RESEARCH CENTRE

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2020 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

Contents

Project-Team MATHERIALS

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

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2 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, 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 material science. Efforts in this direction must address a large variety of questions such as

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

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

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

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

4.2 Computational Statistical Mechanics

The orders of magnitude used in the microscopic representation of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 6 \times 10^{23}$, the typical distances are expressed in Å (10^{-10} m), the energies are of the order of $k_B T \simeq 4 \times 10^{-21}$ 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 how to couple models written at the atomistic scale with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

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

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

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to provide a good description of the materials;

- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

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

5 Highlights of the year

5.1 Awards

T. Lelièvre was awarded a visiting professorship from the Leverhulme Trust, to cover his sabbatical leave at Imperial College from January 2020 to June 2020.

Grégoire Ferré, who did his PhD in the Matherials team from Oct. 2016 to Sept. 2019, was awarded the PhD prize from the doctoral school MSTIC of University Paris Est. His worked focused on large deviation theory and its application in statistical physics, both from theoretical and numerical viewpoints. He is now a research associate at Capital Fund Management.

6 New software and platforms

6.1 New software

6.1.1 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

Contacts: Antoine Levitt, Michael Herbst

6.1.2 gen.parRep

Keywords: Molecular simulation, MPI, HPC, C++

Functional Description: gen.parRep is the first publicly available implementation of the Generalized Parallel Replica method (BSD 3-Clause license), targeting frequently encountered metastable biochemical systems, such as conformational equilibria or dissociation of protein-ligand complexes.

It was shown (hal-01832823) that the resulting C++/MPI implementation exhibits a strong linear scalability, providing up to 70 % of the maximum possible speedup on several hundreds of CPUs.

Release Contributions: The software was modified for reproducibility in its release 1.2.0, see the notes: https://gitlab.inria.fr/parallel-replica/gen.parRep/tags/v1.2.0

URL: https://gitlab.inria.fr/parallel-replica/gen.parRep

Publication: hal-01832823

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7 New results

7.1 Electronic structure calculations

7.1.1 The ground state problem in 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.

In [46], E. Cancès, G. Kemlin and A. Levitt have studied the algebraic structure of the self-consistent problems present in mean-field models such as Hartree-Fock and Kohn-Sham density functional theory. They have showed the local convergence of the damped self-consistent iteration and gradient descent, and have compared explicitly their convergence rates, providing insight into the strengths and weaknesses of different methods.

E. Cancès, M. Herbst and A. Levitt have implemented a posteriori error estimators into the DFTK code, and have demonstrated its use in [26]. They have provided fully guaranteed error estimators (including discretization, algebraic and machine arithmetic errors), albeit under simplifying assumptions (analytic pseudopotentials, and neglecting explicit electron-electron). Work is underway to extend this formalism to the more realistic case of nonlinear mean-field models.

M. Herbst and A. Levitt have investigated numerically the convergence of self-consistent iterations in extended systems, and the impact of various preconditioners. As is well-known, homogeneous preconditioners are unable to reflect various chemical environments such as interfaces or surfaces. Using the density of states as a proxy for the local dielectric properties of the medium, they have proposed in [53] a simple yet cheap and efficient preconditioner that does not need to be tuned manually for each system. Numerical results have shown a consistent improvement over state-of-the-art methods in a variety of systems, with particularly good performance on metallic surfaces.

In [14], E. Cancès, G. Dusson (CNRS and University of Besançon), Y. Maday (Sorbonne University), B. Stamm (University of Aachen, Germany), and M. Vorhalík (Inria Paris, project-team Serena) have proven 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 of the same authors. They have considered a Schrödinger operator $= -\frac{1}{2}\Delta + V$ in a cubic box with periodic boundary conditions, with a regular-enough potential V. 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 have computed first-order corrections for the eigenfunctions, which are turned into corrections on the ground-state density matrix. This increases the accuracy by a factor proportional to the inverse of the kinetic energy cutoff of both the ground-state energy and the ground-state density matrix in Hilbert–Schmidt norm 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 planewave basis and two Fast Fourier Transforms per eigenvalue.

7.1.2 Response properties

The team members have focused on justifying rigorously and computing efficiently the response properties of molecules and materials.

In [45], E. Cancès, A. Levitt and S. Siraj-Dine have studied the time-dependent response properties of crystals to a uniform electric field. Their results present in a unified framework various regimes described in the physical and mathematical literature (quantum Hall effect in insulators, ballistic conduction and Bloch oscillations in metals, residual conductivity of graphene), and shed light on their range of validity.

M. Herbst and T. Fransson (Heidelberg University, Germany) have used the recently developed adcc code to study the error of the core-valence separation (CVS) approximation in the context of simulating X-ray absorption spectra [25]. Using an iterative post-processing procedure they have managed to undo said approximations on obtained computational results and in this way have managed for the first time to study the error of the approximation within the regime of computational parameters employed in practice. Their results show that in the K-edge region of the X-ray spectra errors are negligible and overall only amount to a scalar shift of the simulated spectrum. This shows that the CVS approximation is therefore safe to use for the calculation of core-excited states not lowering the quality of results required for comparison with experimental X-ray absorption spectra.

7.1.3 Various topics

E. Cancès, R. Coyaud and R. Scott (University of Chicago, USA) have pursued their study of van der Waals interactions. In [44], they have extended a method previously introduced by the first and third authors, to compute more terms in the asymptotic expansion of the van der Waals attraction between two hydrogen atoms. These terms are obtained by solving a set of modified Slater–Kirkwood partial differential equations. The accuracy of the method is demonstrated by numerical simulations and comparison with other methods from the literature. It is also shown that the scattering states of the hydrogen atom, that are the states associated with the continuous spectrum of the Hamiltonian, have a major contribution to the C_6 coefficient of the van der Waals expansion.

In [10], R. Benda and E. Cancès, in collaboration with B. Lebental and G. Zucchi (Ecole Polytechnique) have investigated the interaction of polyfluorene and fluorene/carbazole copolymers, bearing various functional groups and side chains, with small to large diameter carbon nanotubes (CNTs) in vacuo, using variable-charge molecular dynamics simulations based on the reactive force field ReaxFF. It is shown that non-covalent functionalization of nanotubes, driven by $\pi-\pi$ interactions, is effective for all the polymers studied, thanks to their conjugated backbone and regardless of the presence of specific functional groups. Both energetic and geometric adsorption features of these polymer/CNT hybrids is analyzed in detail at the scale of each fluorene or carbazole unit. The force field ReaxFF and its available parameterization used for the simulations are validated, thanks to a benchmark and review on higher-level quantum calculations—for simple $\pi-\pi$ interacting compounds made up of polycyclic aromatic molecules adsorbed on a graphene sheet or bilayer graphene. This methodology proves to be a valuable tool for optimal polymer design for nanotube functionalization at no re-parameterization cost and could be adapted to simulate and assist the design of other types of molecular systems.

C. Le Bris has pursued his long term collaboration with P. Rouchon (Ecole des Mines de Paris and Inria/QUANTIC) on the study of high dimensional Lindblad type equations at play in the modelling of open quantum systems. They have co-supervised the M2 internship of L-A. Sellem, that was focused

on the simulation of some simple quantum gates, and has investigated several discretization strategies based upon the choice of suitable basis sets. Following up on the topic of his internship, L-A. Sellem has started in September 2020 his PhD work, under the co-supervision of P. Rouchon and C. Le Bris, at the intersection between the QUANTIC and the MATHERIALS project-teams.

7.2 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 project-team can be divided into four 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 dynamic simulations and gain some insights on the models.

7.2.1 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 averages 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 realizations of certain dynamics. 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 known as hypocoercivity, and usually involves prefactors which are difficult to quantitatively estimate. Bounds on the asymptotic variance on the other hand only require bounds on the resolvent of the generator. An approach to directly obtaining estimates on the resolvent of hypocoercive operators is proposed in [40], using Schur complements, rather than obtaining bounds on the resolvent from an exponential decay of the evolution semigroup. The results can be extended, besides Langevin-like dynamics, to the linear Boltzmann equation (which is also the generator of randomized Hybrid Monte Carlo in molecular dynamics). In particular, the dependence of the resolvent bounds on the parameters of the dynamics and on the dimension is made precise, and the relationships with other hypocoercive approaches are highlighted. This work has been performed while Max Fathi (now at Université de Paris, France) was visiting the MATHERIALS project-team.

Other numerical sampling algorithms were also studied. In [58], T. Lelièvre and G. Stoltz, together with W. Zhang (Zuse Institute Berlin, Germany) have proposed new Markov Chain Monte Carlo (MCMC) algorithms to sample probability distributions on submanifolds. Such target distributions are typically encountered when studying systems with molecular constraints (fixed bond angles or bond lengths), or for free energy computations. The newly proposed method generalizes previous algorithms by allowing the use of set-valued maps in the proposal step of the MCMC algorithms. The motivation for this generalization is that the numerical solvers used to project proposed moves to the submanifold of interest may find several solutions. The unbiasedness of these new algorithms is proven thanks to some carefully enforced reversibility property. The interest of the new MCMC algorithms is illustrated on various numerical examples.

For sampling multimodal and anisotropic distributions in Bayesian inference or statistical physics, T. Lelièvre, G. Robin and G. Stoltz, together with G. Pavliotis (Imperial College, United-Kingdom) are studying a new algorithm based on Langevin dynamics, in the framework of G. Robin's post-doc funded by Inria through the "Programme de Recherche Exploratoire" on "Molecular Dynamics and Learning". They have proposed a new method extending the Metropolis Adjusted Langevin Algorithm (MALA), by introducing a diffusion function allowing a more efficient exploration of the parameter space. This diffusion function is obtained by optimizing the convergence rate of the sampling algorithm, which boils down to solving a spectral problem. The properties of this optimization problem are studied, and a numerical method is developed to compute the corresponding optimal diffusion. Numerical experiments

are also performed to evaluate the gain in terms of convergence speed, in comparison to the original MALA with constant diffusion.

Finally, the team has also pursued its endeavour to study and improve free energy biasing techniques, such as adaptive biasing force or metadynamics. The gist of these techniques is to bias the original metastable dynamics used to sample the target probability measure in the configuration space by an approximation of the free energy along well-chosen reaction coordinates. This approximation is built on the fly, using empirical measures over replicas, or occupations measures over the trajectories of the replicas. In [49], V. Ehrlacher and T. Lelièvre, together with P. Monmarché (Sorbonne Université, France) have introduced a modified version of the Adaptive Biasing Force method, in which the free energy is approximated by a sum of tensor products of one-dimensional functions. This enables to handle a larger number of reaction coordinates than the classical algorithm. It is proven that the algorithm is well-defined, and the long-time convergence of the algorithm is studied. Numerical experiments demonstrate that the method is able to capture correlations between reaction coordinates.

7.2.2 Sampling of dynamical properties and rare events

The theory of quasi-stationary distributions has been used by T. Lelièvre and collaborators over the past years in order to rigorously model the exit event from a metastable state by a jump Markov process, and to study this exit event in the small temperature regime. In [39], T. Lelièvre together with M. Baudel and A. Guyader (Sorbonne Université, France) have illustrated how the Hill relation and the notion of quasi-stationary distribution can be used to analyse the error introduced by many algorithms that are used to compute mean reaction times between metastable states for Markov processes. The theoretical findings are illustrated on various examples demonstrating the sharpness of the error analysis as well as the applicability of the study to elliptic diffusions.

In [55], T. Lelièvre, together with D. Le Peutrec (Université d'Orléans, France) and B. Nectoux (Université Clermont Auvergne, France) have considered the first exit point distribution from a bounded domain of the overdamped Langevin dynamics in the small temperature regime, under rather general assumptions on the potential function. This work is a continuation of a previous paper (part 1, see [19]) where the exit point distribution is studied starting from the quasi-stationary distribution. The proofs are based on analytical results on the dependency of the exit point distribution on the initial condition, large deviation techniques and results on the genericity of Morse functions.

Quasi-stationary distributions can be seen as the first eigenvector associated with the generator of the stochastic differential equation at hand, on a domain with Dirichlet boundary conditions (which corresponds to absorbing boundary conditions at the level of the underlying stochastic processes). Many results on the quasi-stationary distribution hold for non degenerate stochastic dynamics, the associated generator of which is elliptic. The case of degenerate dynamics is less clear. In [57], T. Lelièvre and M. Ramil, together with J. Reygner (Ecole des Ponts, France), have generalized well-known results on the probabilistic representation of solutions to parabolic equations on bounded domains to the so-called kinetic Fokker Planck equation on bounded domains in positions, with absorbing boundary conditions. Furthermore, a Harnack inequality and a maximum principle are provided for solutions to this kinetic Fokker-Planck equation, as well as the existence of a smooth transition density for the associated absorbed Langevin dynamics. The continuity of this transition density at the boundary is studied as well as the compactness, in various functional spaces, of the associated semigroup. This work is a cornerstone to prove the consistency of various algorithms used to simulate metastable trajectories of the Langevin dynamics, in particular the Parallel Replica algorithm and the Adaptive Multilevel Splitting method.

7.2.3 Nonequilibrium systems and transport properties

Many systems in computational statistical physics are not at equilibrium, but rather in a stationary state. 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.

G. Stoltz and U. Vaes, together with G. Pavliotis (Imperial College London, United-Kingdom) have studied in [33] the properties of the mobility for generalized Langevin dynamics. These dynamics can

be seen as Langevin dynamics with some colored noise, and recast in the quasi-Markovian setting as a stochastic differential equation with additional degrees of freedom modeling the structure of the noise. A hypocoercive analysis in the H^1 framework à la Villani allows to obtain sharp bounds on the resolvent of the generator of the dynamics, in various limiting regimes (overdamped regime, Markovian limit corresponding to Langevin dynamics, underdamped or Hamiltonian limit). These bounds can in turn be used to obtain precise asymptotics on the mobility coefficient in these various limiting regimes. These predictions are confirmed by numerical simulations based on a Galerkin discretization of the generator.

Since joining the project-team in November, U. Vaes has also been working with G. Stoltz on variance reduction methods for the computation of mobility coefficients for Langevin dynamics in the underdamped (or Hamiltonian) limit, for two dimensional systems. There is currently no precise numerical or theoretical understanding of the divergent behavior of the mobility as the friction coefficient vanishes. Strong limitations are due to the large computational cost of numerically converging the estimated value of the diffusion coefficient as the friction decreases. U. Vaes and G. Stoltz are studying the use of variance reduction methods to more efficiently compute the mobility.

Finally, G. Stoltz, together with A. Iacobucci and S. Olla (Université Paris-Dauphine, France) have studied in [54] the macroscopic profiles of temperature and angular momentum in the stationary state of chains of rotors under a thermo-mechanical forcing applied at the boundaries. These profiles are solutions of a system of diffusive partial differential equations with boundary conditions determined by the thermo-mechanical forcing. Instead of expensive Monte Carlo simulations of the underlying microscopic physical system, they have performed extensive numerical simulations based on a finite difference method for the system of partial differential equations describing the macroscopic steady state. They have presented a formal derivation of these stationary equations based on a linear response argument and local equilibrium assumptions. This allows to characterize the regime of parameters leading to uphill diffusion, a situation where the energy flows in the direction of the gradient of temperature; and to identify regions of parameters corresponding to a negative thermal conductivity (*i.e.* a positive linear response to a gradient of temperature). The agreement with previous results obtained by numerical simulation of the microscopic dynamics confirms the validity of the macroscopic equations which were derived.

7.2.4 Coarse-graining and model reduction

In [24], T. Lelièvre, G. Stoltz and Z. Belkacemi have reviewed how machine learning techniques are used in molecular dynamics to extract valuable information from the enormous amounts of data generated by simulation of complex systems. They provide a review of the goals, benefits, and limitations of machine learning techniques for computational studies on atomistic systems, focusing on the construction of empirical force fields from ab-initio databases and the determination of reaction coordinates for free energy computation and enhanced sampling. This work is co-authored with P. Gkeka (Sanofi, France) A. Farimani (Carnegie Mellon University, USA), M. Ceriotti (EPFL, Switzerland), J. Chodera (Memorial Sloane Kettering Cancer Center, USA), A. Dinner (University of Chicago, USA), A. Ferguson (University of Chicago, USA), J.B. Maillet (CEA, France), H. Minoux (Sanofi, France), C. Peter (University of Konstanz, Germany), F. Pietrucci (Sorbonne Université, France), A. Silveira (Memorial Sloane Kettering Cancer Center, USA), A. Tkatchenko (University of Luxembourg, Luxembourg), Z. Trstanova (University of Edinburgh, United Kingdom) and R. Wiewiora (Memorial Sloane Kettering Cancer Center, USA).

7.3 Homogenization

7.3.1 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 the context of the PhD work of R. Goudey, who has studied perturbations of periodic systems that do not decay at infinity but become increasingly rare. Another interesting direction studied is that of general algebras for homogenization, introduced by X. Blanc, C. Le Bris and P.-L. Lions two decades ago. Some very illustrative one-dimensional cases have been explored, as well as the case of equations simpler than the diffusion equation, namely elliptic equations with highly oscillatory potentials. A monograph that summarizes the developments completed in the past years, and that combines them with the basic elements of

homogenization theory, is currently in writing by C. Le Bris and X. Blanc (half-time on leave at Inria since September 2019 and until August 2021 from Université de Paris).

Also in the context of homogenization theory, O. Gorynina, C. Le Bris and F. Legoll have pursued 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. The 18 months post-doc (January 2019-July 2020) of O. Gorynina has allowed to complete 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. They have been collected in a publication currently submitted [52]. The theoretical study of the approach is performed in a contribution soon to be submitted.

7.3.2 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. Despite the fact that the approach has 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 C. Le Bris, F. Legoll and A. Lozinski, R. Biezemans (who joined the project-team this year during his M2 internship and is now starting his PhD) has 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. In addition, R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski have undertaken the precise mathematical study of an existing variant of MsFEM, where the standard basis set is enriched using a singular value decomposition of an operator defined for each edge of the coarse mesh, and the range of which is essentially given by the trace on that edge of the oscillatory solutions (for, say, various right-hand sides). This variant has been recently proposed in the literature, and its appealing numerical performances (basis functions that are locally supported, lack of any resonance error in the regime $H \approx \varepsilon, \ldots$) have motivated the team to better understand it from a theoretical perspective. A convergence analysis of this new variant, together with comprehensive numerical tests, are currently in progress.

Second, within the PhD thesis of A. Lesage, Multiscale Finite Element Methods have been developped 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. In a first step, V. Ehrlacher, F. Legoll and A. Lesage, in collaboration with A. Lebée (ENPC, France), have established strong convergence results (between the oscillatory solution and an adequate two-scale expansion) for problems posed on thin heterogeneous plates. After having considered the case of a diffusion equation, the case of linear elasticity has been studied, both in the so-called membrane case (that is, when the loading lies in the in-plane directions) and in the much more challenging case of bending (that is, when the loading is perpendicular to the in-plane directions). In a second step, several MsFEM variants have been proposed and compared numerically. A priori error bounds have been established, assessing the performances of the approaches,

and extensive numerical tests have been performed. All these results are presented in two manuscripts in preparation.

7.4 Various topics

7.4.1 Complex fluids

In 2020, 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. Regarding fluid viscoelasticity (of Maxwell-type), it turns out this can be modeled within the standard framework of classical continuum mechanics, with a symmetric-hyperbolic system of conservation laws unifying the elastodynamics of hyperelastic materials and Newtonian fluid dynamics [41]. To that aim, the viscoelastic system is an extension of elastodynamics using a time-dependent structure tensor that produces friction through relaxation. The new framework is versatile and should be consolidated for extension to other material imperfection beyong viscoelasticity.

7.4.2 Cross-diffusion systems

New results were obtained in 2020 by V. Ehrlacher on the analysis and numerical analysis of cross-diffusion systems, in the context of the ANR project COMODO.

In a joint work [43] with C. Cancès (Inria RAPSODI) and L. Monasse (Inria COFFEE), a finite volume numerical scheme for the so-called Maxwell-Stefan model has been developed. The Maxwell-Stefan model is a cross-diffusion system used to describe the evolution of a mixture of gas, and is used in particular in biomedical applications. The numerical method developed is provably convergent and preserves on the discrete level the main mathematical properties of the continuous system, including mass conservation, non-negativity of the solutions and an entropy-entropy dissipation inequality which accunts for the long-time behaviour of the solutions of the system.

In a joint work with J-F. Pietschmann and G. Marino (Chemnitz, Germany) [50], V. Ehrlacher has proved the existence of weak solutions to a multi-species cross-diffusion degenerate Cahn-Hilliard system, including phase separation effects of one species with respect to the other species composing the mixture. The proof of the existence of weak solutions to such a model requires the development of new analysis tools, in particular due to the degenerate nature of the resulting model.

7.4.3 Tensor methods for high-dimensional problems

In a joint work with D. Lombardi and M. Fuente-Ruiz (Inria COMMEDIA), V. Ehrlacher has developed a new algorithm for the computation of a canonical polyadic approximation of a high-order tensor [48]. The new method is much more efficient and robust that the standard Alternating Least Square method and gave very encouraging results especially for tensors with high order.

8 Bilateral 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.

9 Partnerships and cooperations

9.1 National initiatives

The project-team is involved in several ANR projects:

- S. Boyaval is the PI of the ANR JCJC project SEDIFLO (2016-2021) 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 COMMEDIA 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 (2015-2020), 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),

- 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),

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

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).

9.2 European initiatives

The ERC Synergy Grant EMC2 (ERC Grant Agreement number 810367 , PI 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 been selected for funding.

9.3 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.

10 Dissemination

10.1 Promoting scientific activities

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

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 Cordi-S selection committee of INRIA,
- co-organizes the colloquium of the CERMICS lab.

C. Le Bris

- is a managing editor of Networks and Heterogeneous Media,
- 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-), 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, Series, Springer (2008-), Modelling, Simulations and Applications, Series, Springer (2009-), Springer Monographs in Mathematics, Springer (2016-),
- is a member of the "Conseil de la Faculté des sciences et ingénierie", Sorbonne Université, and the "Conseil scientifique" of SMAI,
- 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.

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

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings and Surveys (with D. Chafai, C. Imbert and P. Lafitte),
- is a member of the 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 SMAI and École des Ponts,
- is the head of the applied mathematics department (CERMICS) at Ecole des Ponts,
- held a visiting professorship position at Imperial College of London (until July 2020).

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

G. Robin

- has co-organized the working group "Machine learning and optimization" of the Labex Bezout (with G. Stoltz, and W. Hachem),
- is president of the "Groupe Jeunes" de la Société Française de Statistique (SFdS),
- has organized the «Young Statisticians and Probabilists» seminar of the SFdS Young Statisticians group in January 2020,
- is a member of the editorial board of the YoungStats blog and webinar, operating under the FENStats organization.

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.

10.2 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 (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, L3 (G. Kemlin)
- Outils mathématiques pour l'ingénieur, (E. Cancès: 18h, V. Ehrlacher: 9h, R. Goudey: 9h, F. Legoll: 9h)
- Parcours recherche, 15h (A. Levitt)
- 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)
- Statistics and data sciences, 24h (G. Stoltz)
- Techniques de développement logiciel, 18h (M. Herbst)

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

- Méthodes de quantification des incertitudes en ingénierie, 18h (V. Ehrlacher)

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:

- Uncertainty quantification and model order reduction, 20h, Imperial College (T. Lelièvre)
- Modal de Mathématiques Appliquées (MAP472A), 10h, Ecole polytechnique (T. Lelièvre)
- Modélisation statistique, 32h, ESSEC Business School (G. Robin)
- Probabilités de 1ère année, 27h, L3, Ecole des Mines (M. Ramil)
- Renormalized solutions of parabolic equations, 21h, University of Chicago (C. Le Bris)

The following HDR theses have been defended by members of the project-team

- Virginie Ehrlacher, Mathematical and numerical analysis of some high-dimensional and multiscale problems in materials science, December 10th
- Antoine Levitt, Mathematical and numerical analysis of models of condensed-matter physics, October 2nd

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

- Qiming Du, Mathematical analysis of splitting methods, Ecole Doctorale Sciences Mathématiques de Paris Centre, defended on June 17th, supervised by A. Guyader (UPMC) and T. Lelièvre
- Adrien Lesage, Multi-scale methods for calculation and optimization of thin structures, Université Paris-Est, École des Ponts, defended on December 16th, supervised by F. Legoll, co-advised by V. Ehrlacher and A. Lebée (Ecole des Ponts, Laboratoire Navier),
- Mouad Ramil, Kinetic processes on cylindrical domains and quasi-stationarity, Université Paris-Est Ecole des Ponts, defended on December 10th, supervised by T. Lelièvre and J. Reygner
- Sami Siraj-Dine, Dynamics of electrons in 2D materials, defended on December 17th, supervised by E. Cancès, C. Fermanian (Univ. Paris-Est) and A. Levitt

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)

- 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)
- 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
- 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)
- Lise Maurin, funding Sorbonne Université, Non reversible and adaptive biasing processes for sampling, since October 2018, supervised by T. Lelièvre and J.-P. Piquemal (Sorbonne Université), together with P. Monmarché (Sorbonne Université)
- 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)
- 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)

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

- S. Boyaval, PhD of Arwa Mrad ("Numerical simulation of sediment dynamics in free surface flows"), defended at EPFL in November 2020
- E. Cancès, PhD of Muhammad Hassan (“Mathematical analysis of boundary integral equations and domain decomposition methods with applications in polarizable electrostatics”), defended at University of Aachen (Germany) in June 2020 (reviewer)
- E. Cancès, PhD of Louis Garrigue (“Contributions mathématiques à la théorie des fonctionnelles de la densité”) defended at Université Paris Dauphine in September 2020 (chair)
- V. Ehrlacher, PhD of Louis Garrigue (“Contributions mathématiques à la théorie des fonctionnelles de la densité”) defended at Université Paris Dauphine in September 2020
- V. Ehrlacher, PhD of Cécile Haberstitch (“ Adaptive approximation of high-dimensional functions with tree tensor networks for Uncertainty Quantification”) defended at Ecole Centrale de Nantes in December 2020
- V. Ehrlacher, PhD of William Margheriti (“Sur la stabilité de transport optimal martingale”) defended at Université Paris-Est in December 2020
- M. Herbst, PhD of Abdallah Ammar ("Représentation des états du continuum par des gaussiennes complexes"), defended at Université de Lorraine in December 2020
- F. Legoll, PhD of Edoardo Paganoni ("Novel corrector problems with exponential decay of the resonance error for numerical homogenization"), defended at EPFL in August 2020

- T. Lelièvre, PhD of Rishabh Sunil Gvalani ("Many-particle systems: phase transitions, distinguished limits, and gradient flows"), defended at Imperial College of London in June 2020 (reviewer)
- T. Lelièvre, PhD of Loucas Pillaud-Vivien ("Learning with Reproducing Kernel Hilbert Spaces: Stochastic Gradient Descent and Laplacian Estimation"), defended at ENS-INRIA Paris-PSL in October 2020
- T. Lelièvre, PhD of Adel Ouled Said ("Analyse asymptotique des paramètres du théorème central limite fonctionnel pour une diffusion dans un flot incompressible rapide"), defended at Université de Bretagne Occidentale and Université de Sfax (Tunisie) in December 2020 (reviewer)
- G. Stoltz, PhD of Anton Martinsson ("Accelerated sampling schemes for high dimensional systems"), defended at University of Edinburgh in February 2020 (reviewer)

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

- E. Cancès, HdR of Cosmin Marinica (“Modélisation multi-échelle des défauts d’irradiation dans les métaux cubiques centrés”), defended at Université de Lille in October 2020 (chair)
- E. Cancès, HdR of Antoine Levitt (“Mathematical and numerical analysis of models of condensed-matter physics”), defended at Université Paris Est in October 2020
- E. Cancès, HdR of Virginie Ehrlacher (“Mathematical and numerical analysis of some high-dimensional and multiscale problems in materials science”), defended at University Paris Dauphine in December 2020
- E. Cancès, HdR of Robert Altmann (“Numerical methods for complex dynamical systems,”), defended at University of Augsburg (Germany) in 2020 (reviewer)
- E. Cancès, HdR of Giuseppe Di Molfetta, (“Quantum walks and their application for the simulation of transport equations”), defended at Université d’Aix-Marseille in December 2020
- V. Ehrlacher, HdR of Fabien Casenave (“Quelques méthodes de réduction de modèle et calcul intensif pour les simulations numériques de grande échelle”), defended at University Paris Sorbonne in July 2020

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

- V. Ehrlacher, Maître de conférences position, Université Paris-Sorbonne
- V. Ehrlacher, Maître de conférences position Université Gustave Eiffel
- T. Lelièvre, Professor position, Université Côte d’Azur
- T. Lelièvre, Professor position, Université de Paris
- G. Stoltz, Associate professor position, University of Aalborg

10.3 Conference participation

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

- R. Biezemans, French-German Workshop on multiscale problems, Augsburg University, June
- R. Biezemans, CAN-J 2020, Online, December
- S. Boyaval, Lille weekly seminar in applied mathematics
- S. Boyaval, BIRS workshop "Multiscale Models for Complex Fluids: Modeling and Analysis"
- E. Cancès, Mathematics colloquium, University of Toulouse, January

- V. Ehrlacher, Applied Mathematics seminar, University of Besançon, January
- V. Ehrlacher, Applied Mathematics seminar, TU München, January
- V. Ehrlacher, EMC2 seminar, University Paris-Sorbonne, February
- V. Ehrlacher, "Mathematics of reduced-order models" workshop, ICERM, Providence (USA), February
- V. Ehrlacher, Séminaire Laboratoire Jacques-Louis Lions, Université Paris-Sorbonne, June
- V. Ehrlacher, Séminaire of the INRIA MOKAPLAN Team, June
- V. Ehrlacher, Applied mathematics colloquium of the University of Mainz (Germany), July
- V. Ehrlacher, Applied mathematics seminar of the University of Massachussets (USA), September
- V. Ehrlacher, Séminaire AN-EDP du Laboratoire de Mathématiques d'Orsay, September
- V. Ehrlacher, One World Numerical Analysis Seminar Series, October
- O. Gorynina, First workshop of the Mathematical center in Akademgorodok, Novosibirsk, Russia, July-August
- O. Gorynina, CAN-J, Online, December
- O. Gorynina, Inria's Junior Seminar, December
- R. Goudey, CAN-J, Online, December
- M. Herbst, 1st GDR NBODY meeting, Lille, France, January
- M. Herbst, EMC2 Seminar, Jussieu, Paris, France, June
- M. Herbst, JuliaCon 2020, Online, July
- M. Herbst, Faraday Discussions: New horizons in density functional theory, Cambridge, September
- M. Herbst, GAMM-MOANSI Meeting, Online, September
- M. Herbst, Theoretical Chemistry group seminar, Universität Braunschweig, Braunschweig, Germany, October
- M. Herbst, Scientific computing seminar, Universität Kaiserslautern, Germany, December
- G. Kemlin, AlgDynQua Workshop, CIRM, Marseille, France, September
- G. Kemlin, GAMM-MOANSI Meeting, Online, September
- G. Kemlin, EMC2 Seminar, Jussieu, Paris, France, October
- G. Kemlin, CAN-J, Online, December
- C. Le Bris, 19th GAMM-Seminar on Microstructures, Freiburg, Germany, January
- C. Le Bris, Opening Conference of the new NSF Institute for Mathematics and Statistics at the University of Chicago, USA, October
- F. Legoll, Workshop on Multiscale methods for deterministic and stochastic dynamics, Geneva, Switzerland, January
- F. Legoll, French-German Workshop on multiscale problems, Augsburg University, June
- F. Legoll, 26th International Domain Decomposition Conference (DD26), Online, December
- T. Lelièvre, Applied Mathematics seminar, Edinburgh, United Kingdom, January

- T. Lelièvre, Numerical Analysis seminar, Bath, United Kingdom, February
- T. Lelièvre, Statistics seminar, Bristol, United Kingdom, February
- T. Lelièvre, Bernoulli-IMS One World Symposium 2020, online, August
- T. Lelièvre, BIRS conference on Multiscale Models for Complex Fluids: Modeling and Analysis, Banff, Canada, November
- M. Ramil, IMS Bernoulli Symposium, Online, August
- M. Ramil, PréGAMM activity group, Online, September
- G. Robin, Statistics seminar, IMT, Université Paul Sabatier, January
- G. Robin, seminar, LIG, Université Grenoble Alpes, January
- G. Robin, Statistics seminar, LMO, Université Paris-Sud, January
- G. Robin, seminar, LPP, ENS de Lyon, February
- G. Robin, Statistics seminar, MAP5, Université de Paris, April
- G. Robin, Statistics seminar, LPSM, Sorbonne Université, April
- G. Robin, Statistics and Probability seminar, Laboratoire Paul Painlevé, Université de Lille, May
- G. Robin, Maths for genomics seminar, LaMME, Université d'Évry Val d'Essonne, June
- G. Robin, seminar, LIP, ENS de Lyon, June
- G. Robin, Bernoulli-IMS One World Symposium, August
- G. Stoltz, Bayes 2020, Gainesville, Florida, USA, January
- G. Stoltz, Probability group seminar, University of Bonn, January
- G. Stoltz, MAC-MIGs students seminar Edinburgh, February
- G. Stoltz, ACM seminar, University of Edinburgh, Feburary
- G. Stoltz, Hypocoercivity workshop, Heilbronn Institute, Bristol, UK, March
- G. Stoltz, Applied mathematics and computation seminar, University of Massachussetts, USA, April
- G. Stoltz, Bernoulli-IMS One World Symposium, online, August,
- U. Vaes, Applied mathematics seminar, University of Franche-Comté, November
- U. Vaes, CAN-J, Online, December

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

- M. Herbst, Introduction to plane-wave DFT and DFTK, 2h, Invited guest lecture, RWTH Aachen University, Aachen, Germany, July
- T. Lelièvre, Leverhulme Trust Research Lectures: Free energy adaptive biasing methods, Sampling measures supported on submanifolds, Splitting methods for rare event simulations, 3h, Imperial College of London, United Kingdom, February
- T. Lelièvre, Ecole d'été de mécanique théorique, "Simulation moléculaire : modèles, calcul d'énergie libre et aspects dynamiques", 7h30, Quiberon, France, September
- T. Lelièvre, Hausdorff School for Advanced Studies in Mathematics, "Sampling problems in computational statistical physics", 3h45, Bonn, Germany, September

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

- G. Kemlin, First meeting of GDR N-BODY, Lille, France, January

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

- E. Cancès, M. Herbst, A. Levitt, G. Kemlin, Mini-school on Numerical analysis of high dimensional quantum dynamics, Université Gustave Eiffel and Ecole des Ponts, France, March
- R. Benda, E. Cancès, A. Levitt, G. Kemlin, Faraday Discussions, Cambridge, September
- J. Cauvin-Vila, CAN-J 2020, December
- G. Kemlin, Mini-school on High-dimensional quantum dynamics using variational methods, Online, September

10.4 Popularization

10.4.1 Internal or external Inria responsibilities

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

10.4.2 Internal actions

- C. Le Bris has organized a research day for the students at École des Ponts on October 21st.

11 Scientific production

11.1 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.

11.2 Publications of the year

International journals

[8] A. Alfonsi, R. Coyaud, V. Ehrlacher and D. Lombardi. 'Approximation of Optimal Transport problems with marginal moments constraints'. In: *Mathematics of Computation* (2020). DOI: 10.1090/mcom/3568. URL: https://hal.archives-ouvertes.fr/hal-02128374.

[9] A. Bakhta, V. Ehrlacher and D. Gontier. 'Numerical reconstruction of the first band(s) in an inverse Hill's problem'. In: *ESAIM: Control, Optimisation and Calculus of Variations* (8th Sept. 2020). DOI: 10.1051/cocv/2019031. URL: https://hal.archives-ouvertes.fr/hal-01591133.

[10] R. Benda, G. Zucchi, E. Cancès and B. Lebental. 'Insights into the π - π interaction driven non-covalent functionalization of carbon nanotubes of various diameters by conjugated fluorene and carbazole copolymers'. In: *Journal of Chemical Physics* 152.6 (14th Feb. 2020), p. 064708. DOI: 10.1063/1.5133634. URL: https://hal.archives-ouvertes.fr/hal-02502707.

[11] X. Blanc, M. Josien and C. Le Bris. 'Precised approximations in elliptic homogenization beyond the periodic setting'. In: *Asymptotic Analysis* 116.2 (13th Jan. 2020), pp. 93–137. DOI: 10.3233/ASY-191537. URL: https://hal.archives-ouvertes.fr/hal-01958207.

[12] E. Cancès, L.-L. Cao and G. Stoltz. 'A reduced Hartree–Fock model of slice-like defects in the Fermi sea'. In: *Nonlinearity* 33.1 (1st Jan. 2020), pp. 156–195. DOI: 10.1088/1361-6544/ab4c7d/meta. URL: https://hal.archives-ouvertes.fr/hal-01891488.

[13] E. Cancès, G. Dusson, Y. Maday, B. Stamm and M. Vohralík. 'Guaranteed a posteriori bounds for eigenvalues and eigenvectors: multiplicities and clusters'. In: *Mathematics of Computation* 89.326 (30th July 2020), pp. 2563–2611. DOI: 10.1090/mcom/3549. URL: https://hal.archives-ouvertes.fr/hal-02127954.

[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* (18th Sept. 2020). DOI: 10.1093/imanum/draa044. URL: https://hal.archives-ouvertes.fr/hal-01908039.

[15] E. Cancès, V. Ehrlacher, D. Gontier, A. Levitt and D. Lombardi. 'Numerical quadrature in the Brillouin zone for periodic Schrödinger operators'. In: *Numerische Mathematik* 144 (7th Jan. 2020), pp. 479–526. DOI: 10.1007/s00211-019-01096-w. URL: https://hal.archives-ouvertes.fr/hal-01796582.

[16] E. Cancès, V. Ehrlacher, F. Legoll, B. Stamm and S. Xiang. 'An embedded corrector problem for homogenization. Part I: Theory'. In: *Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal* 18.3 (2020), pp. 1179–1209. DOI: 10.1137/18M120035X. URL: https://hal.archives-ouvertes.fr/hal-01840993.

[17] E. Cancès, V. Ehrlacher, F. Legoll, B. Stamm and S. Xiang. 'An embedded corrector problem for homogenization. Part II: Algorithms and discretization'. In: *Journal of Computational Physics* 407 (2020), p. 109254. DOI: 10.1016/j.jcp.2020.109254. URL: https://hal.archives-ouvertes.fr/hal-01903486.

[18] 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.

[19] G. Di Gesù, T. Lelièvre, D. Le Peutrec and B. Nectoux. 'The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points'. In: *Journal de Mathématiques Pures et Appliquées* 138 (June 2020), pp. 242–306. DOI: 10.1016/j.matpur.2019.06.003. URL: https://hal.archives-ouvertes.fr/hal-02383232.

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

[21] V. Ehrlacher, D. Lombardi, O. Mula and F.-X. Vialard. 'Nonlinear model reduction on metric spaces. Application to one-dimensional conservative PDEs in Wasserstein spaces'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* (2020). DOI: 10.1051/m2an/2020013. URL: https://hal.inria.fr/hal-02290431.

[22] G. Ferré, M. Rousset and G. Stoltz. 'More on the long time stability of Feynman-Kac semigroups'. In: *Stochastics and Partial Differential Equations: Analysis and Computations* (2020). DOI: 10.1007/s40072-020-00178-3. URL: https://hal.archives-ouvertes.fr/hal-01911620.

[23] G. Ferré and G. Stoltz. 'Large deviations of empirical measures of diffusions in weighted topologies'. In: *Electronic Journal of Probability* 25 (1st Oct. 2020), p. 121. DOI: 10.1214/20-EJP514. URL: https://hal.archives-ouvertes.fr/hal-02164793.

[24] P. Gkeka, G. Stoltz, A. B. Farimani, Z. Belkacemi, M. Ceriotti, J. Chodera, A. R. Dinner, A. Ferguson, J.-B. Maillet, H. Minoux, C. Peter, F. Pietrucci, A. Silveira, A. Tkatchenko, Z. Trstanova, R. Wiewiora and T. Lelièvre. 'Machine learning force fields and coarse-grained variables in molecular dynamics: application to materials and biological systems'. In: *Journal of Chemical Theory and Computation* (2nd July 2020). DOI: 10.1021/acs.jctc.0c00355. URL: https://hal.archives-ouvertes.fr/hal-02544153.

[25] M. F. Herbst and T. Fransson. 'Quantifying the error of the core-valence separation approximation'. In: *Journal of Chemical Physics* (5th Aug. 2020). DOI: 10.1063/5.0013538. URL: https://hal.archives-ouvertes.fr/hal-02571660.

[26] M. F. Herbst, A. Levitt and E. Cancès. 'A posteriori error estimation for the non-self-consistent Kohn-Sham equations'. In: *Faraday Discussions* 224 (16th June 2020), pp. 227–246. DOI: 10.1039/D0FD00048E. URL: https://hal.archives-ouvertes.fr/hal-02557871.

[27] M. F. Herbst, M. Scheurer, T. Fransson, D. R. Rehn and A. Dreuw. 'adcc: A versatile toolkit for rapid development of algebraic-diagrammatic construction methods'. In: *Wiley Interdisciplinary Reviews: Computational Molecular Science* (9th Jan. 2020). DOI: 10.1002/wcms.1462. URL: https://hal.archives-ouvertes.fr/hal-02319517.

[28] T. J. Hudson, F. Legoll and T. Lelièvre. 'Stochastic homogenization of a scalar viscoelastic model exhibiting stress-strain hysteresis'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 54.3 (1st May 2020), pp. 879–928. DOI: 10.1051/m2an/2019081. URL: https://hal.archives-ouvertes.fr/hal-01710772.

[29] F. Legoll, T. Lelièvre, K. Myerscough and G. Samaey. 'Parareal computation of stochastic differential equations with time-scale separation: a numerical convergence study'. In: *Computing and Visualization in Science* 23 (2020), p. 9. DOI: 10.1007/s00791-020-00329-y. URL: https://hal.archives-ouvertes.fr/hal-02421240.

[30] B. Leimkuhler, M. Sachs and G. Stoltz. 'Hypocoercivity properties of adaptive Langevin dynamics'. In: *SIAM Journal on Applied Mathematics* 80.3 (19th May 2020), pp. 1197–1222. DOI: 10.1137/19M1291649. URL: https://hal.archives-ouvertes.fr/hal-02273261.

[31] T. Lelièvre, G. Samaey and P. Zieliński. 'Analysis of a micro-macro acceleration method with minimum relative entropy moment matching'. In: *Stochastic Processes and their Applications* 130.6 (June 2020), pp. 3753–3801. DOI: 10.1016/j.spa.2019.10.008. URL: https://hal.archives-ouvertes.fr/hal-01680761.

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[33] 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.

[34] Z. Trstanova, B. Leimkuhler and T. Lelièvre. 'Local and Global Perspectives on Diffusion Maps in the Analysis of Molecular Systems'. In: *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 476.2233 (15th Jan. 2020). DOI: 10.1098/rspa.2019.0036. URL: https://hal.archives-ouvertes.fr/hal-02104963.

[35] T. Wang, G. Stoltz and P. Plechac. 'Convergence of the likelihood ratio method for linear response of non-equilibrium stationary states'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* (2020). DOI: 10.1051/m2an/2020050. URL: https://hal.archives-ouvertes.fr/hal-02385582.

International peer-reviewed conferences

[36] L. Pillaud-Vivien, F. Bach, T. Lelièvre, A. Rudi and G. Stoltz. 'Statistical Estimation of the Poincaré constant and Application to Sampling Multimodal Distributions'. In: *Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics*. AISTATS 2020 : 23rd International Conference on Artificial Intelligence and Statistics. Palermo / Virtual, Italy, Aug. 2020. URL: https://hal.archives-ouvertes.fr/hal-02327453.

Doctoral dissertations and habilitation theses

[37] S. Siraj-Dine. 'Dynamics of electrons in 2D materials'. Université Paris-Est; Inria, 17th Dec. 2020. URL: https://hal.archives-ouvertes.fr/tel-03164359.

Reports & preprints

[38] A. Alfonsi, R. Coyaud and V. Ehrlacher. *Constrained overdamped Langevin dynamics for symmetric multimarginal optimal transportation*. 4th Feb. 2021. URL: https://hal.archives-ouvertes.fr/hal-03131763.

[39] M. Baudel, A. Guyader and T. Lelièvre. *On the Hill relation and the mean reaction time for metastable processes*. 25th Aug. 2020. URL: https://hal.archives-ouvertes.fr/hal-02921281.

[40] E. Bernard, M. Fathi, A. Levitt and G. Stoltz. *Hypocoercivity with Schur complements*. 1st Dec. 2020. URL: https://hal.archives-ouvertes.fr/hal-03033217.

[41] S. Boyaval. *Viscoelastic flows of Maxwell fluids with conservation laws*. 30th July 2020. URL: https://hal-enpc.archives-ouvertes.fr/hal-02908379.

[42] S. Boyaval, S. Martel and J. Reygner. *Finite-Volume approximation of the invariant measure of a viscous stochastic scalar conservation law*. 6th Jan. 2021. URL: https://hal.archives-ouvertes.fr/hal-02291253.

[43] C. Cancès, V. Ehrlacher and L. Monasse. *Finite Volumes for the Stefan-Maxwell Cross-Diffusion System*. 20th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02902672.

[44] E. Cancès, R. Coyaud and L. R. Scott. *Van der Waals interactions between two hydrogen atoms: The next orders*. 9th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02894550.

[45] E. Cancès, C. Fermanian Kammerer, A. Levitt and S. Siraj-Dine. *Coherent electronic transport in periodic crystals*. 9th Nov. 2020. URL: https://hal.archives-ouvertes.fr/hal-02468564.

[46] E. Cancès, G. Kemlin and A. Levitt. *Convergence analysis of direct minimization and self-consistent iterations*. 27th Oct. 2020. URL: https://hal.inria.fr/hal-02546060.

[47] M.-S. Dupuy and A. Levitt. *Finite-size effects in response functions of molecular systems*. 18th Feb. 2021. URL: https://hal.archives-ouvertes.fr/hal-03145143.

[48] V. Ehrlacher, M. Fuente-Ruiz and D. Lombardi. *CP-TT: using TT-SVD to greedily construct a Canonical Polyadic tensor approximation*. 24th Nov. 2020. URL: https://hal.inria.fr/hal-03018646.

[49] V. Ehrlacher, T. Lelièvre and P. Monmarché. *Adaptive force biasing algorithms: new convergence results and tensor approximations of the bias*. 20th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02314426.

[50] V. Ehrlacher, G. Marino and J.-F. Pietschmann. *Existence of weak solutions to a cross-diffusion Cahn-Hilliard type system*. 3rd July 2020. URL: https://hal.archives-ouvertes.fr/hal-02888479.

[51] S. Gaucher, O. Klopp and G. Robin. *Outliers Detection in Networks with Missing Links*. 29th Nov. 2020. URL: https://hal.archives-ouvertes.fr/hal-02386940.

[52] O. Gorynina, C. Le Bris and F. Legoll. *Some remarks on a coupling method for the practical computation of homogenized coefficients*. 21st May 2020. URL: https://hal.archives-ouvertes.fr/hal-02614896.

[53] M. F. Herbst and A. Levitt. *Black-box inhomogeneous preconditioning for self-consistent field iterations in density functional theory*. 4th Sept. 2020. URL: https://hal.archives-ouvertes.fr/hal-02929951.

[54] A. Iacobucci, S. Olla and G. Stoltz. *Thermo-mechanical transport in rotor chains*. 22nd July 2020. URL: https://hal.archives-ouvertes.fr/hal-02904454.

[55] T. Lelièvre, D. Le Peutrec and B. Nectoux. *The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 2*. 11th Dec. 2020. URL: https://hal.archives-ouvertes.fr/hal-03058529.

[56] 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.

[57] T. Lelièvre, M. Ramil and J. Reygner. *A probabilistic study of the kinetic Fokker-Planck equation in cylindrical domains*. 21st Oct. 2020. URL: https://hal.archives-ouvertes.fr/hal-02974421.

[58] T. Lelièvre, G. Stoltz and W. Zhang. *Multiple projection MCMC algorithms on submanifolds*. 23rd Mar. 2020. URL: https://hal.archives-ouvertes.fr/hal-02515267.

[59] 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.