Multiscale finite element methods for advection diffusion problems, Université Paris-Est, Ecole des Ponts ParisTech, started October 1st, 2013, supervised by C. Le Bris and F. Legoll,
- Boris Nectoux, Métastabilité et distribution quasi-stationnaire, since November 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,
- Rémi Saint, Modèles multi-échelles pour le trafic, since September 2013, supervised by T. Lelièvre and X. Louis,
- 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,
- Zofia Trstanova, A mathematical analysis of some importance sampling strategies in molecular dynamics, Université Joseph Fourier and Inria Grenoble, started June 1st 2013, supervised by S. Redon and G. Stoltz.

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

- E. Cancès was a member (as referee) of the PhD committee of B. Pawilowski (Rennes, Dec. 2015), supervised by F. Nier and N. Mauser.
- F. Legoll was a member (as the opponent) of the PhD committee of D. Elfverson (Univ. Uppsala, Oct. 2015), supervised by A. Malqvist.
- F. Legoll was a member of the PhD committee of M. Capaldo (LMT, ENS Cachan, Nov. 2015), supervised by P. Ladevèze and D. Néron.
- T. Lelièvre was a member (as referee) of the PhD committee of C. Vergé (École Polytechnique, July 2015), supervised by P. Del Moral.
- T. Lelièvre was a member (as referee) of the PhD committee of D. Lesnicki (Paris 6, Sep. 2015), supervised by R. Vuilleumier.
- T. Lelièvre was a member of the PhD committee of O. Zahm (École Centrale de Nantes, Nov. 2015), supervised by A. Zouy.
- T. Lelièvre was a member (as referee) of the HDR committee of J. Tugaut (Dec. 2015, Saint-Étienne).

### 9.3. Conference participation

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

- S. Boyaval, Atelier EDPs stochastiques à Marseilles, June 2015,

- S. Boyaval, Séminaire mathématiques appliquées à Université Versailles Saint-Quentin en Yvelines, October 2015,
- E. Cancès, workshop on Fundamental Aspects of DFT, Oslo, Norway, January 2015,
- E. Cancès, GDR Dynqua Conference on Mathematical Physics, Nantes, France, February 2015,
- E. Cancès, Weekly seminar, ONERA, France, April 2015,
- E. Cancès, distinguished lecture series "Adventures in Theory", Duke University, USA, April 2015,
- E. Cancès, Weekly seminar of the mathematics department, Duke University, USA, April 2015,
- E. Cancès, Weekly seminar of the mathematics department, Michigan State University, Lansing, USA, May 2015,
- E. Cancès, IPAM workshop on materials for a sustainable energy future, Lake Arrowhead, USA, June 2015,
- E. Cancès, SFB conference on Discretization in Geometry and Dynamics, Herrsching am Ammersee, Germany, October 2015
- E. Cancès, Weekly seminar of the mathematics department, University of Metz, France, October 2015,
- E. Cancès, Weekly seminar of the JL Lions laboratory, Paris, France, October 2015,
- L. Chamoin, Séminaire de l'IMT, Toulouse, January 2015,
- L. Chamoin, Séminaire Aristote, École Polytechnique, Palaiseau, February 2015,
- L. Chamoin, 12ième Colloque National en Calcul des Structures, Giens, May 2015,
- L. Chamoin, International conference on Adaptive Modeling and Simulation (ADMOS), Nantes, June 2015,
- L. Chamoin, YIC GACM 2015 (3rd ECCOMAS Young Investigators Conference), Aachen, July 2015,
- L. Chamoin, US National Congress on Computational Mechanics, San Diego, July 2015,
- L. Chamoin, MORE workshop on model reduction, Pilsen, September 2015,
- L. Chamoin, Séminaire de l'équipe-projet POEMS, Palaiseau, December 2015,
- V. Ehrlacher, HIM Workshop: "Gradient flows and entropy methods", Bonn, Germany, February 2015,
- V. Ehrlacher, SIAM CSE 2015, Salt Lake City, USA, March 2015,
- V. Ehrlacher, MSME seminar, Université Marne-la-Vallée, March 2015,
- V. Ehrlacher, MOKAPLAN seminar group, Université Paris-Dauphine, March 2015,
- V. Ehrlacher, Séminaire du groupe de travail "Mécanique des fluides réels", ENS Cachan, May 2015,
- V. Ehrlacher, Séminaire du CMAP, École Polytechnique, Juin 2015,
- V. Ehrlacher, IPAM Workshop on Materials Defects: Mathematics, Computation and Engineering, Lake Arrowhead, USA, June 2015,
- V. Ehrlacher, Numerical Analysis Conference, University of Strathclyde, Glasgow, Great Britain, June 2015,
- V. Ehrlacher, USNCCM 13, San Diego, USA, July 2015,
- V. Ehrlacher, Seminar of the Theoretical Chemistry Group, Johannes Gutenberg Universität, Mainz, Germany, October 2015,
- V. Ehrlacher, 3rd MOKALIEN Meeting, Université Paris-Dauphine, November 2015,
- D. Gontier, workshop on Fundamental Aspects of DFT, Oslo, Norway, January 2015,
- D. Gontier, Oberwolfach workshop Mathematical Methods in Quantum Molecular Dynamics, Germany, June 2015,

- D. Gontier, Nonlinear equations seminar, University Paris 13, November 2015,
- T. Hudson, Workshop on "Analytic approaches to scaling limits for random system", Bonn, January 2015,
- T. Hudson, US National Congress on Computational Mechanics, San Diego, July 2015,
- T. Hudson, ICIAM conference, Beijing, August 2015,
- C. Le Bris, PIRE Workshop, "Design of materials: From grain boundaries to stochastic homogenization", Leipzig, July 2015,
- C. Le Bris, International conference on numerical mathematics and scientific computing, Nanjing (China), August 2015,
- D. Le Peutrec, Séminaire ANEDP au LMO, Université Paris-Sud, 2015,
- D. Le Peutrec, Séminaire Spectral problems in mathematical physics à l'IHP, Paris, 2015,
- D. Le Peutrec, Séminaire EDP à l'IRMAR, Université Rennes 1, 2015,
- F. Legoll, Journées annuelles du GdR ModMat, Lyon, January 2015,
- F. Legoll, Euromech Colloquium on "Multiscale Computational Methods for bridging scales in materials and structures", Eindhoven, February 2015,
- F. Legoll, Workshop "Dimension reduction: mathematical methods and applications", Penn State University, March 2015,
- F. Legoll, Reunion Conference of the Materials Defects IPAM program, Los Angeles, June 2015,
- F. Legoll, Equadiff Conference, Lyon, July 2015,
- F. Legoll, BIRS workshop on "Free-energy calculations: a mathematical perspective", Oaxaca, July 2015,
- F. Legoll, BIRS workshop on "Developments in the Theory of Homogenization", Banff, July 2015,
- F. Legoll, Workshop on "Multiscale Modeling and Analysis in Materials Science", Shanghai, August 2015,
- F. Legoll, ICIAM conference, Beijing, August 2015,
- F. Legoll, SciCADE conference, Potsdam, September 2015,
- F. Legoll, Colloque "Mathématiques appliquées et nanoélectronique", Grenoble, September 2015,
- F. Legoll, Weekly seminar of Numerical Analysis, KTH, Stockholm, October 2015,
- F. Legoll, Workshop "Reduced Basis, POD and PGD Model Reduction Techniques", ENS Cachan, November 2015,
- F. Legoll, Workshop "Gradient flows, Large deviations and Applications", Eindhoven, November 2015,
- F. Legoll, Journée EDP – Probas "Homogénéisation aléatoire", Paris, December 2015,
- F. Legoll, Journées NEEDS – Milieux Poreux, Paris, December 2015,
- T. Lelièvre, Workshop "New Discretization Methods for the Numerical Approximation of PDEs", Oberwolfach, January 2015,
- T. Lelièvre, Séminaire transversal MSME, Paris, January 2015,
- T. Lelièvre, Séminaire Collège de France, January 2015,
- T. Lelièvre, HIM workshop "Analytic approaches to scaling limits for random system", Bonn, January 2015,
- T. Lelièvre, Maxwell mini-symposium, Analysis and its applications, April 2015,
- T. Lelièvre, ADMOS, Nantes, June 2015,
- T. Lelièvre, PASC15, Zurich, June 2015,



- T. Lelièvre, Workshop "Statistical mechanics and computation of large deviation rate functions", Lyon, June 2015,
- T. Lelièvre, Workshop "Probabilistic numerical methods for non-linear PDEs", Imperial College London, July 2015,
- T. Lelièvre, MCM 2015, Linz, July 2015,
- T. Lelièvre, Workshop "Free-energy calculations: A mathematical perspective", BIRS Oaxaca, July 2015,
- T. Lelièvre, CRiSM Workshop "Non reversible dynamics", Warwick, September 2015,
- T. Lelièvre, Scicade 2015, Potsdam, September 2015,
- T. Lelièvre, Set-Oriented Numerics, Imperial College London, September 2015,
- T. Lelièvre, Séminaire de probabilités LJK, Grenoble, November 2015,
- T. Lelièvre, Séminaire analyse numérique, Orsay, November 2015,
- T. Lelièvre, Workshop "Predictive multiscale materials modelling, Cambridge, December 2015,
- T. Lelièvre, Workshop "Mathematical challenges in drug and protein design", MBI Columbus, December 2015,
- S. Lemaire, Workshop on "High order methods on polyhedral meshes", Milano, February 2015,
- S. Lemaire, PANACM conference, Buenos Aires, April 2015,
- S. Lemaire, Weekly seminar of the ANMC group, EPFL, June 2015,
- S. Lemaire, Congrès SMAI 2015, June 2015,
- F. Madiot, Congrès SMAI 2015, June 2015,
- F. Madiot, ICIAM conference, Beijing, August 2015,
- W. Minvielle, Workshop on "Analytic approaches to scaling limits for random system", Bonn, January 2015,
- W. Minvielle, International conference on Adaptive Modeling and Simulation (ADMOS), Nantes, June 2015,
- W. Minvielle, Equadiff Conference, Lyon, July 2015,
- M. Rousset, IRMAR Probability Seminar, Rennes, November 2015,
- M. Rousset, LPMA Probability Seminar, Paris, May 2015,
- M. Rousset, LAMP Proba-EDP GdT, Marseille, February 2015,
- G. Stoltz, workshop "Analytic approaches to scaling limits for random systems", Bonn, January 2015,
- G. Stoltz, workshop "Progress in nonequilibrium statistical mechanics", Nice, France, June 2015,
- G. Stoltz, workshop "Free-energy calculations. A mathematical perspective", Oaxaca, Mexico, July 2015,
- G. Stoltz, workshop NASPDE 2015, Sophia-Antiopolis, France, September 2015,
- G. Stoltz, program "Nonequilibrium Statistical Physics 2015", Bangalore, India, November 2015,
- G. Stoltz, meeting of the GdR ISIS, Paris, November 2015,
- G. Stoltz, workshop "Challenges in statistical mechanics: from mathematics to molecular dynamics to technological applications", London, December 2015.

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

- E. Cancès, Winter School on Computational and Mathematical Methods for Materials Defects and Multiphase Flows, 4h, Singapore, February 2015,
- E. Cancès, International summer School in electronic structure Theory: electron correlation in Physics and Chemistry, 2h, Aussois, France, June 2015,
- E. Cancès and T. Lelièvre, ICS summer school on Computational Chemistry and Applied Mathematics, 10h, Roscoff, France, July 15-August 14, 2015.

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

- F. Madiot, Séminaire CEA GAMNI 2015, Paris, February. 2015

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

- E. Cancès, Oberwolfach workshop on Mathematical Methods in Quantum Molecular Dynamics, Germany, June 2015,
- D. Gontier, GDR DYNAMIQUE QUAntique, Nantes, February 2015,
- D. Gontier, XVIII International Congress on Mathematical Physics, Santiago, July 2015,
- D. Gontier, Summer School on Current Topics in Mathematical Physics, Valparaiso, August 2015,
- M. Josien, PIRE Workshop, "Design of materials: From grain boundaries to stochastic homogenization", Leipzig, July 2015
- M. Josien, BIRS workshop on "Developments in the Theory of Homogenization", Banff, July 2015
- F. Madiot, École de Mécanique des Fluides Numérique 2015, Porquerolles, June 2015
- J. Roussel, Oberwolfach workshop on Mathematical Methods in Quantum Molecular Dynamics, Germany, June 2015
- J. Roussel, Non-equilibrium simulation school, Sheffield, September 2015,
- J. Roussel, Numerical Analysis of Stochastic Partial Differential Equations, Sofia-Antipolis, September 2015,
- J. Roussel, Non-equilibrium statistical physics, Bangalore, Octobre 2015,
- G. Stoltz, Oberwolfach workshop on Mathematical Methods in Quantum Molecular Dynamics, Germany, June 2015.

## 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

### Doctoral Dissertations and Habilitation Theses

- [7] D. GONTIER. *Mathematical contributions to electronic structure calculations*, Universite Paris Est, September 2015, <https://hal.archives-ouvertes.fr/tel-01238627>

### Articles in International Peer-Reviewed Journals

- [8] J. AGHILI, S. BOYAVAL, D. A. DI PIETRO. *Hybridization of mixed high-order methods on general meshes and application to the Stokes equations*, in "Computational Methods in Applied Mathematics", March 2015 [DOI : 10.1515/CMAM-2015-0004], <https://hal.archives-ouvertes.fr/hal-01009723>
- [9] E. AUDUSSE, S. BOYAVAL, N. GOUTAL, M. JODEAU, P. UNG. *Numerical Simulation of the Dynamics of Sedimentary River Beds with a Stochastic Exner Equation*, in "ESAIM: Proceedings and Surveys", January 2015 [DOI : 10.1051/PROC/201448015], <https://hal.archives-ouvertes.fr/hal-01102335>
- [10] X. BLANC, C. LE BRIS, P. L. LIONS. *Local profiles and elliptic problems at different scales with defects*, in "Comptes Rendus Mathématique", January 2015, pp. 203-208 [DOI : 10.1016/J.CRMA.2015.01.003], <https://hal.archives-ouvertes.fr/hal-01143311>
- [11] F. BOUCHUT, S. BOYAVAL. *Unified derivation of thin-layer reduced models for shallow free-surface gravity flows of viscous fluids*, in "European Journal of Mechanics - B/Fluids", January 2016, vol. 55, n<sup>o</sup> 1, pp. 116-131 [DOI : 10.1016/J.EUROMECHFLU.2015.09.003], <https://hal-enpc.archives-ouvertes.fr/hal-00833468>
- [12] C.-E. BRÉHIER, T. LELIÈVRE, M. ROUSSET. *Analysis of Adaptive Multilevel Splitting algorithms in an idealized case*, in "ESAIM: Probability and Statistics", October 2015, vol. 19 [DOI : 10.1051/PS/2014029], <https://hal.archives-ouvertes.fr/hal-00987297>
- [13] E. CANCES, V. EHRLACHER, F. LEGOLL, B. STAMM. *An embedded corrector problem to approximate the homogenized coefficients of an elliptic equation*, in "Comptes Rendus Mathématique", 2015, vol. 353, n<sup>o</sup> 9, pp. 801-806, <https://hal.archives-ouvertes.fr/hal-01100681>
- [14] J. COMER, J. C. GUMBART, J. HÉNIN, T. LELIÈVRE, A. POHORILLE, C. CHIPOT. *The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask*, in "Journal of Physical Chemistry B", January 2015, vol. 119, n<sup>o</sup> 3, pp. 1129–1151 [DOI : 10.1021/JP506633N], <https://hal.archives-ouvertes.fr/hal-01238593>
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- [19] C. LE BRIS, P. ROUCHON, J. ROUSSEL. *Adaptive low-rank approximation and denoised Monte Carlo approach for high-dimensional Lindblad equations*, in "Physical Review", December 2015 [DOI : 10.1103/PHYSREVA.92.062126], <https://hal-mines-paristech.archives-ouvertes.fr/hal-01252664>
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- [24] T. LELIÈVRE, G. SIMPSON. *A generalized parallel replica dynamics*, in "Journal of Computational Physics", March 2015, vol. 284, 21 pages, 14 figures, 5 tables [DOI : 10.1016/J.JCP.2015.01.002], <https://hal.inria.fr/hal-00983282>

### Other Publications

- [25] H. ALRACHID, T. LELIÈVRE. *Long-time convergence of an adaptive biasing force method: Variance reduction by Helmholtz projection*, May 2015, 33 pages, 20 figures, <https://hal.archives-ouvertes.fr/hal-01151894>
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- [28] A. BAKHTA, V. EHRLACHER. *Global existence of bounded weak solutions to degenerate cross-diffusion equations in moving domain*, December 2015, working paper or preprint, <https://hal.archives-ouvertes.fr/hal-01238636>

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- [36] F. CASNAVE, A. ERN, T. LELIÈVRE. *Variants of the Empirical Interpolation Method: symmetric formulation, choice of norms and rectangular extension*, August 2015, 7 pages, <https://hal.archives-ouvertes.fr/hal-01186039>
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- [50] I. G. TEJADA, L. BROCHARD, T. LELIÈVRE, G. STOLTZ, F. LEGOLL, E. CANCES. *Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure*, September 2015, working paper or preprint, <https://hal.archives-ouvertes.fr/hal-01196505>