IN PARTNERSHIP WITH:
Ecole des Ponts ParisTech

Activity Report 2018

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

Table of contents

Project-Team MATHERIALS

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

Keywords:

Computer Science and Digital Science:

A6.1.1. - Continuous Modeling (PDE, ODE)
A6.1.2. - Stochastic Modeling
A6.1.4. - Multiscale modeling
A6.1.5. - Multiphysics modeling
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.2. - Numerical probability
A6.2.3. - Probabilistic methods
A6.2.4. - Statistical methods
A6.2.7. - High performance computing
A6.3.1. - Inverse problems
A6.3.4. - Model reduction
A6.4.1. - Deterministic control

Other Research Topics and Application Domains:

B1.1.2. - Molecular and cellular biology
B4.3.4. - Solar Energy
B5.3. - Nanotechnology
B5.5. - Materials
B9.5.2. - Mathematics
B9.5.3. - Physics
B9.5.4. - Chemistry

1. Team, Visitors, External Collaborators

Research Scientists

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Sébastien Boyaval [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
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Post-Doctoral Fellows

Florent Hédin [Ecole Nationale des Ponts et Chaussées, until Nov 2018]
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PhD Students

Robert Benda [Ecole Polytechnique, from Sep 2018]
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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

Our group, originally only involved in electronic structure computations, continues to focus on many numerical issues in quantum chemistry, but now expands its expertise to cover several related problems at larger scales, such as molecular dynamics problems and multiscale problems. The mathematical derivation of continuum energies from quantum chemistry models is one instance of a long-term theoretical endeavour.

3.1.1. Electronic structure of large systems

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.

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.

3.1.2. Computational Statistical Mechanics

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

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

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

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

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

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

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

3.1.3. Homogenization and related problems

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

The following observation motivates the idea of coupling atomistic and continuum representation of materials. In many situations of interest (crack propagation, presence of defects in the atomistic lattice, ...), using a model based on continuum mechanics is difficult. Indeed, such a model is based on a macroscopic constitutive law, the derivation of which requires a deep qualitative and quantitative understanding of the physical and mechanical properties of the solid under consideration. For many solids, reaching such an understanding is a challenge, as loads they are subjected to become larger and more diverse, and as experimental observations helping designing such models are not always possible (think of materials used in the nuclear industry). Using an atomistic model in the whole domain is not possible either, due to its prohibitive computational cost. Recall indeed that a macroscopic sample of matter contains a number of atoms on the order of 10^{23}. However, it turns out that, in many situations of interest, the deformation that we are looking for is not smooth in *only a small part* of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them, in a domain decomposition spirit. In most of the domain, the

deformation is expected to be smooth, and reliable continuum mechanics models are then available. In the rest of the domain, the expected deformation is singular, so that one needs an atomistic model to describe it properly, the cost of which remains however limited as this region is small.

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

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

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

4. Highlights of the Year

4.1. Highlights of the Year

4.1.1. Awards

Claude Le Bris was selected to deliver the Coxeter lectures at the Fields Institute in Toronto and the Aziz lectures at the University of Maryland.

Florent Hédin received the “Best student/postdoc oral presentation” award at the 7^{th} Workshop on Parallel-in-Time methods, Roscoff, France, May.

5. New Software and Platforms

5.1. simol

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

- Contact: Gabriel Stoltz

6. New Results

6.1. Electronic structure calculations

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

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

6.1.1. Mathematical analysis

The members of the team have continued their systematic study of the properties of materials in the reduced Hartree-Fock approximation, a model striking a good balance between mathematical tractability and the ability to reproduce qualitatively complex effects.

E. Cancès and G. Stoltz have studied with L. Cao models for certain extended defects in materials [37]. These extended defects typically correspond to taking out a slab of finite width in the three-dimensional homogeneous electron gas. The work is performed in the framework of the reduced Hartree-Fock model with either Yukawa or Coulomb interactions, using techniques previously developed to study local perturbations of the free-electron gas. It is shown that the model admits minimizers, and that Yukawa ground state energies and density matrices converge to ground state Coulomb energies and density matrices as the Yukawa parameter tends to zero. These minimizers are unique for Yukawa interactions, and are characterized by a self-consistent equation. Numerical simulations show evidence of Friedel oscillations in the total electronic density.

A. Levitt has examined the phenomenon of screening in materials. In [54] he has studied the effect of adding a small charge to a periodic system modeled by the reduced Hartree-Fock at finite temperature. He has showed that the reaction potential created by the rearrangement of the electrons counteracts exactly the free charge, so that the effective interaction in such systems is short-range. The proof proceeds by studying the properties of the linear response operator, which also sheds some light on the charge-sloshing instability seen in numerical methods to solve the self-consistent equations.

6.1.2. Numerical analysis

E. Cancès has pursued his long-term collaboration with Y. Maday (Sorbonne Université) on the numerical analysis of linear and nonlinear eigenvalue problems. Together with G. Dusson (Warwick, United Kingdom), B. Stamm (Aachen, Germany), and M. Vohralík (Inria SERENA), they have designed *a posteriori* error estimates for conforming numerical approximations of the Laplace eigenvalue problem with homogeneous Dirichlet boundary conditions. In [38], they prove *a priori* error estimates for the perturbation-based post-processing of the plane-wave approximation of Schrödinger equations introduced and tested numerically in previous works. They consider a Schrödinger operator $H = -\frac{1}{2}\Delta + V$ on $L^2(\Omega)$, where Ω is a cubic box with periodic boundary conditions. The quantities of interest are, on the one hand, the ground-state energy defined as the sum of the lowest N eigenvalues of H , and, on the other hand, the ground-state density matrix, that is the spectral projector on the vector space spanned by the associated eigenvectors. Such a problem is central in first-principle molecular simulation, since it corresponds to the so-called linear subproblem in Kohn-Sham density functional theory (DFT). Interpreting the exact eigenpairs of H as perturbations of the numerical eigenpairs obtained by a variational approximation in a plane-wave (i.e. Fourier) basis, they compute first-order corrections for the eigenfunctions, which are turned into corrections on the ground-state density matrix. This allows them to increase the accuracy of both the ground-state energy and the ground-state density matrix at a low computational extra-cost. Indeed, the computation of the corrections only requires the computation of the residual of the solution in a larger plane-wave basis and $2N$ Fast Fourier Transforms.

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 (Sorbonne Université), and B. Stamm (Aachen, Germany) have introduced a few years ago 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 and B. Mennucci (Chemistry, Pisa, Italy) and J.-P. Piquemal (Sorbonne Université), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). Together with L. Lagardère (Sorbonne Université) and G. Scalmani (Gaussian Inc., USA), they illustrate in [29] the domain decomposition COSMO (ddCOSMO) implementation and how to couple it with an existing classical or quantum mechanical (QM) codes. They review in detail what input needs to be provided to ddCOSMO and how to assemble it, describe how the ddCOSMO equations are solved and how to process the results in order to assemble the required quantities, such as Fock matrix contributions for the QM case, or forces for the classical one. Throughout the paper, they make explicit references to the ddCOSMO module, which is an open source, Fortran 90 implementation of ddCOSMO that can be downloaded and distributed under the LGPL license.

E. Cancès, V. Ehrlacher and A. Levitt, together with D. Gontier (Dauphine) and D. Lombardi (Inria REO), have studied the convergence of properties of periodic systems as the size of the computing domain is increased. This convergence is known to be difficult in the case of metals. They have characterized in [39] the speed of convergence for a number of schemes in the metallic case, and have studied the properties of a widely used numerical method that adds an artificial electronic temperature.

A. Levitt has continued his study of Wannier functions in periodic systems. With A. Damle (Cornell, USA) and L. Lin (Berkeley, USA), they have proposed an efficient numerical method for the computation of maximally-localized Wannier functions in metals, and have showed on the example of the free electron gas that they are not in general exponentially localized [42]. With D. Gontier (Dauphine) and S. Siraj-Dine, they proposed a new method for the computation of Wannier functions which applies to any insulator, and in particular to the difficult case of topological insulators [45].

6.2. Computational Statistical Physics

Participants: Grégoire Ferré, Florent Hédin, Frédéric Legoll, Tony Lelièvre, Mouad Ramil, Julien Roussel, Laura Silva Lopes, Gabriel Stoltz, Pierre Terrier.

The objective of computational statistical physics is to compute macroscopic properties of materials starting from a microscopic description, using concepts of statistical physics (thermodynamic ensembles and molecular dynamics). The contributions of the team can be divided into four main topics: (i) the development of methods for sampling the configuration space; (ii) the numerical analysis of such methods; (iii) the efficient computation of dynamical properties which requires to sample metastable trajectories; (iv) coarse-graining techniques to reduce the computational cost of molecular dynamic simulations and gain some insights on the models.

6.2.1. Sampling of the configuration space: new algorithms and applications

New numerical methods in order to sample probability measures on the configuration space have been developed: either measures supported on submanifolds, or stationary states of stochastic dynamics. First, in [51], T. Lelièvre and G. Stoltz, together with M. Rousset (Inria Rennes, France) have studied how to sample probability measures supported on submanifolds, by adding an extra momentum variable to the state of the system, and discretizing the associated Hamiltonian dynamics with some stochastic perturbation in the extra variable. In order to avoid biases in the invariant probability measures sampled by discretizations of these stochastically perturbed Hamiltonian dynamics, a Metropolis rejection procedure can be considered. The so-obtained scheme belongs to the class of generalized Hybrid Monte Carlo (GHMC) algorithms. However, the usual method has to be generalized using a procedure suggested by Goodman, Holmes-Cerfon and Zappa for Metropolis random walks on submanifolds, where a reverse projection check is performed to enforce the reversibility of the algorithm for large timesteps and hence avoid biases in the invariant measure. A full mathematical analysis of such procedures is provided, as well as numerical experiments demonstrating the

importance of the reverse projection check on simple toy examples. Second, the work [55] by J. Roussel and G. Stoltz focuses on the use of control variates for non-equilibrium systems. Whereas most variance reduction methods rely on the knowledge of the invariant probability measure, this latter is not explicit out of equilibrium. Control variates offer an attractive alternative in this framework. J. Roussel and G. Stoltz have proposed a general strategy for constructing an efficient control variate, relying on physical simplifications of the dynamics. The authors provide an asymptotic analysis of the variance reduction in a perturbative framework, along with extensive numerical tests on three different systems.

In terms of applications of such sampling techniques, members of the project-team have been working on two different subjects: random matrices models and adaptive techniques to compute large deviation rate functionals. The paper [16] was written by G. Ferré and D. Chafaï (Université Paris Dauphine, France), following the simple idea: the eigenvalues of random matrices are distributed according to Boltzmann–Gibbs measures, but researchers in this field do not use techniques from statistical physics for numerical investigations. The authors therefore used a Hamiltonian Monte Carlo algorithm to investigate numerically conjectures about random matrices and related Coulomb gases. The next step is to add constraints to these systems to understand better the behavior of random matrices with constraints and the large size limit of their spectra (the algorithm mentioned above to sample probability measures supported on submanifolds may be useful in this context). The work [19] focuses on computing free energies and entropy functions, as they arise in large deviations theory, through adaptive techniques. It is actually in the spirit of techniques used in mathematical finance, adapted to the statistical mechanics context, and enriched with new estimators based on variational representations of entropy functions. These tools have been pioneered by H. Touchette (Stellenbosch University, South Africa), with whom the paper was written by G. Ferré.

6.2.2. Sampling of the configuration space: numerical analysis

Concerning the numerical analysis of sampling techniques of probability measures on the configuration space, let us mention three works.

First, in [44], G. Ferré and G. Stoltz study the numerical errors that arise when a stochastic differential equation (SDE) is discretized in order to compute scaled cumulant functions (or free energy) and ergodic properties of Feynman–Kac semigroups. These quantities naturally arise in large deviations theory, for estimating probabilities of rare events. This analysis is made difficult by the nonlinear (mean field) feature of the dynamics at hand. The obtained estimates generalize previous results on the numerical analysis of ergodic properties of discretized SDEs. As a theoretical extension of the previous work, the purpose of the work [43] by G. Ferré and G. Stoltz, in collaboration with M. Rousset (Inria Rennes, France), is to provide further theoretical investigations on the long time behavior of Feynman–Kac semigroups. More precisely, it aims at giving practical criteria for these nonlinear semigroups to have a limit, and makes precise in which sense this limit is to be understood. This was an open problem so far for systems evolving in unbounded configuration spaces, which was addressed through Lyapunov function techniques. Although theoretical, these results are of practical importance since, if these dynamics do not have a well-defined long time behavior, it is hopeless to try to compute rare events.

Finally, together with C. Andrieu (Univ. Bristol, United-Kingdom), A. Durmus (ENS Saclay, France) and N. Nüsken (Univ. Potsdam, Germany), J. Roussel derived in [32] spectral gap estimates for several Piecewise Deterministic Markov Processes (PDMPs), namely the Randomized Hamiltonian Monte Carlo, the Zig-Zag process and the Bouncy Particle Sampler. The hypocoercivity technique provides estimates with explicit dependence on the parameters of the dynamics. Moreover the general framework considered allows to compare quantitatively the bounds found for the different methods. Such PDMDs are currently more and more used as efficient sampling tools, but their theoretical properties are still not yet well understood.

6.2.3. Sampling of dynamical properties and rare events

The sampling of dynamical properties along molecular dynamics trajectories is crucial to get access to important quantities such as transition rates or reactive paths. This is difficult numerically because of the metastability of trajectories. Members of the project-team are following two numerical approaches to sample

metastable trajectories: the accelerated dynamics *à la* A.F. Voter and the adaptive multilevel splitting (AMS) technique to sample reactive paths between metastable states.

Concerning the mathematical analysis of the accelerated dynamics, in [50], T. Lelièvre reviews the recent mathematical approaches to justify these numerical methods, using the notion of quasi-stationary distribution. Moreover, in [49], T. Lelièvre together with D. Le Peutrec (Université de Paris Saclay, France) and G. Di Gesu and B. Nectoux (TU Wien, Austria) give an overview of the results obtained during the PhD of B. Nectoux. Using the quasi-stationary distribution approach and tools from semi-classical analysis, one can justify the use of kinetic Monte Carlo models parametrized by the Eyring-Kramers formulas to describe exit events from metastable states, for the overdamped Langevin dynamics. Concerning the implementation, in [22], F. Hédin and T. Lelièvre test the Generalized Parallel Replica algorithm to biological systems, and obtain strong linear scalability, providing up to 70% of the maximum possible speedup on several hundreds of CPUs. The "Parallel Replica" (ParRep) dynamics is known for allowing to simulate very long trajectories of metastable Langevin dynamics in the materials science community, but it relies on assumptions that can hardly be transposed to the world of biochemical simulations. The later developed "Generalized ParRep" variant solves those issues, and it had not been applied to significant systems of interest so far. Finally, let us mention the work [27] where T. Lelièvre together with J. Reygner (Ecole des Ponts, France) and L. Pillaud-Vivien (Inria Paris, France) analyze mathematically the Fleming-Viot particle process in the simple case of a finite state space. This Fleming-Viot particle process is a key ingredient of the Generalized ParRep algorithm mentioned above, in order to both approximate the convergence time to the quasi-stationary distribution, and to efficiently sample it.

Concerning the AMS technique, in [36], T. Lelièvre and C.-E. Bréhier (ENS Lyon, France) test new importance functions to compute rare events associated with the law of the solution to a stochastic differential equation at a given fixed time. This can be used for example to estimate the rate functional for large deviation principle applied to time averages.

6.2.4. Coarse-graining

In two related works, members of the project-team have studied the quality of the effective dynamics derived from a high dimension stochastic differential equation on a few degrees of freedom, using a projection approach *à la Mori-Zwanzig*. More precisely, in [48], F. Legoll, T. Lelièvre and U. Sharma obtain precise error bounds in the case of non reversible dynamics. This analysis also aims at discussing what is a good notion of mean force for non reversible systems. In [53], T. Lelièvre together with W. Zhang (ZIB, Germany) extend previous results on pathwise error estimates for such effective dynamics to the case of nonlinear vectorial reaction coordinates.

Once a good coarse-grained model has been obtained, one can try to use it in order to get a better integrator of the original dynamic in the spirit of a predictor-corrector method. In [52], T. Lelièvre together with G. Samaey and P. Zielinski (KU Leuven, Belgium) analyze such a micro-macro acceleration method for the Monte Carlo simulation of stochastic differential equations with time-scale separation between the (fast) evolution of individual trajectories and the (slow) evolution of the macroscopic function of interest.

6.3. Homogenization

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

6.3.1. Deterministic non-periodic systems

In homogenization theory, members of the project-team have pursued their ongoing systematic study of perturbations of periodic problems (by local and nonlocal defects). This has been done in two different directions.

For linear elliptic equations, C. Le Bris has written, in collaboration with X. Blanc (Paris Diderot, France) and P.-L. Lions (Collège de France, France), two manuscripts that present a more versatile proof of the existence of a corrector function for periodic problems with local defects, and also extend the results: the first manuscript [34] addresses the case of an equation (or a system) in divergence form, while the second manuscript [12] extends the analysis to advection-diffusion equations.

Second, they have also provided more details on the quality of approximation achieved by their theory. The fact that a corrector exists with suitable properties allows one to quantify the rate of convergence of the two-scale expansion using that corrector to the actual exact solution, as the small homogenization parameter ε vanishes. These works by C. Le Bris, in collaboration with X. Blanc and M. Josien (and in the context of the PhD thesis of the latter), will be presented in a series of manuscripts in preparation. The precise results have been announced in [11] and proven in [33]. A related study [47] has been performed by M. Josien and addresses issues regarding periodic Green functions.

Also in the context of homogenization theory, C. Le Bris and F. Legoll have initiated a collaboration with R. Cottereau (Ecole Centrale and now CNRS Marseille, France). The topic is in some sense a follow-up on both an earlier work of R. Cottereau and the series of works completed by C. Le Bris and F. Legoll in collaboration with K. Li and next S. Lemaire over the years. Schematically, the purpose of the work is to determine the homogenized coefficient for a medium without explicitly performing a homogenization approach nor using a MsFEM type approach. In earlier works, an approximation approach, somewhat engineering-style, was designed. The purpose now is to examine the performance of this approach in the context of the so-called Arlequin method, a very popular method in the mechanical engineering community. One couples a sub-region of the medium where a homogeneous model is employed, along with a complementary sub-region where the original multiscale model is solved explicitly. The coupling is performed using the Arlequin method. Then, one optimizes a suitable criterion so that optimization leads to an homogeneous sub-region indeed described by the homogenized coefficient seeked for. Some numerical analysis questions, together with practical perspectives for computational enhancements of the approach, are currently examined.

Finally, C. Le Bris has informally participated into the supervision of the master thesis of S. Wolf (Ecole Normale Supérieure, Paris, France), and in this context performed some works in interaction with the student and X. Blanc. The purpose is to investigate perturbations of periodic homogenization problems when the perturbation is geometric in nature. The test case considered is that of a domain perforated by holes the locations of which are not necessarily periodic, but only periodic up to a local perturbation. The results proven, on the prototypical Poisson equation, are natural extensions of the celebrated results by J.-L. Lions published in the late 1960s for the periodic case. This provides a proof of concept, showing that perturbations of a periodic geometry are also possible, a fact that will be more thoroughly investigated in the near future within the above mentioned collaboration.

6.3.2. Stochastic homogenization

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

Using standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the whole space $\mathbb{R}^d$. This equation is therefore delicate and expensive to solve. A standard approach consists in truncating the space $\mathbb{R}^d$ to some bounded domain, on which the corrector problem is numerically solved.

In collaboration with B. Stamm (Aachen University, Germany) and S. Xiang (now also at Aachen University, Germany), E. Cancès, V. Ehrlacher and F. Legoll have studied, both from a theoretical and a numerical standpoints, new alternatives for the approximation of the homogenized matrix. They all rely on the use of an embedded corrector problem, previously introduced by the authors, where a finite-size domain made of the highly oscillatory material is embedded in a homogeneous infinite medium whose diffusion coefficients have to be appropriately determined. In [40], they have shown that the different approximations introduced all converge to the homogenized matrix of the medium when the size of the embedded domain goes to infinity. In [41], they present an efficient algorithm for the resolution of such problems for particular heterogeneous materials, based on the reformulation of the embedded corrector problem as an integral equation, which is discretized using spherical harmonics and solved using the fast multipole method.

Besides the averaged behavior of the oscillatory solution u_ε on large space scales (which is given by its homogenized limit), a question of interest is to describe how u_ε fluctuates. This question is investigated in the PhD thesis of P.-L. Rothé, both from a theoretical and a numerical viewpoints. First, theoretical results

have been obtained for a weakly stochastic setting (where the coefficient is the sum of a periodic coefficient and a small random perturbation). It has been shown that, at the first order and when ε is small, the localized fluctuations (characterized by a test function g) of u_ε are Gaussian. The corresponding variance depends on the localization function g, on the right-hand side f of the problem satisfied by u_ε, and on a fourth order tensor Q which is defined in terms of the corrector. Since the corrector function is challenging to compute, so is Q. A numerical approach has hence been designed to approximate Q and its convergence has been proven. Second, numerical experiments in more general settings (i.e. full stochastic case) following the same approach have been performed. The results are promising, and consistent with the theoretical results obtained in the weakly stochastic setting. These results are collected in a manuscript in preparation.

In collaboration with T. Hudson (University of Warwick, United Kingdom), F. Legoll and T. Lelièvre have considered in [46] a scalar viscoelastic model in which the constitutive law is random and varies on a lengthscale which is small relative to the overall size of the solid. Using stochastic two-scale convergence, they have obtained the homogenized limit of the evolution, and have demonstrated that, under certain hypotheses, the homogenized model exhibits hysteretic behaviour which persists under asymptotically slow loading. This work is motivated by rate-independent stress-strain hysteresis observed in filled rubber.

6.3.3. Multiscale Finite Element approaches

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

During the year, several research tracks have been pursued in this general direction.

The final writing of the various works performed in the context of the PhD thesis of F. Madiot is still ongoing. The issues examined there are on the one hand the application (and adequate adjustment) of MsFEM approaches to the case of an advection-diffusion equation with a dominating convection term posed in a perforated domain, and on the other hand some more general study of a numerical approach based, again in the case of convection-dominated flows, on the introduction of the invariant measure associated to the problem. The final version of the two manuscripts describing the efforts in each of these directions should be completed in a near future.

The MsFEM approach uses a Galerkin approximation of the problem on a pre-computed basis, obtained by solving local problems mimicking the problem at hand at the scale of mesh elements, with carefully chosen right-hand sides and boundary conditions. The initially proposed version of MsFEM uses as basis functions the solutions to these local problems, posed on each mesh element, with null right-hand sides and with the coarse P1 elements as Dirichlet boundary conditions. Various improvements have next been proposed, such as the *oversampling* variant, which solves local problems on larger domains and restricts their solutions to the considered element. In collaboration with U. Hetmaniuk (University of Washington in Seattle, USA), C. Le Bris, F. Legoll and P.-L. Rothé have introduced and studied a MsFEM method improved differently. They have considered a variant of the classical MsFEM approach with enrichments based on Legendre polynomials, both in the bulk of the mesh elements and on their interfaces. A convergence analysis of this new variant has been performed. Promising numerical results have been obtained. These results are currently being collected in a manuscript in preparation.

One of the perspectives of the team, through the PhD thesis of A. Lesage, is the development of Multiscale Finite Element Methods for thin heterogeneous plates. The fact that one of the dimension of the domain of interest scales as the typical size of the heterogeneities within the material induces theoretical and practical difficulties that have to be carefully taken into account. The first steps of the work of V. Ehrlacher, F. Legoll and A. Lesage, in collaboration with A. Lebée (École des Ponts) have consisted in studying the homogenized limit (and the two-scale expansion) of problems posed on thin heterogeneous plates. The case of a diffusion equation has been first dealt with, while the more challenging case of elasticity is currently under study.

6.4. Complex fluids

Participants: Sébastien Boyaval, Dena Kazerani.

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

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

Concerning the first point, new results have been obtained in collaboration with A. Caboussat (HEG, Switzerland) and M. Picasso (EPFL, Switzerland), in the framework of the SEDIFLO project (funded by ANR) and of Arwa Mrad PhD thesis at EPFL. In [13], they have shown numerically inability of some classical incompressible density-dependent Navier-Stokes equations to take into account some multiphase concentration effects in a prototypical set-up of fluvial erosion (in comparison with physical experiments). Hence the need for *new* models, that better describe complex flows associated with heterogeneities in the fluid microstructure. Concerning the second point, new results have been obtained in collaboration with M. Grepl and K. Veroy (Aachen, Germany) regarding the numerical reduction of transport models for data assimilation [25], in the framework of M. Kaercher PhD thesis at Aachen.

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, EDF. 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 is the PI of the ANR JCJC project SEDIFLO (2016-2020) to investigate new numerical models of solid transport in rivers.
- V. Ehrlacher is a member of the ANR project ADAPT (2018-2022), PI: D. Lombardi, Inria REO team-project. This project is concerned with the parallelization of tensor methods for high-dimensional problems.
- F. Legoll is a member of the ANR project CINE-PARA (2015-2019), PI: Y. Maday, Sorbonne Université. This project is concerned with parallel-in-time algorithms.
- G. Stoltz is the PI of the ANR project COSMOS (2014-2019) which focuses on the development of efficient numerical techniques to simulate high-dimensional systems in molecular dynamics and computational statistics. It includes research teams from Institut Mines-Telecom, Inria Rennes and IBPC Paris.

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

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

The project-team is involved in two Labex: 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

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, Institut de Biologie Structurale (Grenoble) and Institut de Biologie Physico-Chimique (Paris). The LIA has been renewed for 4 years, starting January 1st, 2018.

9. Dissemination

9.1. Promoting Scientific Activities

E. Cancès

- is the director of CERMICS, the Applied Mathematics department at École des Ponts,
- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-), SIAM Journal of Scientific Computing (2008-), SIAM Multiscale Modeling and Simulation (2012-), and the Journal of Computational Mathematics (2017-),
- has co-organized an Oberwolfach workshop (March), an IMA workshop (March), the 2018 SIAM MS conference (July), and an ISCD summer school (July - August),
- was a member of the DFG Review Panel “Mathematics” for Clusters of Excellence, Cologne, April.

V. Ehrlacher

- is a member of the “Conseil d’Enseignement et de Recherche” of Ecole des Ponts,
- has co-organized the GdR MASCOT-NUM Working meeting on “Uncertainty quantification in materials science”, at IHP, May (with J. Baccou, J. Reygner and G. Perrin).

G. Ferré and J. Roussel have co-organized the working group J-PSI (Jeunes chercheurs en physique statistique et interactions, until July) at IHP. The working group was provided financial support from the SMAI through a BOUM grant, and ended with a one-day conference in June at Inria Paris.

C. Le Bris 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-), Journal de Mathématiques Pures et Appliquées (2009-), Pure and Applied Analysis (2018-). 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 (until September),
- the "International Scientific Advisory Committee" of the Centre de Recherche Mathématique, Université de Montréal (until mid-2018),
- 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,
- the "Conseil de la Faculté des sciences et ingénierie", Sorbonne Université.

He is the president of the scientific advisory board of the Institut des Sciences du calcul et des données, Sorbonne Université. He has held a regular position of Visiting Professor at the University of Chicago.

F. Legoll

- is a member of the editorial board of SIAM MMS (2012-) and of ESAIM: Proceedings and Surveys (2012-),
- is a member of the ANR committee CES-40 "mathématiques et informatique".

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings and Surveys (with D. Chafai, C. Imbert and P. Lafitte),
- is a member of the editorial boards of IMA: Journal of Numerical Analysis and SIAM/ASA Journal of Uncertainty Quantification,
- is a member of the "Conseil d'Administration" of SMAI and École des Ponts,

Together with G. Stoltz, they have

- co-organized the Workshop "Advances in Computational Statistical Physics", CIRM, September (with G. Pavliotis),
- co-organized the CECAM discussion meeting "Coarse-graining with Machine Learning in molecular dynamics", Sanofi Campus Gentilly, December (with P. Gkeka, P. Monmarché).

G. Stoltz

- is a member of the scientific council of UNIT (Université Numérique Ingénierie et Technologie),
- co-organized with C. Robert the workshop "Computational Statistics and Molecular Simulation: A Practical Cross-Fertilization" (BIRS-Oaxaca, November),
- co-organizes the working group "Machine learning and optimization" of the Labex Bezout (with W. Hachel and R. Elie).

9.1.1. Conference participation

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

- S. Boyaval, weekly seminar of Laboratoire Jean Kuntzmann, Grenoble, February,
- S. Boyaval, GDR EGRIN annual meeting, Clermont-Ferrand, June,
- S. Boyaval, La Trobe University – Kyushu University joint Industrial Math seminar, Melbourne, September,

- E. Cancès, Energy and forces workshop, Cambridge, UK, January,
- E. Cancès, workshop "Mathematical models and computation of nonlinear problems", China, January,
- E. Cancès, weekly seminar of the mathematics department, Sapienza University of Rome, February,
- E. Cancès, weekly seminar of Maison de la Simulation, Saclay, March,
- E. Cancès, 2D materials workshop, Minneapolis, March,
- E. Cancès, Fields Institute workshop, Toronto, May,
- E. Cancès, workshop on computational mathematics, Suzhou, China, June,
- E. Cancès, Centre Henri Lebesgue workshop, Rennes, June,
- E. Cancès, SIAM Materials Science conference, Portland, July,
- E. Cancès, IPAM workshop, Los Angeles, August,
- E. Cancès, GAMM workshop, Aachen, September,
- E. Cancès, Franco-German Meeting Workshop on Mathematical Aspects in Computational Chemistry, Aachen, September,
- E. Cancès, CECAM workshop, Lausanne, November,
- E. Cancès, workshop "Big data challenges for predictive modeling of complex systems", Hong Kong, November,
- V. Ehrlacher, Groupe de travail ENS Rennes, January,
- V. Ehrlacher, workshop on "Mathematical Methods in Quantum Chemistry", Oberwolfach, Germany, March,
- V. Ehrlacher, Séminaire DEFI-MEDISIM-POEMS, October,
- G. Ferré, CERMICS PhD Seminar, Paris, February,
- G. Ferré, Les probabilités de demain, IHP, Paris, March,
- G. Ferré, Congrès National d'Analyse Numérique, Cap d'Agde, May,
- G. Ferré, International Conference in Monte Carlo and Quasi Monte Carlo Methods in Scientific Computing, Rennes, July,
- G. Ferré, SIAM Materials Science conference, Portland, July (two talks),
- G. Ferré, Franco-German Meeting Workshop on Mathematical Aspects in Computational Chemistry, Aachen, September,
- G. Ferré, Student Probability Seminar, Courant Institute of Mathematical Science, New-York, December,
- M. Josien, CANUM conference, Cap d'Agde, May,
- M. Josien, SIAM Materials Science, Portland, USA, July,
- F. Hédin, "PinT 7th Workshop on Parallel-in-Time methods", Roscoff Marine Station, France, May,
- F. Hédin, "CECAM Workshop, Frontiers of coarse graining in molecular dynamics", Zuse Institute Berlin, Germany, July,
- F. Hédin, CIRM Conference "Advances in Computational Statistical Physics", September,
- C. Le Bris, Séminaire Pierre-Louis Lions, Collège de France, January,
- C. Le Bris, Applied Mathematics Colloquium of the University of Maryland, February,
- C. Le Bris, PDE seminar, University of Chicago, April,
- C. Le Bris, Journées de l'Ecole Doctorale Carnot-Pasteur, Université de Besançon, June,
- C. Le Bris, Journées Scientifiques de Marcoule, CEA Marcoule, June,
- C. Le Bris, Journées de Cadarache, CEA Cadarache, June,

- C. Le Bris, (plenary lecture) 25th International Conference on Domain Decomposition Methods, St. John's, Canada, July,
- C. Le Bris, LMS Durham Research Symposium on Homogenization in Disordered Media, Durham, UK, August,
- C. Le Bris, Groupe de travail Calcul des Variations Paris-Ile de France, November
- F. Legoll, EMMC conference, Nantes, March,
- F. Legoll, University of Chicago, CAMP seminar, Chicago, USA, May,
- F. Legoll, AIMS conference, Taipei, Taiwan, July,
- F. Legoll, NumDiff conference, Halle, Germany, September,
- T. Lelièvre, Journée de l'ANR CINE-PARA, Université Paris 13, January,
- T. Lelièvre, Workshop "Interplay of Analysis and Probability in Applied Mathematics", Oberwolfach, Feburary,
- T. Lelièvre, Séminaire de la Maison de la Simulation, Saclay, March,
- T. Lelièvre, Séminaire du LJK, Grenoble, March,
- T. Lelièvre, Séminaire Statistical Machine Learning in Paris, Paris, April,
- T. Lelièvre, Workshop "Data-driven modelling of complex systems", ATI, London, May,
- T. Lelièvre, Workshop "Uncertainty quantification in materials science", IHP, Paris, May,
- T. Lelièvre, Séminaire Mathématiques pour l'Industrie et la Physique, Toulouse, May,
- T. Lelièvre, Fields Institute, "Focus Program on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications", Toronto, May,
- T. Lelièvre, Workshop "Simulation and probability: recent trends", Rennes, June,
- T. Lelièvre, Workshop "Particle based methods", ICMS, Edinburgh, July,
- T. Lelièvre, CECAM workshop "Frontiers of coarse graining in molecular dynamics", Berlin, July,
- T. Lelièvre, Franco-German Workshop on mathematical aspects in computational chemistry, Aachen, September,
- T. Lelièvre, Séminaire "Simulation, Incertitudes et Méta-modèles", CEA Saclay, October,
- T. Lelièvre, Workshop "Computational Statistics and Molecular Simulation: A Practical Cross-Fertilization", Oaxaca, November,
- T. Lelièvre, Groupe de travail Évolution de Populations et Systèmes de Particules en Interaction, Ecole Polytechnique, December,
- A. Levitt, Mathematical Methods in Quantum Chemistry, Oberwolfach, March,
- A. Levitt, Analytical & Numerical Methods in Quantum Transport, Aalborg, May,
- A. Levitt, Beijing Normal University seminar, June,
- A. Levitt, Chinese Academy of Sciences seminar, June,
- A. Levitt, Franco-German Meeting Workshop on Mathematical Aspects in Computational Chemistry, Aachen September,
- P.-L. Rothé, PhD seminar, Inria Paris, June,
- J. Roussel, SIAM Materials Science conference, Portland, July,
- J. Roussel, Monte Carlo & Quasi-Monte Carlo Methods conference, Rennes, France, July,
- L. Silva Lopes, CECAM Coarse Graining Workshop, Berlin, Germany, July,
- L. Silva Lopes, Advances in Computational Statistical Physics, Marseille, September,
- S. Siraj-Dine, SIAM Materials Science conference, Portland, July,
- G. Stoltz, Seminar of the polymer physics group, ETH Zürich, February,

- G. Stoltz, Applied mathematics seminar Duke University, Durham, North Carolina, USA, February,
- G. Stoltz, Statistical Machine Learning in Paris seminar, Paris, April,
- G. Stoltz, Focus Program on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications, Fields institute, Toronto, Canada, May,
- G. Stoltz, Journées scientifiques Inria, Bordeaux, France, June,
- G. Stoltz, Applied mathematics seminar Courant Institute of Mathematical Sciences, New York, October,
- G. Stoltz, Inria-LJLL seminar, December,
- P. Terrier, Minerals, Metals & Materials Society Annual Meeting & Exhibition, Phoenix, March,
- P. Terrier, CANUM, Cap d'Adge, June.

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

- E. Cancès, Fourier transform and applications in quantum physics and chemistry, 9h, GDR CORREL spring school, Paris, April,
- E. Cancès, Optimization problems in molecular simulation, 12h, ISCD summer school, Roscoff, July,
- E. Cancès, Mathematical methods and numerical algorithms for quantum chemistry, 12h, MWM autumn school, Gelsenkirchen, October,
- C. Le Bris, Aziz Lectures, University of Maryland, College Park, February,
- C. Le Bris, Fields Institute Coxeter Lecture Series, Toronto, May,
- T. Lelièvre, Mini-school math/chemistry GDR CORREL, 9h, April,
- T. Lelièvre, Lectures on "Stochastic numerical methods and molecular dynamics simulations" (15h), Ecole d'été ISCD (Sorbonne Université), Roscoff, August.

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

- A. Lesage, Fifth workshop on thin structures, Naples, Italy, September,
- J. Roussel, Advances in Computational Statistical Physics, CIRM, Marseille, France, September,
- G. Ferré, Data-driven modelling of Complex Systems, Alan Turing Institute, London,
- G. Ferré, Simulation Aléatoire : problèmes actuels, Inria Rennes,
- G. Ferré, Advances in Computational Statistical physics, CIRM.

Members of the team have benefited from long-term stays in institutions abroad:

- G. Ferré, Courant Institute of Mathematical Science, New York University, New York, USA, October-November,
- P.-L. Rothé, Department of Applied Mathematics, University of Washington, Seattle, USA, April-May.

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

- G. Ferré YES'X Workshop, Scalable Statistics: Accuracy and computational complexity, March,
- M. Josien, Coxeter Lecture Series, Seminar talks, Toronto, Canada, May
- A. Lesage, CANUM conference, Cap d'Agde, May,
- A. Lesage, 6th European conference on computational mechanics, Glasgow, United Kingdom, June,
- M. Ramil, Perspectives en physique statistique computationnelle au CIRM (Centre International de Recherche Mathématiques), Marseille, September,
- M. Ramil, Journées Kolmogorov, Evry, September,
- M. Ramil, ANR EFI workshop, Lyon, November,
- P.-L. Rothé, 6th European conference on computational mechanics, Glasgow, United Kingdom, June,
- P.-L. Rothé, FreeFem++ days, Paris, December,
- S. Siraj-Dine, Workshop Mathematical Challenges in Quantum Mechanics, Rome, February,
- S. Siraj-Dine, Oberwolfach Workshop on Mathematical Methods in Quantum Chemistry, March,
- S. Siraj-Dine, ICMP XIX Congress on Mathematical Physics, Montréal, July.

9.1.2. Software development and contributions

- A. Levitt has implemented a method to construct maximally-localized Wannier functions for metals. A. Levitt and S. Siraj-Dine have implemented a method for the computation of Wannier functions of topological insulators. Both these methods are available at https://github.com/antoine-levitt/wannier.
- J. Roussel and G. Stoltz have restructured the SIMOL code, in particular separating core functions, routines for quantum simulations and advanced features for molecular dynamics, in order to obtain a simpler and more accessible base code. The code is available at https://gitlab.inria.fr/matherials/simol/.
- A first implementation of the Generalized Parallel Replica algorithm, developed by F. Hédin and T. Lelièvre, is available at https://gitlab.inria.fr/parallel-replica/gen.parRep. The objective of the gen.parRep software is to popularize the use of the Parallel Replica algorithm to biological systems. Molecular dynamics is performed by using external codes linked to this program such as OpenMM. This is the first publicly available implementation of the Generalized Parallel Replica method targeting frequently encountered metastable biochemical systems, such as conformational equilibria or dissociation of protein-ligand complexes. We refer to the preprint [22] for more details.

9.2. Teaching - Supervision - Juries

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

At École des Ponts 1st year (equivalent to L3):

- Analyse et calcul scientifique, 30h (A. Levitt, G. Stoltz),
- Équations aux dérivées partielles et éléments finis, 15h (F. Legoll, P.-L. Rothé),
- Hydraulique numérique, 15h (S. Boyaval),
- Mécanique quantique, 10h (E. Cancès, A. Levitt),
- Méthodes numériques pour les problèmes en grande dimension, 17h30 (V. Ehrlacher, S. Boyaval),
- Optimisation, 15h, L3 (A. Lesage, A. Levitt),
- Outils mathématiques pour l'ingénieur, 15h (E. Cancès, G. Ferré, F. Legoll, T. Lelièvre, P-L. Rothé),
- Probabilités, 27h (M. Ramil)
- Projets de première année, 15h (J. Roussel, P. Terrier),

At École des Ponts 2nd year (equivalent to M1):

- Analyse de Fourier, 15h (A. Levitt),
- Analyse spectrale et application aux Équations aux dérivées partielles, 36h (F. Legoll, V. Ehrlacher),
- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès),
- Projet du département IMI, 12h (G. Ferré, M. Ramil, J. Roussel, L. Silva Lopes),
- Projets Modéliser Programmer Simuler (T. Lelièvre),
- Simulation moléculaire en sciences des matériaux, 6h (A. Levitt),
- Statistics and data sciences, 24h (G. Stoltz).

At École des Ponts 3rd year (equivalent to M2):

- Méthodes de quantification des incertitudes en ingénierie, 18h (V. Ehrlacher),
- Remise à niveau: outils mathématiques, 6h (A. Lesage).

At the M2 "Mathématiques de la modélisation" of Sorbonne Université:

- Introduction à la physique statistique computationnelle, 20h (G. Stoltz),
- Méthodes numériques probabilistes, 24h (T. Lelièvre),
- Problèmes multiéchelles, aspects théoriques et numériques, 24h (F. Legoll),
- Théorie spectrale et variationnelle, 10h (E. Cancès).

At other institutions:

- Analyse variationnelle des équations aux dérivées partielles, 32h, École Polytechnique (T. Lelièvre),
- Aléatoire, 32h, École Polytechnique (T. Lelièvre),
- Maths 1 et 2, 9h, L3, École des Mines (A. Levitt, G. Stoltz),
- Mathématiques pour l'ingénieur, 36h, L2, UPEC (S. Siraj-Dine),
- Numerical methods for partial differential equations, 21h, University of Chicago (C. Le Bris).

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

- Amina Benaceur, Réduction de modèles en thermique et mécanique non-linéaires, Université Paris-Est, École des Ponts, defended on December 21th, 2018, supervised by A. Ern (CERMICS), co-supervised by V. Ehrlacher,
- Marc Josien, Etude mathématique et numérique de quelques modèles multi-échelles issus de la mécanique des matériaux, Université Paris-Est, École des Ponts, defended on November 20th, 2018, supervised by C. Le Bris,
- Julien Roussel, Analyse théorique et numérique de dynamiques non-réversibles en physique statistique computationnelle, Université Paris-Est, École des Ponts, defended on November 27th, 2018, supervised by G. Stoltz,
- Pierre Terrier, Reduced models for defect migration in metals, Université Paris-Est, École des Ponts and CEA Saclay, defended on December 19th, supervised by G. Stoltz and M. Athènes (CEA).

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

- Zineb Belkacemi, Machine learning techniques in molecular simulation, Université Paris-Est, Thèse CIFRE Sanofi, started November 1st, 2018, co-supervised by T. Lelièvre and G. Stoltz,
- Robert Benda, Multiscale modeling of functionalized nanotube networks for sensor applications, Ecole Polytechnique, started September 1st, 2018, supervised by E. Cancès and B. Lebental (École Polytechnique),
- Raed Blel, Monte Carlo methods and model redcution, started October 1st, 2018, supervised by V. Ehrlacher and T. Lelièvre,
- Lingling Cao, Mathematical analysis of models of thermo-electronic transport, Université Paris-Est, École des Ponts, started November 1st, 2016, supervised by E. Cancès and G. Stoltz,
- Rafaël Coyaud, Méthodes numériques déterministes et stochastiques pour le transport optimal, Université Paris-Est, École des Ponts, started October 1st, 2017, supervised by A. Alfonsi (CERMICS) and co-supervised by V. Ehrlacher,
- Qiming Du, Mathematical analysis of splitting methods, École Doctorale Sciences Mathématiques de Paris Centre, started September 1st, 2016, supervised by A. Guyader (Sorbonne Université) and T. Lelièvre,
- Grégoire Ferré, Efficient sampling methods for nonequilibrium systems, Université Paris-Est, École des Ponts started October 1st, 2016, supervised by G. Stoltz,
- Adrien Lesage, Multi-scale methods for calculation and optimization of thin structures, started October 1st, 2017, supervised by F. Legoll, co-supervised by V. Ehrlacher and A. Lebée (École des Ponts),
- Sofiane Martel, Modélisation de la turbulence par mesures invariantes d'EDPS, Université Paris-Est, École des Ponts, started January 1st, 2017, supervised by S. Boyaval and co-supervised by J. Reygner (CERMICS),
- Pierre-Loïk Rothé, Numerical methods for the estimation of fluctuations in multi-scale materials and related problems, started October 1st, 2016, supervised by F. Legoll,
- Mouad Ramil, Metastability for interacting particle systems, started October 1st, 2017, supervised by T. Lelièvre and J. Reygner (CERMICS),
- Laura Silva Lopes, Numerical methods for simulating rare events in molecular dynamics, started October 1st, 2016, supervised by J. Hénin (IBPC) and T. Lelièvre,
- Sami Siraj-Dine, Modélisation mathématique des matériaux 2D, École des Ponts, started October 1st, 2017, supervised by E. Cancès, C. Fermanian and co-supervised by A. Levitt.

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

- E. Cancès, PhD of Marco Vanzini ("Auxiliary systems for observables: dynamical local connector approximation for electron addition and removal spectra"), defended at Ecole Polytechnique in January 2018,
- E. Cancès, PhD of Giovanna Marcelli ("A mathematical analysis of spin and charge transport in topological insulators"), defended at Sapienza University of Rome in February 2018,
- E. Cancès, PhD of Mi-Song Dupuy ("Analyse de la méthode projector augmented-wave pour les calculs de structure électronique en géométrie périodique"), defended at Université Paris Diderot in September 2018,
- E. Cancès, PhD of Carlo Marcati ("Discontinuous hp finite element methods for elliptic eigenvalue problems with singular potentials, with applications in quantum chemistry"), defended at Sorbonne Université in October 2018,
- V. Ehrlacher, PhD of Mi-Song Dupuy, ("Analyse de la méthode projector augmented-wave pour les calculs de structure électronique en géométrie périodique"), defended at Université Paris-Diderot in September 2018.
- V. Ehrlacher, PhD of Nicolas Cagniart, ("Quelques approches non linéaires en réduction de complexité"), defended at Sorbonne Université in November 2018,
- V. Ehrlacher, PhD of Jules Fauque, ("Modèle d'ordre réduit en mécanique du contact. Application à la simulation du comportement des combustibles nucléaires"), defended at Ecole des Mines de Paris in November 2018,
- V. Ehrlacher, PhD of Ahmad Al-Takash, ("Development of numerical methods to accelerate the prediction of the behavior of multiphysics under cyclic loading"), defended at ENSMA in November 2018,
- F. Legoll, PhD of Brian Staber ("Stochastic analysis, simulation and identification of hyperelastic constitutive equations"), defended at Université Paris-Est in June 2018,
- T. Lelièvre, PhD of Bob Pépin ("Time Averages of Diffusion Processes and Applications to Two-Timescale Problems"), défended at Université du Luxembourg, April 2018,
- T. Lelièvre, PhD of Michel Nowak ("Accelerating Monte Carlo particle transport with adaptively generated importance maps"), defended at Université Paris Saclay, September 2018,
- T. Lelièvre, PhD of Ze Lei ("Irreversible Markov Chains for Particle Systems and Spin Models: Mixing and Dynamical Scaling"), défended at Ecole Normale Supérieure, December 2018,
- G. Stoltz, PhD of Sabri Souguir ("Simulation numérique de l'initiation de la rupture à l'échelle atomique"), defended at Ecole des Ponts in November 2018.

9.3. Popularization

9.3.1. Internal or external Inria responsibilities

- A. Levitt is a member of the editorial board of Interstices, Inria's popularization website.

9.3.2. Articles and contents

- E. Cancès has been interviewed in "La Jaune et La Rouge", the journal of the alumni of Ecole Polytechnique, in January.

9.3.3. Internal actions

- C. Le Bris organized an open day at CERMICS in June for the administrative staff of École des Ponts.

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] M. JOSIEN. *Mathematical and numerical study of some multi-scale models from materials science*, Université Paris-Est, November 2018, https://hal.archives-ouvertes.fr/tel-01988719

[8] J. ROUSSEL. *Theoretical and numerical analysis of non-reversible dynamics in computational statistical physics+*, MSTIC graduate school / University of Marne-la-vallée, November 2018, https://tel.archives-ouvertes.fr/tel-01964722

[9] P. TERRIER. *Numerical simulations for predicting the microstructural evolution of ferritic alloys. A study of Cluster Dynamics*, Université Paris-Est, December 2018, https://tel.archives-ouvertes.fr/tel-01990556

Articles in International Peer-Reviewed Journals

[10] A. BENACEUR, V. EHRLACHER, A. ERN, S. MEUNIER. *A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems*, in "SIAM Journal on Scientific Computing", 2018, vol. 40, n^{o} 5, pp. A2930-A2955, https://arxiv.org/abs/1710.00511 , https://hal.archives-ouvertes.fr/hal-01599304

[11] X. BLANC, M. JOSIEN, C. LE BRIS. *Local precised approximation in multiscale problems with local defects*, in "Comptes Rendus Mathématique", 2019, https://arxiv.org/abs/1901.09669 [*DOI :* 10.1016/J.CRMA.2018.12.005], https://hal.archives-ouvertes.fr/hal-01893991

[12] X. BLANC, P.-L. LIONS, C. LE BRIS. *On correctors for linear elliptic homogenization in the presence of local defects: the case of advection-diffusion*, in "Journal de Mathématiques Pures et Appliquées", 2018, https://arxiv.org/abs/1801.10330 [*DOI :* 10.1016/J.MATPUR.2018.04.010], https://hal.archives-ouvertes.fr/hal-01697105

[13] S. BOYAVAL, A. CABOUSSAT, A. MRAD, M. PICASSO, G. STEINER. *A semi-Lagrangian splitting method for the numerical simulation of sediment transport with free surface flows*, in "Computers & Fluids", August 2018, vol. 172, pp. 384-396, https://hal-enpc.archives-ouvertes.fr/hal-01940147

[14] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: a unified framework*, in "Numerische Mathematik", July 2018, vol. 140, n^{o} 4, pp. 1033-1079 [*DOI :* 10.1007/S00211-018-0984-0], https://hal.inria.fr/hal-01483461

[15] P. CARDALIAGUET, C. LE BRIS, P. E. SOUGANIDIS. *Perturbation problems in homogenization of hamilton-jacobi equations*, in "Journal de Mathématiques Pures et Appliquées", 2019, https://arxiv.org/abs/1701.05440 , https://hal.archives-ouvertes.fr/hal-01435744

[16] D. CHAFAÏ, G. FERRÉ. *Simulating Coulomb gases and log-gases with hybrid Monte Carlo algorithms*, in "Journal of Statistical Physics", November 2018, https://arxiv.org/abs/1806.05985 [*DOI :* 10.1007/S10955-018-2195-6], https://hal.archives-ouvertes.fr/hal-01818268

[17] L. CHAMOIN, F. LEGOLL. *A posteriori error estimation and adaptive strategy for the control of MsFEM computations*, in "Computer Methods in Applied Mechanics and Engineering", 2018, vol. 336, pp. 1-38, https://arxiv.org/abs/1709.03624 [*DOI :* 10.1016/J.CMA.2018.02.016], https://hal.archives-ouvertes.fr/hal-01586825

[18] G. FAURE, G. STOLTZ. *Stable and accurate schemes for smoothed dissipative particle dynamics*, in "Applied Mathematics and Mechanics", January 2018, vol. 39, n^{o} 1, pp. 83-102, https://arxiv.org/abs/1707.04232 [*DOI :* 10.1007/S10483-018-2256-8], https://hal.archives-ouvertes.fr/hal-01562490

[19] G. FERRÉ, H. TOUCHETTE. *Adaptive Sampling of Large Deviations*, in "Journal of Statistical Physics", September 2018, vol. 172, n^{o} 6, pp. 1525 - 1544 [*DOI :* 10.1007/S10955-018-2108-8], https://hal.archives-ouvertes.fr/hal-01938825

[20] G. FORT, B. JOURDAIN, T. LELIÈVRE, G. STOLTZ. *Convergence and efficiency of adaptive importance sampling techniques with partial biasing*, in "Journal of Statistical Physics", March 2018, vol. 171, n^{o} 2, pp. 220–268, https://arxiv.org/abs/1610.09194 [*DOI :* 10.1007/S10955-018-1992-2], https://hal.archives-ouvertes.fr/hal-01389996

[21] C. L. HALL, T. HUDSON, P. V. MEURS. *Asymptotic analysis of boundary layers in a repulsive particle system*, in "Acta Applicandae Mathematicae", February 2018, https://arxiv.org/abs/1609.03236 [*DOI :* 10.1007/S10440-017-0119-0], https://hal.archives-ouvertes.fr/hal-01398449

[22] F. HÉDIN, T. LELIÈVRE. *gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems*, in "Computer Physics Communications", 2019, https://arxiv.org/abs/1807.02431 - Accepte version of the article. 37 pages (including references), 13 Figures, 3 Tables [*DOI :* 10.1016/J.CPC.2019.01.005], https://hal.archives-ouvertes.fr/hal-01832823

[23] J. INFANTE ACEVEDO, T. LELIÈVRE. *A non linear approximation method for solving high dimensional partial differential equations: Application in finance*, in "Mathematics and Computers in Simulation", January 2018, vol. 143, pp. 14-34, https://arxiv.org/abs/1309.3731 [*DOI :* 10.1016/J.MATCOM.2016.07.013], https://hal-enpc.archives-ouvertes.fr/hal-00861892

[24] M. JOSIEN, Y.-P. PELLEGRINI, F. LEGOLL, C. LE BRIS. *Fourier-based numerical approximation of the Weertman equation for moving dislocations*, in "International Journal for Numerical Methods in Engineering", 2018, vol. 113, n° 12, pp. 1827-1850, https://arxiv.org/abs/1704.04489 [*DOI :* 10.1002/NME.5723], https://hal.archives-ouvertes.fr/hal-01510158

[25] M. KAERCHER, S. BOYAVAL, M. GREPL, K. VEROY. *Reduced basis approximation and a posteriori error bounds for 4D-Var data assimilation*, in "Optimization and Engineering", June 2018, vol. 2018, n° 3, https://arxiv.org/abs/1802.02328 [*DOI :* 10.1007/S11081-018-9389-2], https://hal.inria.fr/hal-01556304

[26] C. LE BRIS, F. LEGOLL, S. LEMAIRE. *On the best constant matrix approximating an oscillatory matrix-valued coefficient in divergence-form operators*, in "ESAIM: Control, Optimisation and Calculus of Variations", 2018, https://arxiv.org/abs/1612.05807 [*DOI :* 10.1051/COCV/2017061], https://hal.archives-ouvertes.fr/hal-01420187

[27] T. LELIÈVRE, L. PILLAUD-VIVIEN, J. REYGNER. *Central Limit Theorem for stationary Fleming–Viot particle systems in finite spaces*, in "ALEA : Latin American Journal of Probability and Mathematical Statistics", September 2018, vol. 15, pp. 1163-1182, https://arxiv.org/abs/1806.04490 [*DOI :* 10.30757/ALEA.V15-43], https://hal-enpc.archives-ouvertes.fr/hal-01812120

[28] J. ROUSSEL, G. STOLTZ. *Spectral methods for Langevin dynamics and associated error estimates*, in "ESAIM: Mathematical Modelling and Numerical Analysis", September 2018, vol. 52, n° 3, pp. 1051-1083, https://arxiv.org/abs/1702.04718 [*DOI :* 10.1051/M2AN/2017044], https://hal.archives-ouvertes.fr/hal-01470251

[29] B. STAMM, L. LAGARDÈRE, G. SCALMANI, P. GATTO, E. CANCÈS, J.-P. PIQUEMAL, Y. MADAY, B. MENNUCCI, F. LIPPARINI. *How to make continuum solvation incredibly fast in a few simple steps: a practical guide to the domain decomposition paradigm for the Conductor-like Screening Model Continuum Solvation, Linear Scaling, Domain Decomposition*, in "International Journal of Quantum Chemistry", 2018 [*DOI :* 10.1002/QUA.25669], https://hal.archives-ouvertes.fr/hal-01793770

[30] G. STOLTZ, Z. TRSTANOVA. *Langevin dynamics with general kinetic energies*, in "Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal", May 2018, vol. 16, n° 2, pp. 777-806, https://arxiv.org/abs/1609.02891 [*DOI :* 10.1137/16M110575X], https://hal.archives-ouvertes.fr/hal-01364821

[31] G. STOLTZ, E. VANDEN-EIJNDEN. *Longtime convergence of the Temperature-Accelerated Molecular Dynamics Method*, in "Nonlinearity", July 2018, vol. 31, n° 8, pp. 3748-3769, https://arxiv.org/abs/1708.08800 [*DOI :* 10.1088/1361-6544/AAC541], https://hal.archives-ouvertes.fr/hal-01578911

Other Publications

[32] C. ANDRIEU, A. DURMUS, N. NÜSKEN, J. ROUSSEL. *Hypocoercivity of Piecewise Deterministic Markov Process-Monte Carlo*, December 2018, https://arxiv.org/abs/1808.08592 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01941467

[33] X. BLANC, M. JOSIEN, C. LE BRIS. *Precised approximations in elliptic homogenization beyond the periodic setting*, December 2018, https://arxiv.org/abs/1812.07220 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01958207

[34] X. BLANC, C. LE BRIS, P.-L. LIONS. *On correctors for linear elliptic homogenization in the presence of local defects*, January 2018, https://arxiv.org/abs/1801.10335 - working paper or preprint [*DOI :* 10.1080/03605302.2018.1484764], https://hal.archives-ouvertes.fr/hal-01697104

[35] T. BOIVEAU, V. EHRLACHER, A. ERN, A. NOUY. *Low-rank approximation of linear parabolic equations by space-time tensor Galerkin methods*, October 2018, https://arxiv.org/abs/1712.07256 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01668316

[36] C.-E. BRÉHIER, T. LELIÈVRE. *On a new class of score functions to estimate tail probabilities of some stochastic processes with Adaptive Multilevel Splitting*, November 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01923385

[37] E. CANCÈS, L.-L. CAO, G. STOLTZ. *Removing a slab from the Fermi sea: the reduced Hartree-Fock model*, October 2018, https://arxiv.org/abs/1807.06960 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01891488

[38] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Post-processing of the planewave approximation of Schrödinger equations. Part I: linear operators*, November 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01908039

[39] E. CANCÈS, V. EHRLACHER, D. GONTIER, A. LEVITT, D. LOMBARDI. *Numerical quadrature in the Brillouin zone for periodic Schrödinger operators*, May 2018, https://arxiv.org/abs/1805.07144 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01796582

[40] E. CANCÈS, V. EHRLACHER, F. LEGOLL, B. STAMM, S. XIANG. *An embedded corrector problem for homogenization. Part I: Theory*, July 2018, https://arxiv.org/abs/1807.05131 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01840993

[41] E. CANCÈS, V. EHRLACHER, F. LEGOLL, B. STAMM, S. XIANG. *An embedded corrector problem for homogenization. Part II: Algorithms and discretization*, October 2018, https://arxiv.org/abs/1810.09885 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01903486

[42] A. DAMLE, A. LEVITT, L. LIN. *Variational formulation for Wannier functions with entangled band structure*, January 2018, https://arxiv.org/abs/1801.08572 - 26 pages, 10 figures, https://hal.archives-ouvertes.fr/hal-01696529

[43] G. FERRÉ, M. ROUSSET, G. STOLTZ. *More on the long time stability of Feynman-Kac semigroups*, November 2018, https://arxiv.org/abs/1807.00390 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01911620

[44] G. FERRÉ, G. STOLTZ. *Error estimates on ergodic properties of discretized Feynman-Kac semigroups*, January 2018, https://arxiv.org/abs/1712.04013 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01690532

[45] D. GONTIER, A. LEVITT, S. SIRAJ-DINE. *Numerical construction of Wannier functions through homotopy*, December 2018, https://arxiv.org/abs/1812.06746 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01955842

[46] T. J. HUDSON, F. LEGOLL, T. LELIÈVRE. *Stochastic homogenization of a scalar viscoelastic model exhibiting stress-strain hysteresis*, February 2018, https://arxiv.org/abs/1802.05549 - 35 pages, 4 figures, https://hal.archives-ouvertes.fr/hal-01710772

[47] M. JOSIEN. *Decomposition and pointwise estimates of periodic Green functions of some elliptic equations with periodic oscillatory coefficients*, July 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01848268

[48] F. LEGOLL, T. LELIÈVRE, U. SHARMA. *Effective dynamics for non-reversible stochastic differential equations: a quantitative study*, September 2018, https://arxiv.org/abs/1809.10498 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01883330

[49] T. LELIÈVRE, D. LE PEUTREC, B. NECTOUX. *Exit event from a metastable state and Eyring-Kramers law for the overdamped Langevin dynamics*, November 2018, https://arxiv.org/abs/1811.06786 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01696187

[50] T. LELIÈVRE. *Mathematical foundations of Accelerated Molecular Dynamics methods*, January 2018, https://arxiv.org/abs/1801.05347 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01686062

[51] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Hybrid Monte Carlo methods for sampling probability measures on submanifolds*, July 2018, https://arxiv.org/abs/1807.02356 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01832820

[52] T. LELIÈVRE, G. SAMAEY, P. ZIELIŃSKI. *Analysis of a micro-macro acceleration method with minimum relative entropy moment matching*, January 2018, https://arxiv.org/abs/1801.01740 - 40 pages, https://hal.archives-ouvertes.fr/hal-01680761

[53] T. LELIÈVRE, W. ZHANG. *Pathwise estimates for effective dynamics: the case of nonlinear vectorial reaction coordinates*, May 2018, https://arxiv.org/abs/1805.01928 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01794919

[54] A. LEVITT. *Screening in the finite-temperature reduced Hartree-Fock model*, October 2018, https://arxiv.org/abs/1810.03342 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01889411

[55] J. ROUSSEL, G. STOLTZ. *A perturbative approach to control variates in molecular dynamics*, February 2018, https://arxiv.org/abs/1712.08022 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-01709265