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ACTIVITY REPORT

Project-Team
MATHERIALS

MATHematics for MatERIALS

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

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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Creation of the Project-Team: 2015 April 01

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2 Overall objectives

The MATHERIALS project-team was 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, 4, 5, 6, 7] that other scientists may consult in order to enter the field.

3 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.

4 Application domains

4.1 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 materials science. Efforts in this direction must address a large variety of questions such as

- how can one improve the nonlinear iterations that are the basis of any *ab initio* models for computational chemistry?

- how can one more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?

- how can one design a sufficiently small variational space, whose dimension is kept limited while the size of the system increases?

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

- in the former, the results of the model at the lower scale are simply used to evaluate some parameters that are inserted in the model for the larger scale: one example is the parameterized classical molecular dynamics, which makes use of force fields that are fitted to calculations at the quantum level;

- while in the latter, the model at the lower scale is concurrently coupled to the model at the larger scale: an instance of such a strategy is the so called QM/MM coupling (standing for Quantum Mechanics/Molecular Mechanics coupling) where some part of the system (typically the reactive site of a protein) is modeled with quantum models, that therefore accounts for the change in the electronic structure and for the modification of chemical bonds, while the rest of the system (typically the inert part of a protein) is coarse grained and more crudely modeled by classical mechanics.

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

4.2   Computational Statistical Mechanics

The orders of magnitude used in the microscopic representation of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 6 \times 10^{23}$, the typical distances are expressed in Å (10^{-10} m), the energies are of the order of $k_B T \simeq 4 \times 10^{-21}$ 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 O(10^{15}) time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of a few microseconds.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of N particles correctly approximate the macroscopic property, formally obtained in the

thermodynamic limit $N \to +\infty$ (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

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

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

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

4.3   Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on multiscale modeling for materials science at the continuum scale. The presence of numerous length scales in material science problems indeed 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 (the coefficients of the coarse scale equations are thus simply constant, or vary on a coarse length 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 (this is for instance the case for random stationary settings). Our aim is to focus on different settings, all relevant from an applied viewpoint, and leading to practically affordable computational approaches. It is well-known that the case of ordered (that is, in this context, periodic) systems is now well-understood, both from a theoretical and a numerical standpoint. Our aim is to turn to cases, more relevant in practice, where some disorder is present in the microstructure of the material, to take into account defects in crystals, impurities in continuous media... This disorder may be mathematically modeled in various ways.

Such endeavors raise several questions. The first one, theoretical in nature, is to extend the classical theory of homogenization (well developed e.g. in the periodic setting) to such disordered settings. Next, after homogenization, we expect to obtain an effective, macroscopic model, which includes no small scale. A second question is to introduce affordable numerical methods to compute the homogenized coefficients. An alternative approach, more numerical in nature, is to directly attack the oscillatory problem by using discretization approaches tailored to the multiscale nature of the problem (the construction of which is often inspired by theoretical homogenization results).

5 New software and platforms

5.1 New software

5.1.1 DFTK

Keywords: Molecular simulation, Quantum chemistry, Materials

Functional Description: DFTK, short for the density-functional toolkit, is a Julia library implementing plane-wave density functional theory for the simulation of the electronic structure of molecules and materials. It aims at providing a simple platform for experimentation and algorithm development for scientists of different backgrounds.

Release Contributions: In 2020 DFTK has reached maturity, and has been used in three publications in the group. It has been extended to support a variety of features (MPI, threading, arbitrary precision, response properties, Wannier functions, integration with external tools...)

URL: http://dftk.org

Contact: Antoine Levitt

6 New results

6.1 Electronic structure calculations

6.1.1 Density functional theory

The team members have continued their study of algorithms for solving the ground-state problem in Kohn-Sham density functional theory, the long-term goal being the construction of robust and efficient numerical methods with guaranteed error bounds. M. Herbst and A. Levitt have investigated numerically the convergence of self-consistent iterations, and designed a new linesearch strategy. This makes computations more robust and less reliant on user-chosen parameters, without slowing down the algorithms [44]. E. Cancès, G. Dusson, G. Kemlin and A. Levitt have designed and implemented computable error estimates for properties of realistic models of solids. This demonstrates the inaccuracy of standard bounds, and improves them using a two-level splitting of the error in high and low frequencies [32].

The team members have also focused on justifying rigorously and computing efficiently the response properties of molecules and materials. In [38], M-S. Dupuy (Sorbonne Université) and A. Levitt investigate dynamical response properties of a simple model of molecules, the difficulty being that the truncation of the computational domain discretizes the continuous spectrum of the Schrödinger operator, and therefore changes the nature of the response function from a continuous function to a sum of discrete poles. The convergence is proven in an appropriate weak sense, and sharp error estimates for a regularization method are given.

In [41] , L. Garrigue studied the inverse problem of density functional theory. This consists in finding the potential which produces some targeted one-body density, in ground or excited states configurations, and can be seen as a control problem. The theoretical results of the article show that up to some regularization, the problem is well-posed, even for excited states. An algorithm is proposed, and numerical simulations show that in all the cases tested the inverse potential is obtained by a well-posed maximization of a dual functional. This provides a solution to theoretical and numerical problems which were previously solved only in dimension one.

6.1.2   Open quantum systems

In his post-doctoral work co-supervised by Claude Le Bris (MATHERIALS) and Pierre Rouchon (Inria QUANTIC), Masaaki Tokieda addresses various issues related to the numerical simulation and the fundamental understanding of several models of physical systems likely candidates to play a crucial role in quantum computing. More specifically, he studies several pathways to efficiently account for adiabatic elimination in the simulation of composite quantum systems in interactions, modeled by Lindblad type master equations. The specific question currently under study is the expansion up to high orders and the compatibility of such an expansion with the formal requirements of consistency of quantum mechanical evolutions. He is also planning to address various other connected issues, all aiming at better fundamental understanding and a more effective simulation of open quantum systems.

6.1.3   Strongly correlated electrons

The Strictly Correlated Electrons (SCE) limit of the Levy-Lieb functional in Density Functional Theory (DFT) gives rise to a symmetric multi-marginal optimal transport problem with Coulomb cost, where the number of marginal laws is equal to the number of electrons in the system, which can be very large in relevant applications. In [8], we design a numerical method, built upon constrained overdamped Langevin processes to solve previously introduced Moment Constrained Optimal Transport (MCOT) relaxations of symmetric multi-marginal optimal transport problems with Coulomb cost. Some minimizers of such relaxations can be written as discrete measures charging a low number of points belonging to a space whose dimension, in the symmetrical case, scales linearly with the number of marginal laws. We leverage the sparsity of those minimizers in the design of the numerical method and prove that any local minimizer to the resulting problem is actually a global one. We illustrate the performance of the proposed method by numerical examples which solves MCOT relaxations of 3D systems with up to 100 electrons.

Tensor methods have proved to be very powerful tools in order to represent high-dimensional objects with low complexity. Such methods prove to have a wide range of applications in quantum chemistry, for instance for the approximation of the ground state wavefunction of a molecular system when the number of electrons is large. The DMRG method is one example of such a numerical scheme. Research efforts are led in the team so as to propose new methodological developments in order to improve on the current state-of-the-art tensor methods.

In [19], V. Ehrlacher, M. Fuente-Ruiz and D. Lombardi (Inria COMMEDIA) introduce a method to compute an approximation of a given tensor as a sum of Tensor Trains (TTs), where the order of the variates and the values of the ranks can vary from one term to the other in an adaptive way. The numerical scheme is based on a greedy algorithm and an adaptation of the TT-SVD method. The proposed approach can also be used in order to compute an approximation of a tensor in a Canonical Polyadic format (CP), as an alternative to standard algorithms like Alternating Linear Squares (ALS) or Alternating Singular Value Decomposition (ASVD) methods. Some numerical experiments are presented, in which the proposed method is compared to ALS and ASVD methods for the construction of a CP approximation of a given tensor and performs particularly well for high-order tensors. The interest of approximating a tensor as a sum of Tensor Trains is illustrated in several numerical test cases.

In [20], V. Ehrlacher, L. Grigori (Inria ALPINES), Damiano Lombardi (Inria COMMEDIA) and Hao Song propose a numerical method to compress a tensor by constructing a piece-wise tensor approximation. This is constructed by partitioning a tensor into sub-tensors and by constructing a low-rank tensor approximation (in a given format) in each sub-tensor. Neither the partition nor the ranks are fixed a priori, but, instead, they are obtained in order to fulfill a prescribed accuracy and optimize the storage. Some numerical experiments are proposed to illustrate the method.

6.2   Computational statistical physics

The aim 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 five main topics: (i) the development of methods for sampling the configuration space; (ii) the efficient computation of dynamical properties which requires to sample metastable trajectories; (iii) the simulation of nonequilibrium systems and the computation of transport coefficients; (iv) coarse-graining techniques to reduce the

computational cost of molecular dynamics simulations and gain some insights on the models; (v) the use of particle methods for sampling and optimization.

6.2.1   Sampling of the configuration space

Various dynamics are used in computational statistical physics to sample the configurations of the system according to the target probability measure at hand and approximate expectations as time averages along one realization. It is important to have a good theoretical understanding of the performance of sampling methods, in order to choose the optimal parameters in actual numerical simulations, for instance to have a variance as small as possible for time averages along one realization. A common dynamics is the so-called Langevin dynamics, which corresponds to a Hamiltonian dynamics perturbed by an Ornstein–Uhlenbeck process on the momenta. The generator associated with this stochastic differential equation is hypoelliptic (at best). Proving the longtime convergence of the semigroup requires dedicated tools, under a general strategy coined as hypocoercivity, and usually involves prefactors which are difficult to estimate quantitatively; see the review [51] by G. Stoltz. Bounds on the asymptotic variance on the other hand only require bounds on the resolvent of the generator. In the work [13] in collaboration with E. Camrud, D. Herzog (Iowa State, USA) and M. Gordina (University of Connecticut, USA), G. Stoltz derives such estimates for singular potentials such as the ones arising from Lennard–Jones interactions.

For discretizations of Langevin dynamics, hypocoercive techniques cannot be used as such, and other techniques have to be used to obtain quantitative longtime convergence estimates. In a work with A. Durmus, A. Enfroy (ENS Paris Saclay, France) and Eric Moulines (École polytechnique, France), G. Stoltz obtained such estimates by Lyapunov techniques combined with minorization estimates, the key point being that these estimates are uniform in the timestep [39]. From a technical viewpoint, the minorization condition is derived by considering the dynamics on small physical times, in which case it can be seen as some perturbation of a (degenerate) Gaussian process.

Another work which falls into the category of sampling methods is [50], where G. Stoltz shows with I. Sekkat, one of his PhD students, how to correct Langevin dynamics in which the force appearing in the update of the momenta, which corresponds to the opposite of the gradient of the potential energy function, is not computed exactly but approximated with some unbiased estimator. This induces some bias on the probability measure which is sampled. This bias can however be corrected with a method known as Adaptive Langevin dynamics, where the friction coefficient is a variable adjusted by some Nosé–Hoover feedback mechanism. They showed how to extend this method to the case where the covariance of the gradient noise is not constant, and also derived error estimates on the bias incurred on the invariant measure [50].

Multiplicative noises can also be introduced in the case of (overdamped) Langevin dynamics by considering non separable Hamiltonians. G. Stoltz and T. Lelièvre along with R. Santet, one of their PhD students, are actively working on unbiased numerical sampling in those cases, where properties such as time reversibility of the Hamiltonian flow have to be exactly reproduced numerically.

One important aim of sampling methods is to compute free energy differences. In [46], T. Lelièvre, in collaboration with L. Maurin and P. Monmarché (Sorbonne Université), studies the robustness of the Adaptive Biasing Force method under non-conservative forces. In particular, using classical entropy techniques, the exponential convergence to equilibrium is proven.

Let us also mention the work [29] where R. Blel, V. Ehrlacher, and T. Lelièvre analyse the convergence of a variance reduction technique for the computation of parameter-dependent expectations using a reduced basis paradigm.

6.2.2   Sampling of dynamical properties and rare events

One research direction which has been developed over the past ten years in the team is to analyse metastable trajectories using the notion of quasi-stationary distribution. A stochastic process, when trapped in a metastable state, reaches a local equilibrium (the quasi-stationary distribution) before leaving the state. This viewpoint is useful to rigorously justify the use of jump Markov processes to model the exit event, which is interesting both theoretically to provide a sound justification to Markov State models, and numerically to justify a class of algorithms called accelerated molecular dynamics. In [26], T. Lelièvre, M. Ramil and J. Reygner (Ecole des Ponts) prove the existence of a quasi-stationary distribution

for the Langevin process trapped in a bounded domain in position, as well as the exponential convergence towards this distribution for the process conditioned to stay in the bounded domain. Compared to the case of of the overdamped Langevin dynamics, this result requires to circumvent two main difficulties: the Langevin process is a degenerate diffusion process (noise only acts on velocities) and the domain is unbounded in velocity. The high friction limit of this model was further studied by M. Ramil in [49].

6.2.3 Mathematical understanding and efficient simulation of nonequilibrium systems

Many systems in computational statistical physics are not at equilibrium. This is in particular the case when one wants to compute transport coefficients, which determine the response of the system to some external perturbation. For instance, the thermal conductivity relates an applied temperature difference to an energy current through Fourier's law, while the mobility coefficient relates an applied external constant force to the average velocity of the particles in the system.

Petr Plechac (University of Delaware, USA), Ting Wang (Army Research Lab, USA) and G. Stoltz considered in [48] numerical schemes for computing the linear response of steady-state averages of Langevin dynamics with respect to a perturbation of the drift part of the stochastic differential equation. The schemes are based on Girsanov's change-of-measure theory to reweight trajectories with factors derived from a linearization of the Girsanov weights. They investigate both the discretization error and the finite-time approximation error. The designed numerical schemes are shown to be of bounded variance with respect to the integration time, which is a desirable feature for long time simulation. They also show how the discretization error can be improved to second order accuracy in the time step by modifying the weight process in an appropriate way, based on a formulation using a product of discrete martingales.

Another method to compute transport coefficients is based on a direct evaluation of the linear response. From a numerical viewpoint, this method works better when the regime of linear response holds true for forcings as large as possible. Renato Spacek started his PhD work on this topic, the aim being to find (possibly non-physical) forcings which have the desired linear response, while minimizing the nonlinear part of the response.

6.2.4 Analysis and derivation of coarse-grained models

Coarse-grained descriptions of physical systems can be derived once one has a set of so-called reaction coordinates, which is a low dimensional (nonlinear) fonction of the system configuration which describes the main features of the system, and allows in particular to compute free energy profiles. Reaction coordinates are often based on an intuitive understanding of the system, and one would like to complement this intuition or even replace it with automated tools. With Z. Belkacemi and E. Gkeka (Sanofi, France), T. Lelièvre and G. Stoltz studied a machine learning technique to find reaction coordinates to be used in conjunction with free energy biasing techniques such as the adaptive biasing force method. This allows for instance to improve the sampling of configurations of complex proteins. The approach is based on autoencoders, for which the bottleneck layer provides a low dimensional representation of high dimensional atomistic systems. Applications to alanine dipeptive and chignolin are considered.

Thomas Pigeon, a PhD student funded by Inria in the framework of the joint laboratory with IFPEN, is currently working on interpretations of autoencoders based on conditional expectations, and more generally on the use of techniques from machine learning to find reaction coordinates which can be used to sample dynamical properties and rare events, and not only free energy profiles.

In a different direction, it is well-known that molecular dynamics simulations often require extremely long trajectories to be computed, either to reach equilibrium or to see meaningful events such as transitions from one metastable well to another. It is thus tempting to use the parareal algorithm, which has been proposed two decades ago as a method for performing parallel-in-time computations, in order to improve the efficiency of such simulations. In collaboration with U. Sharma (Freie Universitat Berlin, Germany), F. Legoll and T. Lelièvre have introduced in [25] an adaptive variant of the parareal algorithm, specifically tailored to molecular dynamics simulations. The algorithm is adaptive in the sense that the time horizon of the simulation is iteratively adjusted, in order to prevent the algorithm from simulating parts of the trajectory where the accuracy is deemed to be insufficient. A significant gain in efficiency is obtained in comparison to the standard parareal algorithm.

A natural follow-up of this work is to implement this algorithm in LAMMPS (a very well distributed software in the applied communities), that will open the way to the simulation of realistic physical systems. This work is currently performed by O. Gorynina, F. Legoll and T. Lelièvre, in collaboration with D. Perez (Los Alamos Nat. Lab., USA).

6.2.5 Interacting particle methods for sampling and optimization.

This research area was recently developed with the arrival of Urbain Vaes in the project-team. In a first preprint, drawing inspiration from consensus-based methods in the optimization community, U. Vaes together with J. A. Carrillo (University of Oxford, United Kingdom), F. Hoffmann (Hausdorff Center for Mathematics, Germany) and A. M. Stuart (Caltech, USA) proposed a sampling method based on a system of particles interacting via the mean and covariance of the empirical probability distribution, appropriately reweighted by a power of the target probability distribution [34]. They studied the long-time behavior of the mean-field equation describing the evolution of the particle system in the limit of infinitely many particles. A reasoning based on Laplace's method enables to prove, in simple settings, the exponential convergence of the solution to a Gaussian approximation of the target probability distribution. In a second project, U. Vaes together with G. A. Pavliotis (Imperial College London, United Kingdom) and A. M. Stuart studied a Langevin-type sampling method in which the gradient of the potential is approximated using a multiscale particle system [47]. The goal was to develop a method relying on a gradient approximation similar in structure to that of ensemble Kalman-based methods but which, unlike these methods, could be systematically refined in order to reduce the sampling error. Techniques from multiscale analysis were used to prove the convergence of the numerical solution to a preconditioned overdamped Langevin dynamics, in an appropriate limit for the parameters of the method. In another project, U. Vaes together with J. A. Carrillo and C. Totzeck (University of Wuppertal, Germany) investigated the viability of a simple penalization approach for incorporating constraints in consensus-based and ensemble Kalman methods for optimization [35]. The efficiency of the proposed method was studied by means of careful numerical experiments.

6.3 Homogenization

6.3.1 Deterministic non-periodic systems

From the theoretical viewpoint, the project-team has pursued the development of a *general theory for homogenization of deterministic materials modeled as periodic structures with defects.* This work, performed in collaboration with X. Blanc, P.-L. Lions and P. Souganidis, is also the topic of the ongoing PhD thesis of R. Goudey. We recall that the periodic setting is the oldest traditional setting for homogenization. Alternative settings include the quasi- and almost-periodic settings, and the random stationary setting. From a modeling viewpoint, assuming that multiscale materials are periodic is however an idealistic assumption: natural media (such as the subsoil) have no reason to be periodic, and manufactured materials, even though indeed sometimes designed to be periodic, are often not periodic in practice, e.g. because of imperfect manufacturing processes, of small geometric details that break the periodicity and can be critical in terms of industrial performances, . . . Quasi- and almost-periodic settings are not appropriate answers to this difficulty. Using a random stationary setting may be tempting from a modelization viewpoint (in the sense that all what is not known about the microstructure can be "hidden" in a probabilistic description), but this often leads to prohibitively expensive computations, since the model is very general. The direction explored by the project-team consists in considering periodic structures with defects, a setting which is rich enough to fit reality while still leading to affordable computations.

Considering defects in the structure raises many mathematical questions. From an overall perspective, homogenization is based upon the determination of corrector functions, useful to compute the homogenized properties of the materials as well as to provide a fine-scale description of the oscillatory solution. In general, corrector problems are posed on the whole space. In the periodic and random stationary settings, it turns out that the corrector problems can actually be posed on a bounded domain. Powerful tools (e.g. Rellich compactness theorems) can then be used (to establish well-posedness and qualitative properties of the correctors, . . .). The presence of defects breaks this property, making the

corrector problem non-compact. Additional tools (such as the concentration-compactness method or the theory of Calderón-Zygmund operators) are required to circumvent this difficulty.

Starting from the simplest case (localized defects in a purely diffusive equation, a setting for which we were able to show two-scale expansion results), we have followed two directions: (i) considering more complex equations (advection-diffusion equations, Hamilton-Jacobi equations, ...) for which the defects, although localized, may have an impact on a larger and larger neighborhood, and (ii) considering more complex (i.e. less localized) defects, as in [43] (where defects become increasingly rare but do not decay at infinity); defects in the form of interfaces between two perfectly periodic materials also fall within this research direction. A monograph that summarizes the contributions of the project-team on this topic, along with a general perspective on the field, has recently been submitted for publication.

Also in the context of homogenization theory, O. Gorynina, C. Le Bris and F. Legoll have concluded their work on the question of how to determine the homogenized coefficient of heterogeneous media without explicitly performing an homogenization approach. This work is a follow-up on earlier works over the years by C. Le Bris and F. Legoll in collaboration with K. Li and next S. Lemaire. More precisely, they have completed the mathematical study and the numerical improvement of a computational approach initially introduced by R. Cottereau (CNRS Marseille). This approach combines, in the Arlequin framework, the original fine-scale description of the medium (modelled by an oscillatory coefficient) with an effective description (modelled by a constant coefficient) and optimizes upon the coefficient of the effective medium to best fit the response of a purely homogeneous medium. In the limit of asymptotically infinitely fine structures, the approach yields the value of the homogenized coefficient. Various computational improvements have been suggested in [22], while the theoretical study of the approach has been performed in [42].

6.3.2 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 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 (at the time at the University of Washington in Seattle, USA), C. Le Bris, F. Legoll and P.-L. Rothé have completed in [45] the study of 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. In addition, residue type a posteriori error estimators have been proposed and certified, leading to a numerical strategy where the degree of enrichment is *locally* adapted in order to reach, at the smallest computational cost, a given error. Promising numerical results have been obtained.

Within the ongoing PhD of R. Biezemans, several directions of research have been explored. The results obtained are currently being collected in manuscripts in preparation. First, despite the fact that MsFEM approaches have been proposed many years ago, it turns out that not all specific settings are covered by the numerical analyses existing in the literature. Together with A. Lozinski (currently in delegation in the team), R. Biezemans, C. Le Bris and F. Legoll have extended the analysis of MsFEM to the case of rectangular meshes and that of coefficients that are not necessarily Hölder continuous. An ongoing research effort is devoted to further improving the error estimates. Second, many (if not all) MsFEM approaches proposed up to date are *intrusive*. They require to change the finite element basis set, and adjust it to the problem at hand. Obviously, not every software developer will allow such a modification. Motivated by this observation, R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski have investigated how MsFEM approaches can be adapted (at the possible price of a marginal loss in their

efficiency) so that they become as little intrusive as possible (and thus can be easily used in the context of single scale legacy softwares). Promising results have been obtained in that vein for several variants of the MsFEM approach. Third, they have studied how to extend MsFEM approaches to various types of equations, beyond the purely diffusive case, and in particular to the case of multiscale advection-diffusion problems, in the advection-dominated regime. Thin boundary layers are present in the exact solution, and numerical approaches should be carefully adapted to this situation, e.g. using stabilization. How stabilization and the multiscale nature of the problem interplay with one another is a challenging question, and several MsFEM variants have been compared.

In a different direction, we note that many numerical analysis studies of the MsFEM are focused on obtaining a priori error bounds. In collaboration with L. Chamoin, who was in delegation in the project-team a few years ago from ENS Cachan, F. Legoll has been working on a posteriori error analysis for MsFEM approaches, with the aim of developing error estimation and adaptation tools. L. Chamoin and F. Legoll have extended to the MsFEM case approaches (for the control of the error in energy norm and for the control of the error on quantities of interest [18]) that are classical in the computational mechanics community for single scale problems, and which are based on the so-called Constitutive Relation Error (CRE). While performing these works for multiscale problems, they have reviewed the literature on a posteriori error estimation for single scale problems. This work has led to the recent pedagogical review article [36].

6.4 Complex fluids

In 2021, S. Boyaval has pursued his research to improve mathematical models of non-Newtonian fluids for application to large time-space domains, when waves propagate at finite speed. The symmetric-hyperbolic system of conservation laws introduced in 2020 to unify the elastodynamics of hyperelastic materials with viscous fluid dynamics (through viscoelasticity of Maxwell-type) has been extended [30], in particular to cover the *non-isothermal flows* (highly relevant for application to polymer melts).

7 Bilateral contracts and grants with industry

Many research activities of the project-team are conducted in close collaboration with private or public companies: CEA, EDF, IFPEN, Sanofi, OSMOS Group. 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, except the contracts with IFPEN, which are administrated by Inria.

8 Partnerships and cooperations

8.1 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.

Eric Cancès has been awarded a Simons Targeted Grant "Moiré materials magic" (September 2021 - August 2026). His co-PIs are Allan MacDonald (UT Austin, coordinating PI), Svetlana Jitomirskaya (UC Irvine), Efthimios Kaxiras (Harvard), Lin Lin (UC Berkeley), Mitchell Luskin (University of Minnesota), Angel Rubio (Max-Planck Institut), Maciej Zworski (UC Berkeley).

8.2 European initiatives

The ERC Synergy Grant EMC2 (ERC Grant Agreement number 810367, PIs E. Cancès, L. Grigori, Y. Maday, J.-P. Piquemal) has started in September 2019.

The Euro HPC grant TIME-X (PIs: Y. Maday and G. Samaey), focusing on parallel-in-time computations and in which F. Legoll and T. Lelièvre participate, has started on 1st April 2021.

8.3   National initiatives

The project-team is involved in several ANR projects:

- S. Boyaval is the PI of the ANR JCJC project SEDIFLO (2016-2022) to investigate new numerical models of solid transport in rivers.

- V. Ehrlacher is the PI of the ANR project COMODO (2020-2024) which focuses on the development of efficient numerical methods to simulate cross-diffusion systems on moving domains, with application to the simulation of the fabrication process of thin film solar cells. It includes Inria project-teams from Lille and Sophia-Antipolis as well as research teams from Germany.

- V. Ehrlacher is a member of the ANR project ADAPT (2018-2022), PI: D. Lombardi, Inria COM-MEDIA 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 (2015-2021), PI: Y. Maday, Sorbonne Université. This project is concerned with parallel-in-time algorithms.

- T. Lelièvre is responsible of the node "Ecole des Ponts" of the ANR QuAMProcs (2019-2023), to which G. Stoltz also participates, PI: L. Michel, Université de Bordeaux.

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

- AMORE (Advanced Model Order REduction),

- CHOCOLAS (experimental and numerical study of shock waves),

- DYNQUA (time evolution of quantum systems),

- EGRIN (gravity flows),

- MANU (MAthematics for NUclear applications),

- MASCOT-NUM (stochastic methods for the analysis of numerical codes),

- MEPHY (multiphase flows),

- NBODY (electronic structure),

- REST (theoretical spectroscopy).

The project-team is involved in two Labex: the Labex Bezout (2011-) and the Labex MMCD (2012-).
C. Le Bris is a participant to the Inria Challenge EQIP (Engineering for Quantum Information Processors), in particular in collaboration with P. Rouchon (QUANTIC project-team).

9   Dissemination

9.1   Promoting Scientific Activities

R. Benda co-organizes the PhD students and postdocs seminar of CERMICS.

S. Boyaval

- is the director of Laboratoire d'Hydraulique Saint-Venant (Ecole des Ponts ParisTech - EDF R&D - CEREMA), since September 2021;

- is currently a member of the RA1 (scientific committee) and CODIR+ (executive committee) of E4C
  https://www.e4c.ip-paris.fr/

E. Cancès 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-).

V. Ehrlacher

- is a member of the "Conseil d'Enseignement et de Recherche" of Ecole des Ponts,

- is a member of the "Conseil d'Administration" of the COMUE Paris-Est,

- is a member of the Cordi-S selection committee of INRIA,

- has co-organized the CEMRACS 2021 (6 weeks summer school at CIRM, Luminy, on "Data assimilation and reduced-order modeling for high-dimensional problems") and an Oberwolfach workshop together with Jean-David Benamou and Daniel Matthes on "Applications of optimal transportation in the natural sciences".

C. Le Bris

- is a member of the editorial boards of Annales mathématiques du Québec (2013-), Archive for Rational Mechanics and Analysis (2004-), Calcolo (2019-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Networks and Heterogeneous Media (2007-), Nonlinearity (2005-), Journal de Mathématiques Pures et Appliquées (2009-), Pure and Applied Analysis (2018-),

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

- has been a member of the "Conseil de la Faculté des sciences et ingénierie", Sorbonne Université, until October 2021,

- is the president of the scientific advisory board of the Institut des Sciences du calcul et des données, Sorbonne Université, and a member of the Scientific Advisory Committee of the Institute for Mathematical and Statistical Innovation, University of Chicago,

- is a member of several scientific advisory boards in the industrial sector, in particular (since 2020) of the Energy Division of the Atomic Energy Council (CEA) and (since 2019) of *Framatome* senior management,

- holds a position of Visiting Professor at the University of Chicago, for one quarter a year,

- has co-organized (with Q. Du, I. Fonseca, R. James, J. Lu, D. Perez) the workshop Mathematical and Computational Materials Science at the Institute for Mathematical and Statistical Innovation, Chicago, February 15-19, 2021, and (with A.-L. Dalibard, P. Souganidis) the workshop Homogenization theory: periodic and beyond, Oberwolfach, 14-20 March 2021.

F. Legoll

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

- was a member of the DFG review panel for a Collaborative Research Centre on "Multiscale Simulation Methods for Soft-Matter Systems" (dec 2021).

T. Lelièvre

- is a member of the editorial boards of IMA: Journal of Numerical Analysis, SIAM/ASA Journal of Uncertainty Quantification, Communications in Mathematical Sciences, Journal of Computational Physics and ESAIM:M2AN,

- is a member of the "Conseil d'Administration" of École des Ponts,

- is the head of the applied mathematics department (CERMICS) at Ecole des Ponts,

- has organized the 13th International Workshop on Rare-Event Simulation - RESIM 2021, Les Cordeliers Paris, 18th-21st May 2021 (with G. Fort, E. Gobet and A. Guyader).

A. Levitt co-organizes the applied mathematics seminar of the CERMICS lab, and the internal seminar of the EMC2 project (Sorbonne Université).

G. Stoltz

- is a member of the scientific council of UNIT (Université Numérique Ingénierie et Technologie),

- is a member of the "Conseil d'Enseignement et de Recherche" of Ecole des Ponts and of the Faculty Board of EELISA (European Engineering Learning Innovation Science Alliance),

- co-organized with X. Shang (University of Birmingham, United Kingdom) a mini-symposium at SIAM Materials Science'21 (17-28 May) on "Computational Statistical Physics and Related Fields".

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 (R. Biezemans, V. Ehrlacher, R. Goudey, G. Kemlin, G. Stoltz)

- Équations aux dérivées partielles et éléments finis, 15h (R. Biezemans, O. Gorynina, R. Goudey, F. Legoll)

- Hydraulique numérique, 15h (S. Boyaval)

- Mécanique quantique, 15h (E. Cancès, A. Levitt)

- Méthodes numériques pour les problèmes en grande dimension, 17h30 (V. Ehrlacher)

- Optimisation, 15h (O. Gorynina, J. Cauvin-Vila)

- Outils mathématiques pour l'ingénieur (E. Cancès: 18h, V. Ehrlacher, J. Cauvin-Vila, R. Goudey, F. Legoll, A. Levitt: 9h)

- Pratique du calcul scientifique, 15h (A. Levitt)

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

- Analyse de Fourier, 15h (A. Levitt)

- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès)

- Problèmes d'évolution, 36h (F. Legoll, V. Ehrlacher)

- Projets Modéliser Programmer Simuler (V. Ehrlacher, T. Lelièvre, G. Stoltz)

- Projets Semaine IMI, 10h (O. Gorynina)

- Statistics and data sciences, 24h (G. Stoltz)

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

- Introduction to computational statistical physics, 20h (G. Stoltz)

- Méthodes numériques probabilistes, 24h (T. Lelièvre)

- Problèmes multiéchelles, aspects théoriques et numériques, 24h (F. Legoll)

- Théorie spectrale et méthodes variationnelles, 10h (E. Cancès)

At other institutions:

- Modal de Mathématiques Appliquées (MAP472A, MAP463D), 15h, Ecole polytechnique (T. Lelièvre)

- Aléatoire (MAP361), 40h, Ecole Polytechnique (T. Lelièvre)

- Modélisation de phénomènes aléatoires (MAP432), 20 h (T. Lelièvre)

- Probabilités de 1ère année, 27h, L3, Ecole des Mines (M. Ramil)

- Analyse fonctionnelle, 46h, L3 Sorbonne Université (J. Cauvin-Vila)

The following PhD theses supervised by members of the project-team have been defended:

- Rafaël Coyaud, funding Ecole des Ponts, Deterministic and stochastic approaches for multimarginal optimal transport problems, since October 2017, co-supervised by V. Ehrlacher and A. Alfonsi (École des Ponts and Inria MATHRISK), defended in January

- Lise Maurin, funding Sorbonne Université, Adaptive biasing algorithms: mathematical analysis and applications in molecular dynamics, co-supervised by T. Lelièvre and J.P. Piquemal (SU), defended in December

The following PhD theses supervised by members of the project-team are ongoing:

- Zineb Belkacemi, thèse CIFRE SANOFI, Machine learning for model reduction in molecular dynamics, Université Paris-Est, since October 2018, supervised by T. Lelièvre and G. Stoltz

- Robert Benda, funding MTES, Multi-scale modeling of water quality nanosensors based on carbon nanotubes and conjugated polymers, Institut Polytechnique de Paris, since September 2018, supervised by E. Cancès and B. Lebental (Polytechnique)

- Rutger Biezemans, funding DIM Math Innov (Inria), Difficult multiscale problems and non-intrusive approaches, Ecole des Ponts, since October 2020, supervised by C. Le Bris and A. Lozinski (University of Besançon)

- Raed Blel, funding UM6P, Model-order reduction methods for stochastic problems, since October 2018, co-supervised by T. Lelièvre and V. Ehrlacher

- Jean Cauvin-Vila, funding Ecole des Ponts, Cross-diffusion systems on moving boundary domains, since October 2020, co-supervised by V. Ehrlacher and A. Hayat

- Yonah Conjugo-Taumhas, thèse CIFRE CEA, Reduced basis methods for non-symmetric eigenvalue problems, since October 2020, co-supervised by T. Lelièvre and V. Ehrlacher together with G. Dusson (CNRS Besançon) and F. Madiot (CEA)

- Maria Fuente-Ruiz, funding INRIA, Parallel algorithms for tensor methods, since September 2020, supervised by V. Ehrlacher and D. Lombardi (Inria COMMEDIA)

- Rémi Goudey, funding CDSN, Homogenization problems in the presence of defects, Université Paris-Est, since September 2019, supervised by C. Le Bris

- Gaspard Kemlin, Mathematical and numerical analysis for electronic structures, École des Ponts, since September 2019, supervised by E. Cancès and A. Levitt

- Eloïse Letournel, funding Ecole des Ponts, Finite size effects in electronic structure, École des Ponts, since September 2021, supervised by A. Levitt

- Alex Libal, funding Ecole des Ponts, Probabilistic approaches for materials fatigue, Ecole des Ponts, since September 2020, supervised by F. Legoll and J. Reygner (Ecole des Ponts)

- Idrissa Niakh, thèse CIFRE EDF, Reduced basis for variational inequalities, since October 2019, co-supervised by V. Ehrlacher and A. Ern (Inria SERENA)

- Thomas Pigeon, funding Inria, Combining machine learning and quantum computations to discover new catalytic mechanisms, Université de Lyon, since October 2020, supervised by P. Raybaud (IFPEN) and T. Lelièvre, together with G. Stoltz and M. Corral-Vallero (IFPEN)

- Régis Santet, funding Ecole des Ponts, Enhancing the sampling efficiency of reversible and non-reversible dynamics, Ecole des Ponts, since October 2021, supervised by T. Lelièvre and G. Stoltz

- Inass Sekkat, funding UM6P, Large scale Bayesian inference, Université Paris-Est, since March 2018, supervised by G. Stoltz

- Lev-Arcady Sellem, funding Advanced ERC Q-Feedback (PI: P. Rouchon), Mathematical approaches for simulation and control of open quantum systems, Ecole des Mines de Paris, since October 2020, co-supervised by C. Le Bris and P. Rouchon (Inria QUANTIC)

- Renato Spacek, funding FSMP CoFund, Efficient computation of linear response of nonequilibrium stochastic dynamics, ED 386 Sorbonne-Université, since November 2021, supervised by G. Stoltz and P. Monmarché (Sorbonne Université)

- Elisa Beteille, thèse CIFRE EDF, Propagation of Urban Flood waves, since November 2021, supervised by S. Boyaval

- Jana Tarhini, thèse IFPEN, Fast simulation of CO2/H2 storage in geological bassins, since November 2021, supervised by S. Boyaval

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

- S. Boyaval, PhD of Benjamin Streichenberger ("Approches multi-fidélités pour la simulation rapide d'écoulements d'air en milieu urbain"), defended at Université Gustave Eiffel in September

- V. Ehrlacher, PhD of Anne-Françoise Lempereur de Guerny ("De l'influence des conditions aux bords périodiques pour la simulation de quelques quantités d'intérêt pour la chimie séparative"), defended at Sorbonne Université in April (president)

- V. Ehrlacher, PhD of Thomas Daniel ("Apprentissage statistique pour la réduction de modèles non linéaire"), defended at Ecole des Mines de Paris in September (referee)

- V. Ehrlacher, PhD of Benoit Gaudeul ("Approximation numérique entropique pour des systèmes de diffusion croisée issus de la physique"), defended at Université de Lille in August

- V. Ehrlacher, PhD of Gabriele Todeschi ("Finite volume approximation of optimal transport and Wasserstein gradient flows"), defended at Université Paris-Dauphine in December

- G. Stoltz, PhD of Anne-Françoise Lempereur de Guerny ("De l'influence des conditions aux bords périodiques pour la simulation de quelques quantités d'intérêt pour la chimie séparative"), defended at Sorbonne Université in April (referee)

- G. Stoltz, PhD of Louis Thiry ("On the efficiency of local methods in image classification and energy regression in Physics"), defended at ENS Ulm in July (president)

- G. Stoltz, PhD of Lorenz Richter ("Solving high-dimensional PDEs, approximation of path space measures and importance sampling of diffusions"), defended at BTU Cottbus in December (referee)

- G. Stoltz, PhD of Robert Benda ("Multi-scale modeling of water quality nanosensors based on carbon nanotubes and conjugated polymers"), defended at Ecole polytechnique in December

- T. Lelièvre, PhD of Giacomo Garegnani ("Probabilistic and Bayesian methods for uncertainty quantification of deterministic and stochastic differential equations"), defended at EPFL in June (referee)

- T. Lelièvre, PhD of Arthur Macherey ("Approximation et re'duction de modèle pour les e'quations aux de'rive'es partielles avec interpre'tation probabiliste"), defended at Centrale Nantes in June (president)

- T. Lelièvre, PhD of Adrien Laurent ("Algebraic Tools and Multiscale Methods for the Numerical Integration of Stochastic Evolutionary Problems"), defended at Université de Genève in July

- T. Lelièvre, PhD of Louis Thiry ("On the efficiency of local methods in image classification and energy regression in physics") defended at Ecole Normale Supérieure in July (referee)

- T. Lelièvre, PhD of Dario Lucente ("Predicting probabilities of climate extremes from observations and dynamics"), defended at Ecole Normale Supérieure de Lyon in November

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

- T. Lelièvre, HdR of Pierre Monmarché ("Degenerated Markov processes for sampling, optimization and modelling"), defended at Sorbonne Université in January

- T. Lelièvre, HdR of Charles-Edouard Bréhier ("Contributions to stochastic numerics: simulation of SPDEs and rare events") defended at Université de Lyon 1, in June

- T. Lelièvre, HdR of Julien Reygner ("Theoretical analysis and numerical methods for conservation laws, metastability and uncertainty propagation "), defended at Paris Est Sup in September

Project-team members have participated in the following selection committees:

- C. Le Bris has chaired the committee for CEA-INSTN PhD fellowships in the Numerics program at CEA

- C. Le Bris was a member of the committee for CEA-FOCUS PhD fellowships in the Experimentation and Numerical Twins program at CEA.

- T. Lelièvre, Postes en mathématiques appliquées, Ecole Polytechnique.

- T. Lelièvre, Professeur en probabilités et statistiques, Université de Lorraine

9.3 Conference participation

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

- R. Biezemans, CERMICS Young Researchers Seminar, online, April

- R. Biezemans, Congrès SMAI 2021, la Grande-Motte, June

- R. Biezemans, 2nd French-German Workshop on Multiscale Problems, Besançon, September

- J. Cauvin-Vila, Journée école doctorale MSTIC, online, June.

- J. Cauvin-Vila, Congrès des jeunes chercheuses et chercheurs en mathématiques appliquées (CJC-MA), Ecole Polytechnique, October

- J. Dabaghi, WCCM conference, invited in a minisymposium, online, January

- J. Dabaghi, European Finite Element Fair conference, online, September

- J. Dabaghi, SIMRACE conference, Rueil-Malmaison, December

- J. Dabaghi, CEMRACS research project with Christoph Strossner and supervised by Virginie Ehrlacher, Luminy, July-August

- J. Dabaghi, research stay at ACSIOM, invited by M. Daniele Di Pietro, Université de Montpellier, November

- V. Ehrlacher, University of Strathclyde applied mathematics seminar, online, October

- V. Ehrlacher, Rencontres CEA-LJLL, December

- V. Ehrlacher, Plenary talk at the ICOSAHOM 2020 conference, online, July

- V. Ehrlacher, Journées IHP "Réduction de modèles et traitement géométrique des données", November

- V. Ehrlacher, University of Warwick applied mathematics seminar, online, June

- V. Ehrlacher, IPAM Workshop "Tensor Methods and their Applications in the Physical and Data Sciences", online, June

- L. Garrigue, Seminar of the laboratory of mathematics of the university of Bourgogne, Dijon, March

- L. Garrigue, Seminar of mathematical physics of the Centre for theoretical physics of Toulon, Toulon, March

- L. Garrigue, Seminar on multiscale problems in mathematical physics, Angers, June

- L. Garrigue, International congress on mathematical physics, Geneva, August

- L. Garrigue, MOANSI meeting 2021, online, September

- O. Gorynina, Congrès SMAI 2021, la Grande-Motte, June

- R. Goudey, Oberwolfach workshop on "Homogenization Theory: Periodic and Beyond", online, March

- R. Goudey, Congrès SMAI 2021, la Grande-Motte, June

- G. Kemlin, MOANSI meeting 2021, online, September

- G. Kemlin, SIAM MS, online, May

- G. Kemlin, SIAM CSE, online, March

- C. Le Bris, invited keynote lecture at the 2nd Conference of the Collaborative Research Center 1114 "Scaling Cascades in Complex Systems" (Freie Universitat - Zuse Institute Berlin), online, March

- C. Le Bris, Mittag-Leffler Institute workshop on "New trends in numerical multiscale methods and beyond", online, July

- T. Lelièvre, IMSI workshop on Mathematical and Computational Materials Science, online, February

- T. Lelièvre, SIAM MS conference, online, May

- T. Lelièvre, IPAM conference, online, June

- T. Lelièvre, Franco-Dutch Eurandom meeting, IHP, July

- T. Lelièvre, CEMRACS conference, CIRM, July

- T. Lelièvre, Lorentz Center, August

- T. Lelièvre, Analysis and probability seminar, Université Mohammed VI Polytechnique, online, September

- T. Lelièvre, CECAM Workshop on Generalized Langevin Equations, Berlin, online, September

- T. Lelièvre, Swiss numerics day, EPFL, September

- T. Lelièvre, Neutron Transport Days of the Bath-Beijing-Paris Branching Structures Meeting, online, September

- T. Lelièvre, Probability and Stochastic Processes seminar, University of Delaware, September

- T. Lelièvre, Workshop On Future Synergies for Stochastic and Learning Algorithms, CIRM, September

- T. Lelièvre, Statistical modeling for stochastic processes and related fields, ISM Japan, online, September

- T. Lelièvre, CECAM discussion meeting Generalized Langevin Equations in classical and quantum simulations, Paris, October

- T. Lelièvre, Séminaire LAMA, Université Gustave Eiffel, November

- T. Lelièvre, Séminaire PHIMECA l'aléatoire par les chemins de traverse, November

- T. Lelièvre, Séminaire LAGA, Université Sorbonne Paris Nord, November

- T. Lelièvre, Matherials Research Society fall meeting, online, December

- T. Lelièvre, Workshop Interaction Mechanisms in Monte Carlo Beyond Resampling, Bristol, online, December

- A. Levitt, GDR DYNQUA general meeting, online, March

- A. Levitt, UM6P seminar, online, April

- A. Levitt, GDR REST general meeting, online, May

- A. Levitt, SIAM Linear Algebra, online, May

- A. Levitt, Solid Math 2021, ENPC, August

- A. Levitt, Numerical analysis seminar, University of Besançon, October

- A. Levitt, Numerical analysis seminar, IMO, University Paris-Saclay, October

- A. Levitt, Chemistry seminar, ICP, University Paris-Saclay, October

- F. Legoll, WCCM congress, online, January

- F. Legoll, SIAM conference on Mathematical Aspects of Materials Science, online, May

- F. Legoll, 10th International Conference On Adaptive Modeling and Simulation (ADMOS), online, June

- F. Legoll, Mittag-Leffler Institute workshop on "New trends in numerical multiscale methods and beyond", online, July

- F. Legoll, 16th US National Congress on Computational Mechanics, online, July

- F. Legoll, Complas conference, Barcelona, September

- F. Legoll, 2nd French-German Workshop on Multiscale Problems, Besançon, September

- F. Legoll, workshop on "Generalized Langevin Equations in classical and quantum simulations", Paris, October

- E.Letournel, MOANSI meeting 2021, online, September

- G. Stoltz, MPI Polymer Research public seminar (online), January

- G. Stoltz, ERC Synergy workshop (online), February

- G. Stoltz, Probability seminar, University of Delaware (online), April

- G. Stoltz, SIAM Materials (online), May

- G. Stoltz, Probability seminar, University of Bristol (online), May

- G. Stoltz, MAC-MIGS afternoon on Mathematical Research Topics in Machine Learning (online), June

- G. Stoltz, Summer school "From kinetic equations to statistical mechanics", St Jean de Monts, France, June

- G. Stoltz, One World Stochastic Numerics and Inverse Problems seminar (online), July

- G. Stoltz, Workshop "On Future Synergies for Stochastic and Learning Algorithms", CIRM, France, October

- G. Stoltz, Workshop ANR EFI, Université Paris Dauphine, October

- G. Stoltz, Data Science and Computational Statistics Seminar, University of Birmingham, October

- U. Vaes, Séminaire de Dynamique Quantique et Classique, CPT (online), April

- U. Vaes, CECAM workshop on generalized Langevin equations, Sorbonne Université, October

- U. Vaes, Working group on consensus-based optimization and sampling, Simons Institute (online), October

- U. Vaes, Rencontres Inria–LJLL, Inria Paris, October

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

- T. Lelièvre, T. Pigeon and G. Stoltz, Constructing collective variables using Machine Learning and free energy biased simulations, 3h lecture + 3h hands-on session, AlgoSB Winter school 2021, CIRM, France, November

- T. Lelièvre, Brummer & Partners MathDataLab, "Sampling problems in computational statistical physics" (3h), KTH (online), Sweden, January 2021.

- T. Lelièvre, Lecture Series in Probability Theory, "Jump Markov models and transition state theory: the quasi-stationary distribution approach", Seoul National University, South Korea, August 2021.

- T. Lelièvre, T. Pigeon and G. Stoltz, Constructing collective variables using Machine Learning and free energy biased simulations, 3h lecture + 3h hands-on session, AlgoSB Winter school 2021, CIRM, France, November 2021.

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

- J. Cauvin-Vila, Congrès SMAI 2021, la Grande-Motte, June.

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

- R. Biezemans, Le Monde des Mathématiques Industrielles, online, March

- R. Biezemans, ECCOMAS Young Investigators Conference, online, July

- R. Biezemans, CEMRACS Summer School, July

- R. Biezemans, Congrès des Jeunes Chercheuses et Chercheurs en Mathématiques Appliquées, Palaiseau, October

- G. Kemlin, Online workshop on wave-function methods in quantum chemistry and nuclear physics, online, Frebruary

- G. Kemlin, CEMRACS 2021, Marseille, July-August

- G. Kemlin, Congrès des Jeunes Chercheuses et Chercheurs en Mathématiques Appliquées, Palaiseau, October

- E. Letournel, Solid Math 2021, Marne la Vallée, August

- R. Santet, QuAMProcs working group #3, seminar on metastable processes, Institut Denis Poisson, France, October

- L. Vidal, CEMRACS 2021, Marseille, July-August

9.4 Popularization

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

10 Scientific production

10.1 Major publications

[1]   E. Cancès, M. Defranceschi, W. Kutzelnigg, C. Le Bris and Y. Maday. *Computational Quantum Chemistry: A Primer*. English. Le Bris, Claude (ed.), Special Volume: Computational Chemistry. Amsterdam: North-Holland. Handb. Numer. Anal. 10, 3-270 (2003). 2003.

[2]   E. Cancès, C. Le Bris and Y. Maday. *Mathematical Methods in Quantum Chemistry. An Introduction. (Méthodes mathématiques en chimie quantique. Une introduction.)* French. Mathématiques et Applications (Berlin) 53. Berlin: Springer. xvi, 409~p., 2006.

[3]   I. Catto, C. Le Bris and P.-L. Lions. *The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models*. English. Oxford Mathematical Monographs. Oxford: Clarendon Press. xiii, 277~p., 1998.

[4]   J.-F. Gerbeau, C. Le Bris and T. Lelièvre. *Mathematical Methods for the Magnetohydrodynamics of Liquid Metals*. English. 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.)* French. Mathématiques et Applications (Berlin) 47. Berlin: Springer. xi, 212~p., 2005.

[6]   C. Le Bris and P.-L. Lions. *Parabolic Equations with Irregular Data and Related Issues: Applications to Stochastic Differential Equations*. Vol. 4. De Gruyter Series in Applied and Numerical Mathematics, 2019.

[7]   T. Lelièvre, M. Rousset and G. Stoltz. *Free Energy Computations: A Mathematical Perspective*. Imperial College Press, 458~p., 2010.

10.2 Publications of the year

International journals

[8]   A. Alfonsi, R. Coyaud and V. Ehrlacher. 'Constrained overdamped Langevin dynamics for symmetric multimarginal optimal transportation'. In: *Mathematical Models and Methods in Applied Sciences* (2021). URL: https://hal.archives-ouvertes.fr/hal-03131763.

[9]   C. Andrieu, A. Durmus, N. Nüsken and J. Roussel. 'Hypocoercivity of Piecewise Deterministic Markov Process-Monte Carlo'. In: *Annals of Applied Probability* (29th Oct. 2021). DOI: 10.1214/20-AAP1653. URL: https://hal.archives-ouvertes.fr/hal-01941467.

[10] Z. Belkacemi, P. Gkeka, T. Lelièvre and G. Stoltz. 'Chasing Collective Variables using Autoencoders and biased trajectories'. In: *Journal of Chemical Theory and Computation* 18.1 (1st Jan. 2022), pp. 59–78. DOI: 10.1021/acs.jctc.1c00415. URL: https://hal.archives-ouvertes.fr/hal-03207673.

[11]   X. Blanc and S. Wolf. 'Homogenization of the Poisson equation in a non-periodically perforated domain'. In: *Asymptotic Analysis* (29th Oct. 2021). DOI: 10.3233/ASY-201667. URL: https://hal.archives-ouvertes.fr/hal-02019504.

[12]   S. Boyaval, S. Martel and J. Reygner. 'Finite-Volume approximation of the invariant measure of a viscous stochastic scalar conservation law'. In: *IMA Journal of Numerical Analysis* (2021). DOI: 10.1093/imanum/drab049. URL: https://hal.archives-ouvertes.fr/hal-02291253.

[13]   E. Camrud, D. P. Herzog, G. Stoltz and M. Gordina. 'Weighted L^2-contractivity of Langevin dynamics with singular potentials'. In: *Nonlinearity* 35.2 (1st Jan. 2022), pp. 998–1035. URL: https://hal.archives-ouvertes.fr/hal-03205253.

[14]   E. Cancès, G. Dusson, Y. Maday, B. Stamm and M. Vohralík. 'Post-processing of the planewave approximation of Schrödinger equations. Part I: linear operators'. In: *IMA Journal of Numerical Analysis* 41.4 (Oct. 2021), pp. 2423–2455. DOI: 10.1093/imanum/draa044. URL: https://hal.archives-ouvertes.fr/hal-01908039.

[15]   E. Cancès, C. Fermanian Kammerer, A. Levitt and S. Siraj-Dine. 'Coherent electronic transport in periodic crystals'. In: *Annales Henri Poincaré* 22 (8th Mar. 2021), pp. 2643–2690. URL: https://hal.archives-ouvertes.fr/hal-02468564.

[16]   E. Cancès, G. Kemlin and A. Levitt. 'Convergence analysis of direct minimization and self-consistent iterations'. In: *SIAM Journal on Matrix Analysis and Applications* 42.1 (2021), 243–274 (32 pages). DOI: 10.1137/20M1332864. URL: https://hal.inria.fr/hal-02546060.

[17]   D. Chafaï, G. Ferré and G. Stoltz. 'Coulomb gases under constraint: some theoretical and numerical results'. In: *SIAM Journal on Mathematical Analysis* 53.1 (7th Jan. 2021), pp. 181–220. DOI: 10.1137/19M1296859. URL: https://hal.archives-ouvertes.fr/hal-02184896.

[18]   L. Chamoin and F. Legoll. 'Goal-oriented error estimation and adaptivity in MsFEM computations'. In: *Computational Mechanics* 67.4 (2021), pp. 1201–1228. DOI: 10.1007/s00466-021-01990-x. URL: https://hal.archives-ouvertes.fr/hal-02262423.

[19]   V. Ehrlacher, M. Fuente-Ruiz and D. Lombardi. 'SoTT: greedy approximation of a tensor as a sum of Tensor Trains'. In: *SIAM Journal on Scientific Computing* (2021). URL: https://hal.inria.fr/hal-03018646.

[20]   V. Ehrlacher, L. Grigori, D. Lombardi and H. Song. 'Adaptive hierarchical subtensor partitioning for tensor compression'. In: *SIAM Journal on Scientific Computing* (2021). DOI: 10.1137/19M128689X. URL: https://hal.inria.fr/hal-02284456.

[21]   V. Ehrlacher, G. Marino and J.-F. Pietschmann. 'Existence of weak solutions to a cross-diffusion Cahn-Hilliard type system'. In: *Journal of Differential Equations* 286 (2021), pp. 578–623. URL: https://hal.archives-ouvertes.fr/hal-02888479.

[22]   O. Gorynina, C. Le Bris and F. Legoll. 'Some remarks on a coupling method for the practical computation of homogenized coefficients'. In: *SIAM Journal on Scientific Computing* 43.2 (2021), A1273–A1304. DOI: 10.1137/20M1339076. URL: https://hal.archives-ouvertes.fr/hal-02614896.

[23]   A. Iacobucci, S. Olla and G. Stoltz. 'Thermo-mechanical transport in rotor chains'. In: *Journal of Statistical Physics* 183 (4th May 2021), article number 26. URL: https://hal.archives-ouvertes.fr/hal-02904454.

[24]   B. Jourdain, T. Lelièvre and P.-A. Zitt. 'Convergence of metadynamics: discussion of the adiabatic hypothesis'. In: *Annals of Applied Probability* 31.5 (Oct. 2021), pp. 2441–2477. DOI: 10.1214/20-AAP1652. URL: https://hal.archives-ouvertes.fr/hal-02104961.

[25]   F. Legoll, T. Lelièvre and U. Sharma. 'An adaptive parareal algorithm: application to the simulation of molecular dynamics trajectories'. In: *SIAM Journal on Scientific Computing* (2021). URL: https://hal.archives-ouvertes.fr/hal-03189428.

[26]   T. Lelièvre, M. Ramil and J. Reygner. 'Quasi-stationary distribution for the Langevin process in cylindrical domains, part I: existence, uniqueness and long-time convergence'. In: *Stochastic Processes and their Applications* 144 (Feb. 2022), pp. 173–201. URL: https://hal.archives-ouvertes.fr/hal-03123442.

[27] G. A. Pavliotis, G. Stoltz and U. Vaes. 'Scaling limits for the generalized Langevin equation'. In: *Journal of Nonlinear Science* 31 (2nd Jan. 2021), p. 8. DOI: `10.1007/s00332-020-09671-4`. URL: `https://hal.archives-ouvertes.fr/hal-02911852`.

Reports & preprints

[28] R. Benda, E. Cancès, V. Ehrlacher and B. Stamm. *Multi-center decomposition of molecular densities: a mathematical perspective*. 9th Sept. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03338862`.

[29] M.-R. Blel, V. Ehrlacher and T. Lelièvre. *Influence of sampling on the convergence rates of greedy algorithms for parameter-dependent random variables*. 23rd Sept. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03238244`.

[30] S. Boyaval and M. Dostalík. *Non-isothermal viscoelastic flows with conservation laws and relaxation*. 22nd Apr. 2021. URL: `https://hal-enpc.archives-ouvertes.fr/hal-03206116`.

[31] C. Cancès, V. Ehrlacher and L. Monasse. *Finite Volumes for the Stefan-Maxwell Cross-Diffusion System*. 2021. URL: `https://hal.archives-ouvertes.fr/hal-02902672`.

[32] E. Cancès, G. Dusson, G. Kemlin and A. Levitt. *Practical error bounds for properties in plane-wave electronic structure calculations*. 29th Oct. 2021. URL: `https://hal.inria.fr/hal-03408321`.

[33] É. Cancès, L. Garrigue and D. Gontier. *Second-order homogenization of periodic Schrödinger operators with highly oscillating potentials*. 23rd Dec. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03501482`.

[34] J. A. Carrillo, F. Hoffmann, A. M. Stuart and U. Vaes. *Consensus Based Sampling*. 11th Nov. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03425993`.

[35] J. A. Carrillo, C. Totzeck and U. Vaes. *Consensus-based Optimization and Ensemble Kalman Inversion for Global Optimization Problems with Constraints*. 11th Nov. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03425989`.

[36] L. Chamoin and F. Legoll. *A pedagogical review on a posteriori error estimation in Finite Element computations*. 6th Oct. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03368356`.

[37] J. Dabaghi, V. Ehrlacher and C. Strössner. *Computation of the self-diffusion coefficient with low-rank tensor methods: application to the simulation of a cross-diffusion system*. 22nd Nov. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03441986`.

[38] M.-S. Dupuy and A. Levitt. *Finite-size effects in response functions of molecular systems*. 3rd Dec. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03145143`.

[39] A. Durmus, A. Enfroy, É. Moulines and G. Stoltz. *Uniform minorization condition and convergence bounds for discretizations of kinetic Langevin dynamics*. 3rd Sept. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03333501`.

[40] V. Ehrlacher, T. Lelièvre and P. Monmarché. *Adaptive force biasing algorithms: new convergence results and tensor approximations of the bias*. 19th Nov. 2021. URL: `https://hal.archives-ouvertes.fr/hal-02314426`.

[41] L. Garrigue. *Building Kohn-Sham potentials for ground and excited states*. 6th Jan. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03099868`.

[42] O. Gorynina, C. Le Bris and F. Legoll. *Mathematical analysis of a coupling method for the practical computation of homogenized coefficients*. 10th June 2021. URL: `https://hal.archives-ouvertes.fr/hal-03256156`.

[43] R. Goudey. *A periodic homogenization problem with defects rare at infinity*. 14th Sept. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03343281`.

[44] M. F. Herbst and A. Levitt. *A robust and efficient line search for self-consistent field iterations*. 30th Sept. 2021. URL: `https://hal.inria.fr/hal-03359244`.

[45] F. Legoll, P.-L. Rothe, C. Le Bris and U. Hetmaniuk. *An MsFEM approach enriched using Legendre polynomials*. 3rd Sept. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03333670`.

[46]   T. Lelièvre, L. Maurin and P. Monmarché. *The Adaptive Biasing Force algorithm with non-conservative forces and related topics.* 22nd Feb. 2021. URL: https://hal.archives-ouvertes.fr/hal-03148328.

[47]   G. A. Pavliotis, A. M. Stuart and U. Vaes. *Derivative-free Bayesian Inversion Using Multiscale Dynamics.* 29th Apr. 2021. URL: https://hal.archives-ouvertes.fr/hal-03211852.

[48]   P. Plechac, G. Stoltz and T. Wang. *Martingale product estimators for sensitivity analysis in computational statistical physics.* 2nd Dec. 2021. URL: https://hal.archives-ouvertes.fr/hal-03462697.

[49]   M. Ramil. *Quasi-stationary distribution for the Langevin process in cylindrical domains, part II: overdamped limit.* 6th Mar. 2021. URL: https://hal.archives-ouvertes.fr/hal-03161373.

[50]   I. Sekkat and G. Stoltz. *Removing the mini-batching error in Bayesian inference using Adaptive Langevin dynamics.* 19th Oct. 2021. URL: https://hal.archives-ouvertes.fr/hal-03386488.

[51]   G. Stoltz. *Computational statistical physics and hypocoercivity.* 16th Dec. 2021. URL: https://hal.archives-ouvertes.fr/hal-03482498.