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2022 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

Inria

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Project-Team MATHERIALS

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 2022 has gained support for GPU acceleration, norm-conserving pseudopotentials, and many other smaller features. It has been used for several publications both inside and outside the project-team.

URL: http://dftk.org

Contact: Antoine Levitt

6 New results

6.1 Electronic structure calculations

Participants: Andrea Bordignon, Eric Cancès, Virginie Ehrlacher, Louis Garrigue, Gaspard Kemlin, Antoine Levitt, Eloïse Letournel, Solal Perrin-Roussel, Etienne Polack, Laurent Vidal.

6.1.1 Density functional theory

A track of the project-team's activity this year has been the investigation of continuum eigenstates, as opposed to the bound states that form much of the project-team's usual focus. Such states are relevant to the study of processes where electrons propagate away from the system under consideration, such as ionization. They are delocalized, complicating their discretization. In [35] and [36], together with colleagues from the Laboratoire de Chimie Théorique at Sorbonne Université, É. Cancès and A. Levitt have proposed a method to compute the photoionization spectrum for atoms in time-dependent density functional theory (TDDFT) in the Sternheimer formalism. This method, inspired by similar schemes in numerical wave propagation, employs an analytic Dirichlet-to-Neumann map to impose correct boundary conditions on the Sternheimer equations, which appears mathematically as a perturbation of an Helmholtz equation with a Coulomb potential. In [56], E. Letournel and A. Levitt, together with physicist colleagues from CEA Grenoble, have proposed a method to compute electronic resonances in crystals with defects. The method involves the computation of analytic continuations of Green functions of periodic operators, which is accomplished by a complex deformation of the Brillouin zone.

E. Cancès, G. Kemlin and A. Levitt have studied the numerical properties of response computations in density functional theory at finite temperature. They have proposed a method based on a Schur complement to increase the stability and efficiency of iterative solvers for the Sternheimer equations [48].

Together with D. Gontier (U. Paris Dauphine and ENS Paris), E. Cancès and L. Garrigue provided a formal derivation of a reduced model for twisted bilayer graphene (TBG) from Density Functional Theory. This derivation is based on a variational approximation of the TBG Kohn-Sham Hamiltonian and asymptotic limit techniques. In contrast with other approaches, it does not require the introduction of an intermediate tight-binding model. The so-obtained model is similar to that of the Bistritzer-MacDonald (BM) model but contains additional terms. Its parameters can be easily computed from Kohn-Sham calculations on single-layer graphene and untwisted bilayer graphene with different stackings. It allows one in particular to estimate the parameters w_{AA} and w_{AB} of the BM model from first-principles. The resulting numerical values, namely $w_{\mathrm{AA}} = w_{\mathrm{AB}} \simeq 126$ meV for the experimental interlayer mean distance are in good agreement with the empirical values $w_{\mathrm{AA}} = w_{\mathrm{AB}} = 110$ meV obtained by fitting to experimental data. We also show that if the BM parameters are set to $w_{\mathrm{AA}} = w_{\mathrm{AB}} \simeq 126$ meV, the BM model is an accurate approximation of this new reduced model.

With G. Dusson (CNRS and U. of Franche-Comté) E. Cancès, G. Kemlin and L. Vidal proposed in [46] general criteria to construct optimal atomic centered basis sets in quantum chemistry. They focuses in particular on two criteria, one based on the ground-state one-body density matrix of the system and the other based on the ground-state energy. The performance of these two criteria was numerically tested and compared on a parametrized eigenvalue problem, which corresponds to a one-dimensional toy version of the ground-state dissociation of a diatomic molecule.

In solid state physics, electronic properties of crystalline materials are often inferred from the spectrum of periodic Schrödinger operators. As a consequence of Bloch's theorem, the numerical computation of electronic quantities of interest involves computing derivatives or integrals over the Brillouin zone of so-called energy bands, which are piecewise smooth, Lipschitz continuous periodic functions obtained by solving a parametrized elliptic eigenvalue problem on a Hilbert space of periodic functions. Classical discretization strategies for resolving these eigenvalue problems produce approximate energy bands that are either non-periodic or discontinuous, both of which cause difficulty when computing numerical derivatives or employing numerical quadrature. In a paper with M. Hassan (Sorbonne Université) [47], E. Cancès and L. Vidal studied an alternative discretization strategy based on an ad hoc operator modification approach. While specific instances of this approach have been proposed in the physics literature, they introduced a systematic formulation of this operator modification approach. They derived *a priori* error estimates for the resulting energy bands and showed that these bands are periodic and can be made arbitrarily smooth (away from band crossings) by adjusting suitable parameters in the operator modification approach.

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 funda-

mental 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 Tensor methods

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 [20], 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.

6.2 Computational statistical physics

Participants: Noé Blassel, Shiva Darshan, Olga Gorynina, Frédéric Legoll, Tony Lelièvre, Antoine Levitt, Thomas Pigeon, Mohamad Rachid, Régis Santet, Renato Spacek, Gabriel Stoltz, Urbain Vaes.

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 improvement of techniques to sample the configuration space; (ii) the study of simulation methods to efficiently simulate nonequilibrium systems; (iii) the sampling of dynamical properties and rare events; (iv) the use and development of machine learning tools in molecular dynamics and sampling; (v) the use of particle methods for sampling and optimization.

6.2.1 Sampling of the configuration space

There is still a need to improve techniques to sample the configuration space. In [25], Tony Lelièvre together with Lucie Delemotte (KTH, Sweden), J. Hénin (IBPC, France), Michael Shirts (University of Colorado, USA) and Omar Valsson (MPI Mainz, Germany) provide on overview of enhanced sampling algorithms. These algorithms have emerged as powerful methods to extend the potential of molecular dynamics simulations and allow the sampling of larger portions of the configuration space of complex systems. This "living" review is intended to be updated to continue to reflect the wealth of sampling methods as they emerge in the literature.

6.2.2 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. G. Stoltz reviewed in [66] the motivations and mathematical framework involved in the computation of transport coefficients, with a particular emphasis on the numerical analysis of the estimators at hand.

The main limitations of usual methods to compute transport coefficients is the large variance of the estimators, which motivates searching for dedicated variance reduction strategies. Such a method was proposed by G. Pavliotis (Imperial College London, United-Kingdom), G. Stoltz and U. Vaes in the context of the estimation of the mobility via Einstein's method in [65], although the method can be adapted to other transport coefficients. The fundamental idea is to approximate the solution to some Poisson equation determining the transport coefficient, and relying on Ito calculus to construct a random variable strongly correlated to the square displacement from the position at origin. The motivation of this work was to estimate the mobility of underdamped Langevin dynamics of two dimensional systems for low values of the friction, in an attempt to (in)validate physical conjectures about the divergence of the mobility as the friction goes to zero.

6.2.3 Sampling dynamical properties and rare events

Sampling trajectories which link metastable states of the target probability measure, and estimating the associated transition rates from one metastable state to another, is a difficult task, which requires dedicated numerical methods. Various works along these lines were preprinted this year.

In [62], Tony Lelièvre, together with Mouad Ramil (Seoul National University, South Korea) and Julien Reygner (CERMICS, France), propose and analyze a simple and complete numerical method to estimate statistics of transitions between metastable states for the Langevin dynamics, based on the so-called Hill relation. More precisely, they prove the Hill relation in the fairly general context of positive Harris recurrent chains, and show that this formula applies to the Langevin dynamics. Moreover, they provide an explicit expression of the invariant measure involved in the Hill relation for the Langevin dynamics, and describe an elementary exact simulation procedure.

In [61], Tony Lelièvre, together with Boris Nectoux (Laboratoire de Mathématiques Blaise Pascal, France) and Dorian Le Peutrec (Institut Denis Poisson, France), conclude a series of papers which aim at providing firm mathematical grounds to jump Markov models which are used to model the evolution of molecular systems, as well as to some numerical methods which use these underlying jump Markov models to efficiently sample metastable trajectories of the overdamped Langevin dynamics. More precisely, using the quasi-stationary distribution approach to analyze the metastable exit from the basin of attraction of a local minimum of the potential energy function, they prove that the exit event (exit position and exit time) of the overdamped Langevin dynamics in the small temperature regime can be accurately modeled by a jump Markov model parameterized by the Eyring–Kramers rates. From a mathematical viewpoint, the proof relies on tools from the semiclassical analysis of Witten Laplacians on bounded domains. The main difficulty is that, since they consider as metastable states the basins of attraction of the local minima of the energy, the exit regions are neighborhoods of saddle points of the energy, and many standard techniques (such as WKB approximations) cannot handle critical points on the boundary.

In [34], Tony Lelièvre, together with Mouad Ramil (Seoul National University, South Korea) and Julien Reygner (CERMICS, France), give an overview of some of the results obtained during the PhD work of Mouad Ramil. More precisely, the paper provides a self-contained analysis of the Parallel Replica algorithm applied to the Langevin dynamics. This algorithm was designed to efficiently sample metastable trajectories relying on a parallelization in time technique. The analysis relies on results on the existence of quasi-stationary distributions of the Langevin dynamics in domains bounded in positions. The article also contains some discussions about the overdamped limit of the quasi-stationary distribution.

Another approach to sampling reactive trajectories is to allow for longer integration times, thanks to dedicated algorithmic developments. In [58], Frédéric Legoll and Tony Lelièvre, together with Olga Gorynina (WSL-SLF, Switzerland) and Danny Perez (Los Alamos National Laboratory, USA) numerically investigate an adaptive version of the parareal algorithm in the context of molecular dynamics. This method allows to more efficiently integrate in time the dynamics under consideration. The parareal algorithm uses a family of machine-learning spectral neighbor analysis potentials (SNAP) as fine, ref-

erence, potentials and embedded-atom method potentials (EAM) as coarse potentials. The numerical results (obtained using LAMMPS, a very broadly used software within the materials science community) demonstrate significant computational gains when using the adaptive parareal algorithm in comparison to a sequential integration of the Langevin dynamics.

6.2.4 Machine-learning approaches in molecular dynamics

Together with G. Robin (CNRS & Université d'Evry), I. Sekkat (CERMICS) and G. Victorino Cardoso (CMAP, Ecole polytechnique & IHU LIRYC), T. Lelièvre and G. Stoltz considered in [63] how to generate reactive trajectories linking two metastable states. More precisely, they investigated the capabilities and limitations of supervised and unsupervised methods based on variational autoencoders to generate such paths. Bottleneck autoencoders are however somewhat limited in describing reactive paths, which is why alternative approaches based on an importance sampling function determined by a reinforcement learning strategy were also studied. The potential of the approach was demonstrated on simple low dimensional examples.

A. Levitt and G. Stoltz studied in [17] with F. Bottin (CEA/DAM), A. Castellano (CEA/DAM), J. Bouchet (CEA Cadarache) how to train simple empirical force fields on ab-initio data, in order to reproduce thermodynamic properties at finite temperature. The method iterates between exploration phases where new configurations are efficiently sampled and generated, using the current version of the simple empirical potential at hand, and a training phase where the empirical potential is updated with new ab-initio data. Thermodynamic consistency is ensured via some nonlinear reweighting procedure.

6.2.5 Interacting particle methods for sampling

In some situations, stochastic numerical methods can be made more efficient by using various replicas of the system. The ensemble Kalman filter is a methodology for incorporating noisy data into complex dynamical models to enhance predictive capability. It is widely adopted in the geophysical sciences, underpinning weather forecasting for example, and is starting to be used throughout the sciences and engineering. For high dimensional filtering problems, the ensemble Kalman filter has a robustness that is not shared by the particle filter; in particular it does not suffer from weight collapse. However, there is no theory which quantifies its accuracy as an approximation of the true filtering distribution, except in the Gaussian setting. In order to address this issue, 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) provided in [51] an analysis of the accuracy of the ensemble Kalman filter beyond the Gaussian setting. The analysis is developed for the mean field ensemble Kalman filter, which can be rewritten in terms of maps on probability measures. These maps are proved to be locally Lipschitz in an appropriate weighted total variation metric, which enables to demonstrate that, if the true filtering distribution is close to Gaussian after appropriate lifting to the joint space of state and data, then it is well approximated by the ensemble Kalman filter.

In [60], Tony Lelièvre and Panos Parpas (Imperial College London, United Kingdom) introduce a new stochastic algorithm to locate the index-1 saddle points of a potentiel energy function. Finding index-1 saddle points is crucial to build kinetic Monte Carlo models. These models describe the evolution of the molecular system by a jump Markov model with values in the local minima of the energy function, the jumps between these states being parameterized by the Eyring–Kramers laws. This paramaterization thus requires to identify the index-1 saddle points which connect local minima. The proposed algorithm can be seen as an equivalent of the stochastic gradient descent which is a natural stochastic process to locate local minima. It relies on two ingredients: (i) the concentration properties on index-1 saddle points of the first eigenmodes of the Witten Laplacian on 1-forms and (ii) a probabilistic representation of the solution to a partial differential equation involving this differential operator. The resulting algorithm is an interacting particle system, where the particles populate neighborhoods of the index-1 saddle points. Numerical examples on simple molecular systems illustrate the efficacy of the proposed approach.

6.3 Homogenization

Participants: Yves Achdou, Rutger Biezemans, Rémi Goudey, Claude Le Bris, Albéric Lefort, Frédéric Legoll, Alexei Lozinski, Simon Ruget.

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, has also been the topic of the PhD thesis of R. Goudey, defended this year. 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 that 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:

- In line with the first direction, and in the context of the "délégation" of Y. Achdou (on partial leave from Université Paris-Cité), C. Le Bris has studied in [38] a homogenization theory for a general first order Hamilton-Jacobi equation in the presence of defects. The study extends to the fully nonlinear setting previous studies performed by X. Blanc, C. Le Bris and P.-L. Lions in the linear (mostly elliptic) setting. It also extends the class of problems previously addressed by Y. Achdou and his collaborators in the periodic setting only. The study complements, in a slightly different but related regime, results obtained a few years ago by P.-L. Lions and P. Souganidis.

- The works [23] (where defects become increasingly rare but do not decay at infinity) and [24], both by R. Goudey, fall within the second direction. Defects in the form of interfaces between two perfectly periodic materials also fall within this research direction. In the same vein, R. Goudey and C. Le Bris have studied in [59] the homogenized limit of a Schroedinger equation with an highly oscillatory potential, when the latter potential belongs to a general class of non-periodic functions that are global perturbations of a periodic function. Such a class of functions is reminiscent of classes constructed two decades ago, in collaboration with X. Blanc and P.-L. Lions, in the context of thermodynamic limit problems. The result obtained may be seen as a first step toward similar studies for other types of equations.

A monograph that summarizes the contributions of the project-team on this topic, along with a general perspective on the field, has been written by C. Le Bris, in collaboration with X. Blanc. The French and English versions of this textbook are respectively in print for the series "Maths & Applications" and "MS&A, Modeling, Simulation and Applications", both at Springer. In addition, C. Le Bris has written a short text that summarizes the major results obtained and that will be published in the "Séminaire Laurent Schwartz 2022-2023 volume".

6.3.2 Inverse multiscale problems

In the context of the PhD of S. Ruget, which started this year, C. Le Bris and F. Legoll have pursued their work on the question of how to determine the homogenized coefficient of a multiscale problem without explicitly performing an homogenization approach. This work is a follow-up on earlier works over the years in collaboration with K. Li, S. Lemaire and O. Gorynina, in the case of a diffusion equation with highly oscillatory diffusion coefficients. Here, this question is revisited in the setting of Schroedinger equations with rapidly oscillating potentials. The motivation for this work is that Schroedinger equations, besides their own interest, show some *specific* features (in comparison e.g. to diffusion equations) bringing hope that further progress can be achieved. To address these questions is the objective of the PhD of S. Ruget.

6.3.3 Multiscale Finite Element approaches

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

The MsFEM 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. This basis differs from standard (e.g. polynomial) bases that are generally used in existing legacy codes in industry. As a result, the MsFEM approach is *intrusive*, which hinders its adoption in industrial (and, more generally, non-academic) environments.

To overcome this obstacle, R. Biezemans, C. Le Bris and F. Legoll, together with A. Lozinski (in delegation in the team for the first half of the year), have designed modified MsFEM approaches that allow for a non-intrusive implementation, i.e., using any existing legacy code for a Galerkin approximation on a piecewise affine basis. The key principles of the approach are presented in [12]. The technique is reminiscent of the classical approach to homogenization: "corrector" functions are computed in each element of the mesh, from which slowly varying effective coefficients are computed. This leads to an effective PDE that can indeed be solved by standard finite element approaches.

A more comprehensive study of the non-intrusive MsFEM technique has subsequently been finalized in [41], where R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski show that the non-intrusive approach can be extended to a wide variety of problems and more advanced, state of the art MsFEM variants. Indeed, this work provides non-intrusive MsFEMs for general linear second order PDEs, and with various choices for the local problems, in particular the use of an oversampling technique (where the local problems are solved on domains that are larger than a single mesh element) and a Crouzeix-Raviart MsFEM. This work is also the first to propose and test a new MsFEM variant, namely by developing an oversampling technique for the Crouzeix-Raviart MsFEM. Further, it is proved there that the non-intrusive approach is equivalent to the original MsFEM for a Petrov-Galerkin variant of the MsFEM with affine test functions, and for the Galerkin MsFEM, numerical experiments show that the non-intrusive approach preserves the same accuracy as the original MsFEM.

A second research direction pursued in the PhD of R. Biezemans is the question of how to design accurate MsFEM approaches for various types of equations, beyond the purely diffusive case, and in particular for 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 by R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. The main results are being prepared for publication, showing in particular the stabilization of an MsFEM with weak continuity conditions of

Crouzeix-Raviart type by adding specific bubble functions, satisfying the same type of weak boundary conditions, to the approximation space.

Finally, R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski have continued their study of the convergence analysis of MsFEMs. Indeed, despite the fact that MsFEM approaches have been proposed more than two decades ago, it turns out that not all specific settings are covered by the numerical analyses existing in the literature. The research team have previously extended the analysis of MsFEM to the case of rectangular meshes and that of periodic diffusion coefficients that are not necessarily Hölder continuous. An ongoing research effort is devoted to further generalizing the analysis to non-periodic settings and to provide a fully rigorous convergence proof of various MsFEMs with the oversampling technique.

In the context of the PhD of A. Lefort, which started this year, C. Le Bris and F. Legoll have undertaken the study of a multiscale, time-dependent, reaction-diffusion equation. This problem is different from the equations previously studied by the team by the fact that it is *time-dependent* and that it includes a *reaction term* (in addition to the diffusive term). From a numerical perspective, two difficulties are present in the problem. First, the coefficients of the equation (and therefore the solution) oscillate at a small spatial scale. In addition, the problem in time is stiff: a standard marching scheme such as the backward Euler scheme would need a small time-step to provide an accurate solution. Several directions of research have been identified, such as establishing the homogenized limit of the problem and designing efficient numerical approaches.

6.4 Various topics

6.4.1 Complex fluids

Participants: Sébastien Boyaval.

In 2022, S. Boyaval has improved the mathematical understanding of the symmetric-hyperbolic system of conservation laws introduced in 2020 to model non-Newtonian fluids [43]. Precisely, he has established rigorously the structural stability of the model: Newtonian fluids are recovered in one asymptotic limit of the PDE parameters, while the elastodynamics of hyperelastic materials is also recovered in another asymptotic limit of the parameters [44]. Researches are pursued for efficient numerical simulations.

6.4.2 Model-order reduction methods

Participants: Jad Dabaghi, Virginie Ehrlacher.

The objective of a reduced-order model reduction method is the following: it may sometimes be very expensive from a computational point of view to simulate the properties of a complex system described by a complicated model, typically a set of PDEs. This cost may become prohibitive in situations where the solution of the model has to be computed for a very large number of values of the parameters involved in the model. Such a parametric study is nevertheless necessary in several contexts, for instance when the value of these parameters has to be calibrated so that numerical simulations give approximations of the solutions that are as close as possible to some measured data. A reduced-order model method then consists in constructing, from a few complex simulations which were performed for a small number of well-chosen values of the parameters, a so-called *reduced model*, much cheaper and quicker to solve from a numerical point of view, and which enables to get an accurate approximation of the solution of the model for any other values of the parameters.

In [64], together with Idrissa Niakh, Guillaume Drouet (EDF) and Alexandre Ern (SERENA), a new stable model reduction method for linear variational inequalities with parameter-dependent constraints. The method was applied for the reduction of various parametrized contact mechanical problems.

In [39], a new model-order reduction method based on optimal transport theory was investigated by Virginie Ehrlacher together with B. Battisti, T. Blickhan (Garching, Germany), G. Enchéry (IFPEN), D.

Lombardi (INRIA COMMEDIA) and O. Mula (Eindhoven University). This approach, based on the use of Wasserstein barycenters, was successfully applied to the reduction of parametrized porous medium flow problems.

6.4.3 Cross-diffusion systems

Participants: Jean Cauvin-Vila, Jad Dabaghi, Virginie Ehrlacher.

Cross-diffusion systems are nonlinear degenerate parabolic systems which naturally arise in diffusion models of multi-species mixtures in a wide variety of applications: tumor growth, population dynamics, materials science etc. In materials science they typically model the evolution of local densities or volumic fractions of chemical species within a mixture.

In [53], Jad Dabaghi and Virginie Ehrlacher investigated a new structure-preserving model reduction methods for parametrized cross-diffusion systems. The proposed numerical method is analyzed from a mathematical point of view and proved to satisfy the same mathematical properties as the high fidelity modelity (preserving for instance the non-negativeness of the solutions). The method consists in introducing an appropriate nonlinear transformation of the set of solutions, based on the use of entropy variables associated to the system, before applying reduced-basis techniques to the parametrized problem.

In [52], Jean Cauvin-Vila, Virginie Ehrlacher and Amaury Hayat analyzed from a mathematical point of view the boundary stabilization of one-dimensional (linearized) cross-diffusion system in a moving domain. They prove that the system can be stabilized in any arbitrary finite time by using the so-called backstepping stabilization technique.

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, SAFRANTech. 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 is one of the PIs of the 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 International research visitors

8.2.1 Visits of international scientists

Danny Perez (Los Alamos National Laboratory, USA) visited the team in September and October. This was the opportunity to discuss new research directions for accelerated molecular dynamics algorithms.

8.2.2 Visits to international teams

Research stays abroad

Claude Le Bris

Visited institution: Freie Universitat, Humboldt-Universitat, Technische Universitat, Weierstrass Institute for Applied Analysis and Stochastics, and Zuse Institute Berlin

Country: Germany

Dates: November-December

Context of the visit: MATH+ Distinguished Visiting Scholar, Berlin Mathematics Research Center

Mobility program/type of mobility: Research stay

8.3 European initiatives

8.3.1 H2020 projects

EMC2

Participants: Noé Blassel, Eric Cancès, Shiva Darshan, Gaspard Kemlin, Alfred Kirsch, Eloïse Letournel, Antoine Levitt, Solal Perrin-Roussel, Régis Santet, Renato Spacek, Gabriel Stoltz, Laurent Vidal, Urbain Vaes.

EMC2 project on cordis.europa.eu

Title: Extreme-scale Mathematically-based Computational Chemistry

Duration: From September 1, 2019 to February 28, 2026

Partners:

- Institut National de Recherche en Informatique et Automatique (INRIA), France
- École Nationale des Ponts et Chaussées (ENPC), France
- Centre National de la Recherche Scientifique (CNRS), France
- Sorbonne Université, France

Inria contact: Laura Grigori (Inria Alpines)

Coordinators: Eric Cancès (ENPC), Laura Grigori (Inria Alpines), Yvon Maday (Sorbonne Université), J.-P. Piquemal (Sorbonne Université)

Summary: Molecular simulation has become an instrumental tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. It will allow to propose de novo design of e.g. new drugs or materials provided that the efficiency of underlying software is accelerated by several orders of magnitude.

The ambition of the EMC2 project is to achieve scientific breakthroughs in this field by gathering the expertise of a multidisciplinary community at the interfaces of four disciplines: mathematics, chemistry, physics, and computer science. It is motivated by the twofold observation that, i) building upon our collaborative work, we have recently been able to gain efficiency factors of up to 3 orders of magnitude for polarizable molecular dynamics in solution of multi-million atom systems, but this is not enough since ii) even larger or more complex systems of major practical interest (such as solvated biosystems or molecules with strongly-correlated electrons) are currently mostly intractable in reasonable clock time. The only way to further improve the efficiency of the solvers, while preserving accuracy, is to develop physically and chemically sound models,

mathematically certified and numerically efficient algorithms, and implement them in a robust and scalable way on various architectures (from standard academic or industrial clusters to emerging heterogeneous and exascale architectures).

EMC2 has no equivalent in the world: there is nowhere such a critical number of interdisciplinary researchers already collaborating with the required track records to address this challenge. Under the leadership of the 4 PIs, supported by highly recognized teams from three major institutions in the Paris area, EMC2 will develop disruptive methodological approaches and publicly available simulation tools, and apply them to challenging molecular systems. The project will strongly strengthen the local teams and their synergy enabling decisive progress in the field.

TIME-X

Participants: Olga Gorynina, Frédéric Legoll, Tony Lelièvre.

TIME-X project on openaire.eu

Title: TIME parallelisation: for eXascale computing and beyond

Duration: From April 1, 2021 to March 31, 2024

Partners:

- KU Leuven, Belgium
- École Nationale des Ponts et Chaussées (ENPC), France
- Sorbonne Université, France
- University of Wuppertal, Germany
- Forschungszentrum Jülich, Germany
- Universita della Svizzera Italiana, Switzerland
- University of Geneva, Switzerland
- TU Darmstadt, Germany
- TU Munich, Germany
- Hamburg University of Technology, Germany

Coordinators: Yvon Maday (Sorbonne Université) and Giovanni Samaey (KU Leuven)

Summary: Recent successes have established the potential of parallel-in-time integration as a powerful algorithmic paradigm to unlock the performance of Exascale systems. However, these successes have mainly been achieved in a rather academic setting, without an overarching understanding. TIME-X will take the next leap in the development and deployment of this promising new approach for massively parallel HPC simulation, enabling efficient parallel-in-time integration for real-life applications. We will:

(i) provide software for parallel-in-time integration on current and future Exascale HPC architectures, delivering substantial improvements in parallel scaling;

(ii) develop novel algorithmic concepts for parallel-in-time integration, deepening our mathematical understanding of their convergence behaviour and including advances in multi-scale methodology;

(iii) demonstrate the impact of parallel-in-time integration, showcasing the potential on problems that, to date, cannot be tackled with full parallel efficiency in three diverse and challenging application fields with high societal impact: weather and climate, medicine and fusion.

To realise these ambitious, yet achievable goals, the inherently inter-disciplinary TIME-X Consortium unites top researchers from numerical analysis and applied mathematics, computer science

and the selected application domains. Europe is leading research in parallel-in-time integration. TIME-X unites all relevant actors at the European level for the first time in a joint strategic research effort. A strategic investment from the European Commission would enable taking the necessary next step: advancing parallel-in-time integration from an academic/mathematical methodology into a widely available technology with a convincing proof of concept, maintaining European leadership in this rapidly advancing field and paving the way for industrial adoption.

8.4 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 (2020-2025) 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 the PI of the ANR Tremplin-ERC project HighDim (2022-2025) which focuses on the development of efficient numerical methods for the resolution of high-dimensional partial Differential Equations, using machine learning and neural networks.
- V. Ehrlacher is a member of the ANR project ADAPT (2018-2023), PI: D. Lombardi, Inria COMMEDIA team-project. This project is concerned with the parallelization of tensor methods for high-dimensional problems.
- 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.
- G. Stoltz is the PI of the ANR project SINEQ (2022-2025), whose aim is to improve the mathematical understanding and numerical simulation of nonequilibrium stochastic dynamics, in particular their linear response properties. This project involves researchers from CEREMADE, Université Paris-Dauphine and the SIMSART project-team of Inria Rennes.

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),
- IAMAT (Artificial Intelligence for MATerials),
- 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

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.

E. Cancès

- is a member of the MFO scientific committee (Oberwolfach),
- 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-),
- is a member of the editorial board of the Springer series "Mathematics and Molecular Modeling",
- is a member of the committees of the GDRs DynQua, NBody, and REST,
- has co-organized the IPAM program on "Advancing Quantum Mechanics with Mathematics and Statistics" (UCLA, March-June 2022), as well as two workshops in this program, a mini-school on mathematics for theoretical chemistry and physics (Jussieu, May 30-June 1), the 2022 DFTK summer school (Jussieu, Aug. 29-31), and the 2022 Solid Math workshop (Trieste, Sept. 6-9).

V. Ehrlacher

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

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-), Communications in Partial Differential Equations (2022-), 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-),
- 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.

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 review panel for research area proposals for several German universities.

T. Lelièvre

- is a member of the editorial boards of Foundations of Computational Mathematics, 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 (until October 2022),
- is the head of the applied mathematics department (CERMICS) at Ecole des Ponts,
- has co-organized the workshop Machine Learning-Assisted Sampling for Scientific Computing - Applications in Physics, Collège de France - site Ulm, Paris, October 3-4th 2022 (with M. Gabrié and V. de Bortoli).

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),
- is a member of the executive board of GDR IAMAT,
- co-organized with M. Bianciotto (Sanofi), F. Gervasio (UCL London), P. Gkeka (Sanofi), C. Hartmann (BTU Cottbus), a CECAM workshop on “Chasing CVs using Machine Learning: from methods development to biophysical applications”, which took place at Inria Paris from June 28th to 30th.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

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, J. Cauvin-Vila, V. Ehrlacher, E. Letournel, R. Santet, G. Stoltz)
- Équations aux dérivées partielles: approches variationnelles, 15h (R. Biezemans, J. Cauvin-Vila, F. Legoll, R. Santet)
- Probabilités, 24h (N. Blassel)
- Hydraulique numérique, 15h (S. Boyaval)
- Outils mathématiques pour l’ingénieur (E. Cancès: 18h, V. Ehrlacher, E. Letournel, F. Legoll, A. Levitt, G. Stoltz, L. Vidal: 9h)
- Mécanique quantique, 15h (E. Cancès, A. Levitt)
- Méthodes numériques pour les problèmes en grande dimension, 17h30 (V. Ehrlacher)
- Pratique du calcul scientifique, 15h (A. Levitt)

- Initiation au travail en projet, 13h (R. Santet, R. Spacek, L. Vidal)
- PAMS project, 16h (R. Spacek)

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

- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès)
- Statistiques numériques et analyse de données, 26h (S. Darshan)
- Problèmes d'évolution, 36h (V. Ehrlacher, F. Legoll)
- Projets Modéliser Programmer Simuler (T. Lelièvre)
- Statistics and data sciences, 30h (G. Stoltz)
- Projet de physique statistique et mécanique quantique, 10h (G. Stoltz, L. Vidal)

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

- Théorie spectrale et méthodes variationnelles, 10h (E. Cancès)
- Problèmes multiéchelles, aspects théoriques et numériques, 24h (F. Legoll)
- Introduction to computational statistical physics, 20h (G. Stoltz)

At other institutions:

- Modal de Mathématiques Appliquées (MAP473D), 15h, Ecole Polytechnique (T. Lelièvre)
- Aléatoire (MAP361), 40h, Ecole Polytechnique (T. Lelièvre)
- Gestion des incertitudes et analyse de risque (MAP568), 20h, Ecole Polytechnique (T. Lelièvre)
- Théorie spectrale et mécanique quantique, 30h, ENS Paris (S. Perrin-Roussel)
- Modélisation, 40h, ENS Paris (S. Perrin-Roussel)
- Numerical Analysis (in Spring and Fall), 2×56h, NYU Paris (U. Vaes)

9.2.2 Supervision

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

- Zineb Belkacemi, funding CIFRE SANOFI, Deciphering protein function with artificial intelligence, co-supervised by T. Lelièvre and G. Stoltz, defended in July
- Raed Blel, funding UM6P, Model-order reduction methods for stochastic problems, co-supervised by V. Ehrlacher and T. Lelièvre, defended in June
- Rémi Goudey, funding CDSN, Homogenization problems in the presence of defects, supervised by C. Le Bris, defended in October
- Gaspard Kemlin, funding ERC Synergy EMC2, Mathematical and numerical analysis for electronic structures, co-supervised by E. Cancès and A. Levitt, defended in December
- Idrissa Niakh, thèse CIFRE EDF, Reduced basis for variational inequalities, co-supervised by V. Ehrlacher and A. Ern (Inria SERENA), defended in December
- Inass Sekkat, funding UM6P, Large scale Bayesian inference, supervised by G. Stoltz, defended in September

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

- Hichem Belbal, thèse CIFRE EDF, Understanding suspended matter measures in Loire river, since September 2022, supervised by S. Boyaval
- Elisa Beteille, thèse CIFRE EDF, Propagation of Urban Flood waves, since November 2021, supervised by S. Boyaval
- Rutger Biezemans, funding DIM Math Innov (Inria), Difficult multiscale problems and non-intrusive approaches, Ecole des Ponts, since October 2020, co-supervised by C. Le Bris and A. Lozinski (University of Besançon)
- Noé Blassel, funding ERC Synergy EMC2, Approximation of the quasi-stationnary distribution, Ecole des Ponts, since October 2022, co-supervised by T. Lelièvre and G. Stoltz
- Andrea Bordignon, Mathematical and numerical analysis for Density Functional Theory, funding ERC Synergy EMC2, co-supervised by E. Cancès and A. Levitt
- 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)
- Shiva Darshan, funding ANR SINEQ, Linear response of constrained stochastic dynamics, since October 2022, co-supervised by G. Stoltz and S. Olla (Université Paris-Dauphine)
- Maria Fuente-Ruiz, funding INRIA, Parallel algorithms for tensor methods, since September 2020, co-supervised by V. Ehrlacher and D. Lombardi (Inria COMMEDIA)
- Abbas Kabalan, thèse CIFRE SAFRANTech, Reduced-order models for problems with non-parametric geometrical variations, since November 2022, co-supervised by V. Ehrlacher and F. Casenave (SAFRANTech)
- Albéric Lefort, funding CERMICS-ENPC, Multiscale numerical methods for reaction-diffusion equations and related problems, Ecole des Ponts, since November 2022, co-supervised by F. Legoll and C. Le Bris
- Eloïse Letournel, funding DIM Math Innov (Inria), Finite size effects in electronic structure, École des Ponts, since September 2021, supervised by A. Levitt
- Alfred Kirsch, funding Simons foundation, Mathematical and numerical analysis of interacting electrons models, École des Ponts, since September 2021, co-supervised by E. Cancès and D. Gontier (Paris-Dauphine CEREMADE)
- Solal Perrin-Roussel, funding École des Ponts, Mathematical anlaysis and numerical simulation of electronic transport in moiré materials, co-supervised by É. Cances and by D. Gontier (CEREMADE, Université Paris-Dauphine PSL)
- Thomas Pigeon, funding Inria, Combining machine learning and quantum computations to discover new catalytic mechanisms, Université de Lyon, since October 2020, co-supervised by P. Raybaud (IFPEN) and T. Lelièvre, together with G. Stoltz and M. Corral-Vallero (IFPEN)
- Simon Ruget, funding Inria, Coarse approximation for a Schrödinger problem with highly oscillatory coefficients, Ecole des Ponts, since October 2022, co-supervised by F. Legoll and C. Le Bris
- Régis Santet, funding Ecole des Ponts, Enhancing the sampling efficiency of reversible and non-reversible dynamics, Ecole des Ponts, since October 2021, co-supervised by T. Lelièvre and 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, co-supervised by G. Stoltz and P. Monmarché (Sorbonne Université)
- Jana Tarhini, thèse IFPEN, Fast simulation of CO2/H2 storage in geological bassins, since November 2021, supervised by S. Boyaval
- Jean-Paul Travert, thèse CIFRE EDF, Data assimilation for flood predictions, since November 2022, supervised by S. Boyaval
- Laurent Vidal, funding ERC Synergy EMC2, Model reduction in physics and quantum chemistry, since February 2021, supervisd by E. Cancès and A. Levitt.

9.2.3 Juries

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

- S. Boyaval, PhD of Omar Mokhtari (“Écoulement de solutions de polymères en milieux poreux: impact des effets viscoélastiques à l’échelle du pore sur les propriétés effectives à l’échelle de Darcy”), defended at INP Toulouse in July
- E. Cancès, PhD of Etienne Polack (“ Development of efficient multiscale methods and extrapolation techniques for multiphysics molecular chemistry”), defended at Sorbonne University in January (chair)
- E. Cancès, PhD of Augustin Blanchet (“De la surface au cœur des étoiles: vers une modélisation unifiée de la matière condensée aux plasmas”), defended at the University of Paris Saclay in February (chair)
- E. Cancès, PhD of Michele Nottoli (“Fast and accurate multi- layer polarizable embedding strategies for the static and dynamic modeling of complex systems”), defended at the University of Pisa in February (referee)
- E. Cancès, PhD of Martin Mrovec (“Mathematical Methods of Modelling Electronic Structure of Large Systems”), defended at the University of Ostrava in April (referee)
- V. Ehrlacher, PhD of Kiran Kollepara ("Low-rank and sparse approximations for contact mechanics"), defended at Nantes University in July (referee)
- V. Ehrlacher, PhD of Philip Edel ("Reduced basis method for parameter-dependent linear equations. Application to time-harmonic problems in electromagnetism and in aeroacoustics."), defended at Sorbonne University in October (referee)
- V. Ehrlacher, PhD of Emilie Bourne ("Non-Uniform Numerical Schemes for the Modelling of Turbulence in the 5D GYSELA Code"), defended at CEA Cadarache in December (referee)
- V. Ehrlacher, PhD of Katharina Eichinger ("Problèmes variationnels pour l’interpolation dans l’espace de Wasserstein"), defended at University Paris-Dauphine in December (referee)
- T. Lelièvre, PhD of Aurélien Enfroy ("Contributions à la conception, l’étude et la mise en œuvre de méthodes de Monte Carlo par chaîne de Markov appliquées à l’inférence bayésienne"), defended at Institut Polytechnique de Paris in July (chair)
- T. Lelièvre, PhD of Fiona Desplats ("Development of a hybrid method coupling deterministic and stochastic neutronic calculations: Applications to heterogeneous PWR and SFR calculations"), defended at Université Grenoble Alpes in October (referee)

- T. Lelièvre, PhD of Loris Felardos ("Data-free Generation of Molecular Configurations with Normalizing Flows"), defended at Université Grenoble Alpes in December (referee)
- A. Levitt, PhD of Jean Cazalis (“Systèmes quantiques non linéaires en dissociation : l’exemple du graphène”), defended at Université Paris Dauphine in July
- G. Stoltz, PhD of Paul Rohrbach ("Multilevel Monte Carlo simulation of soft matter using coarse-grained models"), defended at the University of Cambridge in October (referee)
- G. Stoltz, PhD of Benjamin Stottrup ("Spectral, scattering, and regularity properties related to various functional and differential equations"), defended at Aalborg University in April (referee)
- G. Stoltz, PhD of Lorenzo Campana ("Stochastic modeling of non-spherical particles in turbulence"), defended at Inria Sophia in March (referee)
- G. Stoltz, PhD of Clovis Lapointe ("Modélisation multi-échelles des défauts d’irradiation dans les métaux cubiques centrés"), defended at INSTN Saclay in February (referee)

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

- V. Ehrlacher and T. Lelièvre (referee), HdR of Marie Billaud-Friess ("Contributions for the approximation and model order reduction of partial differential equations"), defended at Nantes University in October

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

- V. Ehrlacher, MCF position at Laboratoire de Mathématiques d’Orsay.
- V. Ehrlacher, member of the 2022 ANR project selection committee CE46 ("Modeling and simulation").
- T. Lelièvre, positions in applied mathematics, Ecole Polytechnique.

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, Champs-sur-Marne, June
- R. Biezemans, ECCOMAS Congress 2022, Oslo (Norway), June
- R. Biezemans, CANUM 2022, Evian-les-Bains, June
- R. Biezemans, SciCADE 2022, Reykjavik (Iceland), July
- R. Biezemans, Journées Scientifiques des Jeunes du Cermics (First edition), Provins, October
- S. Boyaval, HYP 2022, Malaga (Spain), June
- S. Boyaval, WAVES 2022, Palaiseau, July
- E. Cancès, IMA workshop on Nonlocal and Singular Problems: Recent Advances and Outlook, Singapore, February
- E. Cancès, IPAM workshop on Model Reduction in Quantum Mechanics, Los Angeles (USA), April
- E. Cancès, IPAM workshop on Moiré Materials, Los Angeles (USA), May
- E. Cancès, Séminaire de Mathématiques Appliquées, Collège de France, Paris, June
- E. Cancès, Séminaire des Mathématiques, Ecole Normale Supérieure, Paris, November

- E. Cancès, Mathematical Challenges in Quantum Mechanics, online, December
- J. Cauvin-Vila, CANUM 2022, Evian-les-Bains, June
- J. Cauvin-Vila, Workshop on “Nonlinear evolutionary equations and applications”, TU Chemnitz (Germany), September
- S. Darshan, CECAM Mixed-Gen Season 3 – Session 2: Theory and numerical simulation of transport processes in condensed matter, online, December
- V. Ehrlacher, Séminaire du Collège de France, January
- V. Ehrlacher, SIAM Conference on Imaging Sciences, online, March
- V. Ehrlacher, Erwin Schrödinger Institute Program on "Computational Uncertainty Quantification: Mathematical Foundations, Methodology & Data", Vienna (Austria), May
- V. Ehrlacher, IPAM workshop on Large-Scale Certified Numerical Methods in Quantum Mechanics, Los Angeles (USA), May
- V. Ehrlacher, MATHICSE seminar, EPFL (Switzerland), June
- V. Ehrlacher, 2022 Curves and Surfaces conference, Arcachon, June
- V. Ehrlacher, Congrès pour honorer la mémoire de Roland Glowinski, Sorbonne Université, July
- V. Ehrlacher, CEMRACS 2022 seminar, CIRM Luminy, August
- V. Ehrlacher, plenary talk at the 2022 MORE Conference, Berlin (Germany), September
- V. Ehrlacher, GdT Optimal Transport, Orsay, October
- V. Ehrlacher, Journée de la Fédération Bourgogne-Franche-Comté, Besançon, November
- V. Ehrlacher, Séminaire MACS, Lyon, November
- V. Ehrlacher, Séminaire MOCO, Strasbourg, November
- V. Ehrlacher, SFB Colloquium, RWTH Aachen University (Germany), December
- V. Ehrlacher, Journée IFPEN-INRIA, December
- L. Garrigue, GDR quantum N-body problem, online, January
- L. Garrigue, Séminaire de théorie spectrale, Institut Henri Poincaré, March
- L. Garrigue, Séminaire de physique mathématique, Dijon, March
- L. Garrigue, Séminaire de physique mathématique, Grenoble, April
- L. Garrigue, Workshop at the Norwegian Center for Advanced Study, Oslo (Norway), June
- L. Garrigue, 92th annual meeting of the International association of applied mathematics and mechanics, Aachen (Germany), August
- L. Garrigue, Conference Aspect’22, Oldenbourg (Germany), September
- L. Garrigue, Séminaire EDP, Besançon, December
- L. Garrigue, Séminaire physique mathématique, Stuttgart (Germany), December
- C. Le Bris, Séminaire Laurent Schwartz, Ecole Polyetchnique / IHES, October
- C. Le Bris, CRC-1114 Colloquium, Berlin (Germany), December
- F. Legoll, workshop of the ANR QuAMProcs project, Paris, March

- F. Legoll, European Mechanics of Materials Conference (EMMC), Oxford (United Kingdom), April
- F. Legoll, Annual meeting of the TIME-X project, Leuven (Belgium), April
- F. Legoll, ECCOMAS Congress 2022, Oslo (Norway), June
- F. Legoll, seminar within the CEA-EDF-INRIA summer school on "Certification d'erreurs dans des simulations numériques", Saclay, June
- F. Legoll, Parallel-in-Time (PinT) conference, Marseille, July
- F. Legoll, World Congress on Computational Mechanics (WCCM), online meeting organized by Yokohama University (Japan), August
- F. Legoll, Congrès Français de Mécanique (CFM), Nantes, August
- F. Legoll, Numerical Analysis seminar of the Department of Mathematics of the University of Hong Kong, online, October
- T. Lelièvre, Workshop LIA CNRS-University of Illinois, Hauteluce, January
- T. Lelièvre, CMAP Seminar, Ecole Polytechnique, January
- T. Lelièvre, Workshop on Pólya urns and quasi-stationary distributions, Bath (United Kingdom), April
- T. Lelièvre, Journée Analyse Appliquée Hauts-de-France, May
- T. Lelièvre, Conference 30 years of Acta Numerica, Bedelewo (Poland), June
- T. Lelièvre, ICMMES conference, La Rochelle, June
- T. Lelièvre, CECAM meeting on the development of coarse-grained models, Lyon, November
- T. Lelièvre, Thematic meeting of the GT MASIM - GDR BIM, Paris, December
- E. Letournel, IPAM QMM2022, Los Angeles (USA), March to May
- E. Letournel, WAVES 2022, Palaiseau, July
- E. Letournel, CERMICS Young Researchers Seminar, Champs-sur-Marne, October
- A. Levitt, GDR NBODY, Toulouse, January
- A. Levitt, IPAM QMM2022, Los Angeles (USA), April
- A. Levitt, Collège de France, Paris, May
- A. Levitt, CECAM workshop, Error control in first-principles modelling, Lausanne (Switzerland), June
- A. Levitt, Lab seminar, Orsay, September
- R. Santet, CECAM Mixed-Gen Season 2 - Session 7: Simulating non-equilibrium phenomena and rare-events, online, April
- R. Santet, MCQMC 2022, Linz (Austria), July
- R. Spacek, CECAM Numerical Techniques for Nonequilibrium Steady States, Mainz (Germany), April
- R. Spacek, MCQMC 2022, Linz (Austria), July
- G. Stoltz, CECAM workshop "Numerical Techniques for Nonequilibrium Steady States", Mainz (Germany), April

- G. Stoltz, NOMATEN International Conference on Materials Informatics, Warsaw (Poland), June
- G. Stoltz, Probability seminar, Université de Rennes, June
- G. Stoltz, CNRS-ICL workshop, London (United-Kingdom), July
- G. Stoltz, plenary talk at MCQMC 2022, Linz (Austria), July
- G. Stoltz, workshop “Machine-learning assisted scientific computing”, Paris, October
- G. Stoltz, MASIM ML & sampling workshop, Paris, December
- U. Vaes, Mathematics of Machine Learning Seminar at UMass Amherst, online, December
- U. Vaes, Applied PDE Seminar, Imperial College London (United Kingdom), September
- U. Vaes, SIAM Mathematics of Data Science, online, September
- U. Vaes, MCQMC 2022, Linz (Austria), July
- U. Vaes, SIAM Annual Meeting, online, July
- U. Vaes, LMS-Birmingham Workshop on “Stochastic/Partial Differential Equations: Analysis and Computations”, University of Birmingham (United Kingdom), June
- U. Vaes, Hausdorff Center for Mathematics workshop on “Synergies between Data Science and Partial Differential Equations”, Bonn (Germany), June
- U. Vaes, Erwin Schrödinger Institute workshop on “PDE-constrained Bayesian inverse uncertainty quantification”, online, May
- U. Vaes, Isaac Newton Institute workshop on “Frontiers in kinetic equations for plasmas and collective behaviour”, Cambridge (United Kingdom), April
- L. Vidal, CERMICS Young Researchers Seminar, "Direct minimization for wave-function methods", Champs-sur-Marne, April
- L. Vidal, GAMM 2022 meeting, "On the approximation of energy bands in the Brillouin zone", Aachen (Germany), August

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

- E. Cancès, Mathematical aspects of electronic structure theory, 3h lecture, Aussois, June
- E. Cancès, Planewave DFT calculations, 2h lecture, DFTK summer school, Paris, August
- C. Le Bris, Block course, Berlin Mathematical School, "Multiscale Problems and Homogenization", 15h lecture, Berlin (Germany), November and December
- G. Stoltz, High Dimensional Sampling and Applications, 2h lecture + 1h seminar, MAC-MIGS tutorial, Edinburgh (United Kingdom), November

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

- N. Blassel, CECAM online workshop, “Theory and numerical simulation of transport processes in condensed matter”, December
- E. Letournel, DFTK summer school, Sorbonne Université, August
- E. Letournel, ISTCP 2022, Aussois, June
- R. Santet, CECAM workshop “Numerical Techniques for Nonequilibrium Steady States”, Mainz (Germany), April

- R. Santet, Journée des doctorants MSTIC 2022, Noisy-le-Grand, June
- R. Spacek, CECAM Mixed-Gen Season 2 - Session 7: Simulating non-equilibrium phenomena and rare-events, online, April
- R. Spacek, CECAM online workshop, “Theory and numerical simulation of transport processes in condensed matter”, December

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

- R. Biezemans, Semaine d’Etude Mathématiques-Entreprises, Rennes, May
- A. Bordignon, ISTCP 2022, Aussois, June
- A. Bordignon, GDR N-body minischool, Sorbonne Université, June
- A. Bordignon, Journées Scientifiques des Jeunes du Cermics (First edition), Provins, October
- J. Cauvin-Vila, Hausdorff Center for Mathematics School on “Diffusive Systems Part II”, Bonn (Germany), April
- S. Darshan, Statistical Physics of Complex Systems, Bangalore (India), December
- A. Kirsch, IPAM QMM2022, Los Angeles (USA), April
- A. Kirsch, International Summer School on Computational Quantum Materials, Sherbrooke University (USA), June
- A. Lefort, Journées Scientifiques des Jeunes du Cermics (First edition), Provins, October
- E. Letournel, GDR N-body minischool, Sorbonne Université, June
- E. Letournel, ERC Synergy EMC2 workshop, September
- E. Polack, L. Vidal, ERC Synergy EMC2 workshop, September
- S. Perrin-Roussel, ISTCP 2022, Aussois, June
- S. Perrin-Roussel, Solid Math 2022, Trieste (Italy), September
- S. Perrin-Roussel, ERC Synergy EMC2 workshop, September
- M. Rachid, Rencontre ANR QuAMProcs, Paris, March
- M. Rachid, EDPs et Probabilités, Bordeaux, October
- S. Ruget, Journées Scientifiques des Jeunes du Cermics (First edition), Provins, October
- L. Vidal, ISTCP 2022, Aussois, June
- L. Vidal, ERC Synergy EMC2 workshop, September

9.4 Popularization

- G. Stoltz co-realized a video of the webmagazine Ingenius from Ecole des Ponts on "What is numerical statistical physics?"
- Three researchers of the team (Virginie Ehrlacher, Tony Lelièvre, Gabriel Stoltz) realized videos explaining their scientific activities. Those are available on the webpage of CERMICS.

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] M. Baudel, A. Guyader and T. Lelièvre. 'On the Hill relation and the mean reaction time for metastable processes'. In: *Stochastic Processes and their Applications* 155 (Jan. 2023), pp. 393–436. DOI: 10.1016/j.spa.2022.10.014. URL: https://hal.science/hal-02921281.

[9] 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.

[10] R. Benda, E. Cancès, V. Ehrlacher and B. Stamm. 'Multi-center decomposition of molecular densities: a mathematical perspective'. In: *Journal of Chemical Physics* 156 (28th Apr. 2022), p. 164107. DOI: 10.1063/5.0076630. URL: https://hal.archives-ouvertes.fr/hal-03338862.

[11] E. Bernard, M. Fathi, A. Levitt and G. Stoltz. 'Hypocoercivity with Schur complements'. In: *Annales Henri Lebesgue* 5 (1st May 2022), pp. 523–557. DOI: 10.5802/ahl.129. URL: https://hal.archives-ouvertes.fr/hal-03033217.

[12] R. A. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. 'Non-intrusive implementation of Multiscale Finite Element Methods: an illustrative example'. In: *Journal of Computational Physics* (2023). URL: https://hal.archives-ouvertes.fr/hal-03643103.

[13] 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* 42.3 (July 2022), pp. 2710–2770. DOI: 10.1093/imanum/drab049. URL: https://hal.archives-ouvertes.fr/hal-02291253.

[14] 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.

[15] E. Cancès, G. Dusson, G. Kemlin and A. Levitt. 'Practical error bounds for properties in plane-wave electronic structure calculations'. In: *SIAM Journal on Scientific Computing* 44.5 (17th Oct. 2022). DOI: 10.1137/21M1456224. URL: https://hal.inria.fr/hal-03408321.

[16] J. A. Carrillo, F. Hoffmann, A. M. Stuart and U. Vaes. 'Consensus Based Sampling'. In: *Studies in Applied Mathematics* 148.3 (5th Jan. 2022), pp. 1069–1140. DOI: 10.1111/sapm.12470. URL: https://hal.archives-ouvertes.fr/hal-03425993.

[17] A. Castellano, F. Bottin, J. Bouchet, A. Levitt and G. Stoltz. 'Ab initio Canonical Sampling based on Variational Inference'. In: *Physical Review B* 106.16 (20th Oct. 2022), p. L161110. DOI: 10.1103/PhysRevB.106.L161110. URL: https://hal.archives-ouvertes.fr/hal-03826195.

[18] L. Chamoin and F. Legoll. 'An introductory review on a posteriori error estimation in Finite Element computations'. In: *SIAM Review* (2022). URL: https://hal.science/hal-03368356.

[19] M.-S. Dupuy and A. Levitt. 'Finite-size effects in response functions of molecular systems'. In: *SMAI Journal of Computational Mathematics* (16th Dec. 2022). URL: https://hal.archives-ouvertes.fr/hal-03145143.

[20] 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* 44.2 (21st Mar. 2022). DOI: 10.1137/20M1381472. URL: https://hal.inria.fr/hal-03018646.

[21] V. Ehrlacher, T. Lelièvre and P. Monmarché. 'Adaptive force biasing algorithms: new convergence results and tensor approximations of the bias'. In: *The Annals of Applied Probability* 32.5 (1st Oct. 2022). DOI: 10.1214/21-AAP1775. URL: https://hal.science/hal-02314426.

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