

# 2025 Activity Report

RESEARCH CENTRE: Inria Paris Centre

IN PARTNERSHIP WITH: Ecole Nationale des Ponts et Chaussées

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Project-Team

# MATERIALS

MATHeMatics for MatERIALS

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*In collaboration with* Centre d'Enseignement et de Recherche en Mathématiques  
et Calcul Scientifique (CERMICS)



## **Project-Team MATHERIALS**

*Creation of the Project-Team: 2015 April 01*

Each year, Inria research teams publish an Activity Report presenting their work and results over the reporting period. These reports follow a common structure, with some optional sections depending on the specific team. They typically begin by outlining the overall objectives and research programme, including the main research themes, goals, and methodological approaches. They also describe the application domains targeted by the team, highlighting the scientific or societal contexts in which their work is situated. The reports then present the highlights of the year, covering major scientific achievements, software developments, or teaching contributions. When relevant, they include sections on software, platforms, and open data, detailing the tools developed and how they are shared. A substantial part is dedicated to new results, where scientific contributions are described in detail, often with subsections specifying participants and associated keywords. Finally, the Activity Report addresses funding, contracts, partnerships, and collaborations at various levels, from industrial agreements to international cooperations. It also covers dissemination and teaching activities, such as participation in scientific events, outreach, and supervision. The document concludes with a presentation of scientific production, including major publications and those produced during the year.

## Keywords

### Computer sciences and digital sciences

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

### Other research topics and application domains

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

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# 1 Team members, visitors, external collaborators

## Research Scientists

- Claude Le Bris [Team leader, ENPC, Senior Researcher, HDR]
- Sébastien Boyaval [ENPC, Senior Researcher, HDR]
- Eric Cancès [ENPC, Senior Researcher, HDR]
- Virginie Ehrlacher (Galland) [ENPC, Senior Researcher, HDR]
- David Gontier [ENPC, Researcher, HDR]
- Frederic Legoll [ENPC, Senior Researcher, HDR]
- Tony Lelièvre [ENPC, Senior Researcher, HDR]
- Gabriel Stoltz [ENPC, Senior Researcher, HDR]
- Urbain Vaes [INRIA, ISFP]

## Faculty Member

- Francis Nier [UNIV PARIS XIII, Professor Delegation, from Feb 2025 until Jul 2025]

## Post-Doctoral Fellows

- Thomas Borsoni [ENPC, Post-Doctoral Fellow]
- Lois Delande [INRIA, Post-Doctoral Fellow, from Sep 2025]
- Antonin Dellanoce [INRIA, Post-Doctoral Fellow]
- Laura Grazioli [ENPC]
- Rodrigue Lelotte [ENPC, Post-Doctoral Fellow, until Oct 2025]
- Annamaria Massimini [ENPC, Post-Doctoral Fellow]
- Giulia Merlini [ENPC, Post-Doctoral Fellow, from Apr 2025]
- Thomas Normand [INRIA, Post-Doctoral Fellow, until Aug 2025]
- Giulia Sambataro [ENPC, Post-Doctoral Fellow, until Jan 2025]

## PhD Students

- Noe Blassel [ENPC]
- Yann Bouchereau [ENPC, from Sep 2025]
- Louis Carillo [ENPC]
- Antonin Coatantiec [ENPC, from Oct 2025]
- Shiva Darshan [ENPC, until Sep 2025]
- François Escolan [ENPC]
- Sofiane Ezzehi [ENPC]
- Raphael Gastaldello [ENPC]

- Baptiste Guilbery [INRIA, from Oct 2025]
- Clement Guillot [ENPC]
- Jean-Baptiste Himbert [ENPC, from Sep 2025]
- Alberic Lefort [ENPC, until Oct 2025]
- Pierre Marmey [IFPEN]
- Alicia Negre [INRIA]
- Solal Perrin-Roussel [ENPC, until Aug 2025]
- Thaddeus Roussigne [Université Paris-Dauphine]
- Simon Ruget [INRIA, until Nov 2025]
- Jonte Weixler [Université Paris-Dauphine, from Sep 2025]

### **Interns and Apprentices**

- Yann Bouchereau [ENPC, Intern, from Mar 2025 until Jul 2025]
- Oscar Demont [INRIA, Intern, from Mar 2025 until Sep 2025]
- Thomas Lambert [INRIA, Intern, from Apr 2025 until Sep 2025]

### **Administrative Assistants**

- Derya Gok [INRIA, from Nov 2025]
- Julien Guieu [INRIA, until Nov 2025]

### **Visiting Scientists**

- Theron Guo [MIT, from Nov 2025]
- Theron Guo [MIT, from Apr 2025 until Jul 2025]
- Panagiotis Parpas [IMPERIAL COLLEGE LDN, until Feb 2025]
- Wei Zhang [Zuse Institute Berlin, from Feb 2025 until Apr 2025]

## **2 Overall objectives**

The MATHERIALS project-team was created jointly by the École nationale des ponts et chaussées (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 [3, 4, 5, 6, 7, 8, 9] 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<sup>3</sup>) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability of minerals to naturally split along crystal surfaces (e.g. mica yields to thin flakes), is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time-dependent form or in its time-independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;

- also present into these equations is the wavefunction of the system; it completely describes its state; its  $L^2$  norm is set to one.

The time-dependent equation is a first-order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of  $L^2(\mathbb{R}^d)$ , with  $d = 3(M + N)$ ,  $M$  and  $N$  respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter  $d$  is already 39 for a single water molecule and rapidly reaches  $10^6$  for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is  $10^4$  times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on  $L^2(\mathbb{R}^3)$ . The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales.

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<sup>3</sup> of water in the oceans, *i.e.*  $7 \times 10^{22}$  mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating  $\mathcal{N}_A$  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  $N \rightarrow +\infty$  (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

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

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

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

### 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). For a comprehensive account of many of the research efforts of the team on these topics, we refer to [1, 2].

## 5 Highlights of the year

### 5.1 Awards

Virginie Ehrlacher was distinguished as “chevalier dans l’ordre national du mérite”.

## 6 Latest software developments, platforms, open data

### 6.1 Latest software developments

#### 6.1.1 DFTK

**Keywords:** Molecular simulation, Quantum chemistry, Materials

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

**Release Contributions:** In 2025 DFTK continued to be actively developed, and it received several contributions from members of MATHERIALS. The library has been used for several publications both inside and outside the project-team.

**URL:** <http://dftk.org>

**Contact:** Antoine Levitt

## 7 New results

### 7.1 Electronic structure calculations and related quantum-scale problems

**Participants:** Eric Cancès, Théo Duez, Mathias Dus, Virginie Ehrlacher, Laura Grazioli, Clément Guillot, Alfred Kirsch, Claude Le Bris, Solal Perrin-Roussel, Etienne Polack.

#### 7.1.1 Density functional theory

The team continued its long-standing project to study density functional theory from an applied mathematics perspective.

In a joint work with A. Levitt and J. Thomas (University Paris Saclay), E. Cancès studies the decay of the interatomic force constants (equivalently, the smoothness properties of the dynamical matrix) in perfect crystals both at finite electronic temperature, and for insulators at zero temperature, within the reduced Hartree–Fock approximation (also called Random Phase Approximation). This model is obtained by setting to zero the exchange-correlation energy functional is Kohn–Sham Density Functional Theory. At finite temperature the electrons are mobile, leading to exponential decay of the force constants. In insulators, there is incomplete screening, leading to an algebraic decay of dipole-dipole interaction type. This is the first fully rigorous mathematical proof of a well-known phenomenon in solid-state physics.

#### 7.1.2 Electronic excited states

Computing excited states of many-body quantum Hamiltonians is a fundamental challenge in computational physics and chemistry, with state-of-the-art methods broadly classified into variational (critical point search) and linear response approaches. The Kähler manifold formalism provides a uniform framework which naturally accommodates both strategies for a wide range of variational models, including Hartree-Fock, CASSCF, Full CI, and adiabatic TDDFT. In particular, this formalism leads to a systematic and straightforward way to obtain the final equations of linear response theory for nonlinear models, which provides, in the case of mean-field models (Hartree-Fock and DFT), a simple alternative to Casida’s derivation. In a joint work with Y. Hu (Ecole des Ponts IPP), E. Cancès and L. Grazioli detail the mathematical structure of Hamiltonian dynamics on Kähler manifolds, establish connections to standard quantum chemistry equations, and provide theoretical and numerical comparisons of excitation energy computation schemes at the Hartree-Fock level of theory.

#### 7.1.3 Strongly-correlated systems

The treatment of strongly correlated quantum systems is a long-standing challenge in computational chemistry and physics.

Quantum embedding methods enable the study of large, strongly correlated quantum systems by (usually self-consistent) decomposition into computationally manageable subproblems, in the spirit of divide-and-conquer methods.

The first contribution on the mathematical and numerical analysis of this family of methods is concerned with the Dynamical Mean-Field Theory (DMFT), the most famous quantum embedding methods method introduced by A. Georges and G. Kotliar in 1992. In a previous contribution, E. Cancès, A. Kirsch and S. Perrin-Roussel had proven the existence of a solution to the DMFT equations under the Iterated Perturbation Theory (IPT-DMFT) approximation. In view of numerical simulations, these equations need to be discretized. In a follow-up contribution, they studied a discretization of the IPT-DMFT functional equations, based on the restriction of the hybridization function and local self-energy to a finite number of Matsubara frequencies. They first prove the existence of solutions to the discretized equations in some parameter range depending on the Matsubara frequency cut-off. They then prove uniqueness for a smaller range of parameters. They also study more in depth the case of bipartite systems exhibiting particle-hole symmetry. In this case, the discretized IPT-DMFT equations have purely imaginary solutions, which can be obtained by solving a real algebraic system. They provide a complete characterization of the solutions in the simple case of the

Hubbard dimer for discretizations on the lowest two values of the Matsubara frequency cut-off and numerical simulations for larger values. First, they describe how a conductor-to-insulator transition occurs in the Matsubara frequency discretized IPT-DMFT model in the small temperature regime. Finally, they show that for some parameters ( $U, T$ ) of the considered Hubbard model, this discretization method may provide values of the Green's function at the lowest Matsubara frequencies which cannot be interpolated by a Pick function.

The second contribution is concerned with Density Matrix Embedding Theory (DMET), a popular method in quantum chemistry introduced by Ksanyi and Chang in 2012. DMET is an efficient approach that enforces self-consistency at the level of one-particle reduced density matrices (1-RDMs), facilitating applications across diverse quantum systems. However, conventional DMET is constrained by the requirement that the global 1-RDM (low-level descriptor) be an orthogonal projector, limiting flexibility in bath construction and potentially impeding accuracy in strongly correlated regimes. In a joint work [58] with T. Ayrál (Eviden, now Ecole Polytechnique), F. Faulstich (RPI, USA), R. Kim and L. Lin (UC Berkeley, USA), E. Cancès and A. Nègre introduced a generalized DMET framework in which the low-level descriptor can be an arbitrary 1-RDM and the bath construction is based on optimizing a quantitative criterion related to the maximal disentanglement between different fragments. This yields an alternative yet controllable bath space construction for generic 1-RDMs, lifting a key limitation of conventional DMET. They demonstrate its consistency with conventional DMET in appropriate limits and exploring its implications for bath construction, downfolding (impurity Hamiltonian construction), low-level solvers, and adaptive fragmentation. We expect that this more flexible framework, which leads to several new variants of DMET, can improve the robustness and accuracy of DMET.

#### 7.1.4 Electronic structure of moiré materials

Computing the electronic structure of incommensurate materials is a central challenge in condensed matter physics, requiring efficient ways to approximate spectral quantities such as the density of states (DoS). In a joint work with D. Massatt (NJIT, USA), L. Meng (Zhejiang University, China), Etienne Polack (former member of Matherials, now at CEA Grenoble) X. Zhang (Beijing Normal University, China), E. Cancès numerically investigate two distinct approaches for approximating the DoS of incommensurate Hamiltonians for small values of the incommensurability parameters  $\epsilon$  (e.g., small twist angle, or small lattice mismatch): the first employs a momentum-space decomposition, and the second exploits a semiclassical expansion with respect to  $\epsilon$ . In particular, these two methods are compared using a 1D toy model. We check their consistency by comparing the asymptotic expansion terms of the DoS, and it is shown that, for full DoS, the two methods exhibit good agreement in the small  $\epsilon$  limit, while discrepancies arise for less small  $\epsilon$ , which indicates the importance of higher-order corrections in the semiclassical method for such regimes. These discrepancies are found to be caused by oscillations in the DoS at the semiclassical analogues of Van Hove singularities, which can be explained qualitatively, and quantitatively for  $\epsilon$  small enough, by a semiclassical approach.

#### 7.1.5 Optimal transport and quantum chemistry

Recent research efforts have been carried out in the team on the development of efficient numerical methods for quantum chemistry using optimal transport theory.

## 7.2 Computational statistical physics

**Participants:** Noé Blassel, Louis Carillo, Antonin Coatantiec, Shiva Darshan, Raphaël Gastaldello, Jean-Baptiste Himbert, Tony Lelièvre, Pierre Marmey, Panos Parpas, Régis Santet, Gabriel Stoltz, Urbain Vaes, Wei Zhang.

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 development of simulation methods to efficiently simulate nonequilibrium systems; (iii) the study of dynamical properties and rare event sampling; (iv) the

development of enhanced sampling methods using machine learning techniques; (v) the use of particle methods for sampling and optimization.

### 7.2.1 Sampling of the configuration space

There is still a need to improve techniques to sample the configuration space, and to understand their performance. This includes the development of sampling techniques, and their numerical analysis.

To quantify the performance of sampling methods based on ergodic stochastic differential equations, bounds on the resolvent of the generator of the dynamics under consideration are useful, as one can derive upper bounds on the asymptotic variance for time averages. Such bounds can in turn be deduced from decay estimates on the semigroup. Together with G. Brigati (ISTA, Austria), A. Wang (University of Warwick United-Kingdom) and L. Wang (NUS, Singapore), G. Stoltz studied in [43] how to obtain constructive decay estimates for the semigroup associated with hypoelliptic generators associated with Langevin dynamics, using hypocoercive techniques based on space time averages and Lions' lemma, in the setting where a Poincaré inequality does not hold, but weak or weighted Poincaré inequalities are satisfied by the marginal distributions in positions and momenta.

Besides, together with X. Lin and P. Monmarché (Université Gustave Eiffel), T. Lelièvre explores in [57] a new approach to study the convergence of free-energy-based adaptive biasing methods, such as Metadynamics and their variants. These are enhanced sampling algorithms which are widely used in molecular simulations. Although their efficiency has been empirically acknowledged for decades, providing theoretical insights via a quantitative convergence analysis is a difficult problem, in particular for the kinetic Langevin diffusion, which is non-reversible and hypocoercive. They obtain the first exponential convergence result for such a process, in an idealized setting where the dynamics can be associated with a mean-field non-linear flow on the space of probability measures. A key of the analysis is the interpretation of the (idealized) algorithm as the gradient descent of a suitable functional over the space of probability distributions.

### 7.2.2 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. 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. Let us next describe the efforts of the team done in the previous year.

In [53], R. Gastaldello, G. Stoltz and U. Vaes proposed a variance reduction method for calculating transport coefficients using an importance sampling method via Girsanov's theorem applied to Green–Kubo's formula. They optimized the magnitude of the perturbation applied to the reference dynamics by means of a scalar parameter  $\alpha$  and proposed an asymptotic analysis to fully characterize the long-time behavior in order to evaluate the possible variance reduction. Theoretical results were corroborated by numerical results and show that this method allows for some reduction in variance, although rather modest in most situations.

In [17], S. Darshan and G. Stoltz studied with A. Iacobucci and S. Olla (CEREMADE, France) the behavior of  $\beta$ -FPUT chains under time-periodic forcings. Recent works proved a hydrodynamic limit for periodically forced atom chains with harmonic interaction and pinning, together with momentum flip. When energy is the only conserved quantity, one would expect similar results in the anharmonic case, as conjectured for the temperature profile and energy flux. However, outside the harmonic case, explicit computations are generally no longer possible, thus making a rigorous proof of this hydrodynamic limit difficult. This motivated the numerical investigation of the plausibility of this limit for the particular case of a chain with  $\beta$ -FPUT interactions and harmonic pinning. The results suggest that the conjectured PDE for the limiting temperature profile and Green–Kubo type formula for the limiting energy current conjectured are correct. This Green–Kubo type formula is then used to investigate the relationship between the energy current and period of the forcing. This relationship is investigated in the case of significant rate of momentum flip, small rate of momentum flip and no momentum flip.

### 7.2.3 Modeling and sampling dynamical properties and rare events

Sampling transitions from one metastable state to another is a difficult task. The work of the team here consists in analyzing and developing new numerical methods to this end, and provide the associated mathematical analysis.

In [39] N. Blassel, T. Lelièvre and G. Stoltz studied the optimization of the shape of metastable states. The work is motivated by—and is relevant to—the problem of finding optimal hyperparameters for accelerated molecular dynamics algorithms. The definition of metastable states is indeed an ubiquitous task in the design and analysis of molecular simulation, and is a crucial input in a variety of acceleration methods for the sampling of long configurational trajectories. Although standard definitions based on local energy minimization procedures can sometimes be used, these definitions are typically suboptimal, or entirely inadequate when entropic effects are significant, or when the lowest energy barriers are quickly overcome by thermal fluctuations. This work proposed an approach to the definition of metastable states, based on the shape-optimization of a local separation of timescale metric directly linked to the efficiency of a class of accelerated molecular dynamics algorithms. To realize this approach, analytic expressions were derived for shape-variations of Dirichlet eigenvalues for a class of operators associated with reversible elliptic diffusions, and used to construct a local ascent algorithm, explicitly treating the case of multiple eigenvalues. Two methods were proposed to make the method tractable in high-dimensional systems: one based on dynamical coarse-graining, the other on recently obtained low-temperature shape-sensitive spectral asymptotics. The method was validated on a benchmark biomolecular system, showcasing a significant improvement over conventional definitions of metastable states.

In [38] N. Blassel, T. Lelièvre and G. Stoltz derived novel sharp low-temperature asymptotics for the spectrum of the infinitesimal generator of the overdamped Langevin dynamics. The novelty was that the operator is endowed with homogeneous Dirichlet conditions at the boundary of a domain which depends on the temperature, having in mind the shape optimization problem discussed in the previous paragraph. From the point of view of stochastic processes, this gives information on the long-time behavior of the diffusion conditioned on non-absorption at the boundary, in the so-called quasistationary regime. The results provide sharp estimates of the spectral gap and principal eigenvalue, extending the Eyring–Kramers formula. The phenomenology is richer than in the case of a fixed boundary and gives new insight into the sensitivity of the spectrum with respect to the shape of the domain near critical points of the energy function.

### 7.2.4 Machine learning approaches in molecular dynamics

The team is investigating how machine learning techniques can be used in order to design new sampling techniques. Indeed, neural networks can efficiently approximate high dimensional functions which can then be used as importance functions in various sampling algorithms. Moreover, generative models can complement standard sampling techniques in order to propose innovative moves.

In [60] T. Lelièvre and G. Stoltz developed with C. Schönle (Ecole polytechnique), D. Carbone and M. Gabrié (ENS Paris) Monte-Carlo samplers for metastable systems using non-local collective variable updates. This addresses the problem of sampling a high dimensional multimodal target probability measure, assuming that a good proposal kernel to move only a subset of the degrees of freedoms (also known as collective variables) is known a priori. This proposal kernel can for example be built using normalizing flows. The work shows how to generalize the extension of the move from the collective variable space to the full space and how to implement an accept-reject step in order to get a reversible chain with respect to a target probability measure – namely for situations when non-linear CVs and underdamped Langevin dynamics are considered. Performance is demonstrated on several numerical examples, observing a substantial improvement compared to methods based on overdamped Langevin dynamics as considered previously.

In [35] G. Stoltz proposed together with F.-Z. Akhyar, W. Zhang (ZIB, Germany) and C. Schütte (FU Berlin, Germany) a generative method for conditional probability distributions on the level-sets of collective variables. More precisely, given a probability distribution  $\mu$  in  $\mathbb{R}^d$  represented by data, they studied the generative modeling of its conditional probability distributions on the level-sets of a collective variable  $\xi$ . They developed a general and efficient learning approach able to learn generative models on different level-sets of  $\xi$  simultaneously. To improve the learning quality on level-sets in low-probability regions, they also proposed a strategy for data enrichment by utilizing data from enhanced sampling techniques. They demonstrated the effectiveness of the proposed learning approach through concrete numerical examples,

including molecular systems in biophysics.

### 7.2.5 Interacting particle methods for sampling

A number of stochastic numerical methods for optimization and sampling are based on interacting stochastic dynamics. Methods of this type are convenient because they can usually be implemented in parallel, and they may possess desirable properties that single-replica methods do not enjoy, such as faster convergence or invariance under affine transformations.

A well-known numerical method based on an interacting particle system is the ensemble Kalman filter, a methodology for incorporating noisy data into complex dynamical models to enhance predictive capability. This filter is widely adopted in the geophysical sciences, and is starting to be used throughout the sciences and engineering, but there is no theory which quantifies its accuracy as an approximation of the true filtering distribution, except in the Gaussian setting. Study of the statistical accuracy of the ensemble Kalman filter is inherently technical, as it involves the evolution of probability measures according to a nonlinear and nonautonomous dynamical system. In [44], U. Vaes together with E. Calvello (Caltech, USA), José A. Carrillo (University of Oxford, United Kingdom), Franca Hoffmann (Caltech, USA), P. Monmarché (Université Gustave Eiffel) and Andrew M. Stuart (Caltech, USA) provide an accessible overview of previous work in which they took first steps to analyze the accuracy of the filter beyond the linear Gaussian setting [62].

In a different work [54], U. Vaes together with N. J. Gerber (Hausdorff Center for Mathematics, Germany), D. Kim (Caltech, USA) and F. Hoffmann (Caltech, USA) prove a quantitative, uniform-in-time propagation of chaos result for a consensus-based optimization method, generalizing previous results in [65]. The analysis relies on the classical synchronous coupling method by Sznitman and McKean, together with several novel auxiliary results, including a stability estimate for the weighted mean and novel concentration estimates for the interacting particle system.

In a third work on interacting particle systems [55], U. Vaes together with N. J. Gerber (Hausdorff Center for Mathematics, Germany) establish uniform-in-time propagation of chaos for the Cucker–Smale model, a well-known model for flocking behavior. This extends an existing finite-time propagation of chaos result from [64] to infinite time horizons, by leveraging long-time stability properties of the Cucker–Smale interacting particle system. The result can be interpreted as a long-time error estimate for a stochastic particle method for the Vlasov–Fokker–Planck equation associated with the Cucker–Smale model.

## 7.3 Homogenization

**Participants:** Yann Bouchereau, Claude Le Bris, Albéric Lefort, Frédéric Legoll, Giulia Merlini, Simon Ruget.

### 7.3.1 Homogenization theory

In collaboration with Yves Achdou (Université Paris Cité), C. Le Bris has pursued the study of some homogenization problems for a class of stationary Hamilton–Jacobi equations in which the Hamiltonian is obtained by perturbing an otherwise periodic Hamiltonian. Homogenization then leads to an effective Hamilton–Jacobi equation supplemented with effective Dirichlet boundary conditions. After the case of a perturbation at the origin, the case of a perturbation near a half-line of the state space has been considered. In all these cases, the limiting problem belongs to the class of stratified problems introduced by Alberto Bressan and Yunho Hong and later studied by Guy Barles and Emmanuel Chasseigne. The work has been published in *Nonlinear Differential Equations and Applications*, Volume 32, 119 (2025).

On the other hand, and this time in a series of works in collaboration with Andrea Braides and Gianni Dal Maso (SISSA Trieste, Italy), C. Le Bris has used the tools of Gamma convergence to study several homogenization problems he has considered in the past using the tools of PDE theory, notably in collaboration with Xavier Blanc (Université Paris Cité) and Pierre-Louis Lions (Collège de France). In a first work, the stability of some classes of integrals, with respect to homogenization, was examined. Stability theorems in homogenization which comprise the case of perturbations with zero average on the whole space were then deduced. The results were also extended to the stochastic case, and several other cases. In a second work, the

stability with respect to homogenization of classes of integrals arising in the control-theoretic interpretation of some Hamilton–Jacobi equations were investigated. The study revisits and, depending on the different assumptions, complements results obtained by Pierre-Louis Lions and various collaborators using PDE techniques. This second work has been accepted for publication in *SIAM Journal on Mathematical Analysis*. A third work, in the same vein, is ongoing and this time addresses the case of viscous Hamilton-Jacobi equations.

A third research effort, also connected to the area of homogenization theory, has been conducted by C. Le Bris in collaboration with Anthony T. Patera (MIT), Kento Kaneko (MIT) and Theron Guo (MIT). The general context of the study is heat transfer, and more specifically the dunking problem: a solid body, at uniform temperature and possibly with heterogeneous material composition, is placed in an environment characterized by far field temperature and spatially uniform time independent heat transfer coefficient. The problem is described by a heat equation with Robin boundary conditions. The crucial parameter is the Biot number – a nondimensional heat transfer (Robin) coefficient. Various approximations were introduced, justified theoretically and tested numerically. Error estimates for these approximations were also provided and companion numerical solutions of the heat equation confirm the effectiveness of the error estimates for small Biot number. The work is described in the following three documents: a chapter submitted to Springer MS&A series, a second preprint and a manuscript submitted to ESAIM: M2AN.

V. Ehrlacher and F. Legoll, together with A. Lesage and A. Lebéé (ENPC), have considered in [52] elasticity equations posed in thin domains (such as plates) and including highly oscillatory periodic coefficients. The aim of the work is to establish strong convergence results on the difference between the solution to the reference oscillatory problem and its two-scale expansion. Under some classical assumptions on the symmetries of the elasticity tensor, the problem can be split into two independent problems, the membrane problem and the bending problem. The membrane case can actually be addressed using a careful adaptation of classical arguments. The bending case turned out to be much more challenging. A different strategy of proof is introduced to handle it.

### 7.3.2 Inverse multiscale problems

In the context of the PhD of S. Ruget, C. Le Bris and F. Legoll have completed their work on the question of how to determine the homogenized coefficient of a multiscale problem without explicitly performing a homogenization approach. This work is a follow-up on earlier works over the years in collaboration with Kun Li, Simon Lemaire and Olga Gorynina. The robustness of the proposed approach with respect to the available data, and with respect to noise in measurements, has been thoroughly investigated. In particular, an attractive situation is to assume to only have access to coarse information on the solution, such as the global energy stored in the physical system for any given load (such inverse problems with partial information available are indeed relevant to engineering situations). While the reconstruction of the microstructure is known to be an ill-posed problem, the reconstruction of effective parameters based only on this aggregated information is possible. A manuscript collecting various theoretical and numerical results is currently in preparation (see also [34]).

### 7.3.3 Multiscale Finite Element approaches

From a numerical perspective, the Multiscale Finite Element Method (MsFEM) is a classical strategy to address the situation where 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.

In the context of the PhD of A. Lefort, C. Le Bris and F. Legoll have undertaken the study of a multiscale, reaction-diffusion equation. This problem is different from the equations previously studied by the team by the fact that it includes a *large reaction term* which competes with the diffusive term. To start with, the associated eigenvalue problem has been considered. A promising MsFEM-type approach, which uses an oversampling procedure based on filtering ideas investigated by the team several years ago, has been introduced. This MsFEM approach has next been successfully extended to vector-valued reaction-diffusion eigenvalue problems, a very relevant case from the application viewpoint which presents the mathematical

difficulty of being non self-adjoint. The time-dependent version of the problem has next been investigated, using two possible approaches: a spectral approach, where the solution is written as a linear combination of the eigenmodes of the stationary problem, or a time-marching scheme. A manuscript collecting the theoretical and numerical results is currently being prepared.

In the context of the M2 internship and then PhD of Y. Bouchereau, C. Le Bris and F. Legoll have studied the wave equation in heterogeneous periodic media. Classical homogenization results indicate that the solution to the wave equation converges to the solution to a simple homogenized problem when the final time is fixed and independent of the characteristic length  $\varepsilon$  of the medium. It is also well-known that, over larger time horizons (say times of the order of  $\varepsilon^{-2}$ ), the homogenized equation should be complemented by corrective terms to remain an accurate approximation of the reference model. Y. Bouchereau, C. Le Bris and F. Legoll have investigated how to design efficient MsFEM-type approaches in that context. Adapted basis functions are introduced on the basis of the sole diffusion operator. A spatial Galerkin approximation of the wave equation is then performed, leading to a second-order ODE which can be integrated using different techniques. Different regimes of time horizons have been explored, as well as different settings such as periodic, quasi-periodic and general heterogeneous media. Encouraging preliminary results have been obtained that now need to be consolidated.

In parallel to the exploration of reaction-diffusion equations and wave equations, another direction of research is devoted to hyperbolic multiscale conservation laws. From the viewpoint of asymptotic analysis, it is known that introducing a vanishing viscosity in the conservation law leads to a problem, the homogenized limit of which again reads as a conservation law with effective parameters defined in terms of a corrector function, solution to an elliptic cell problem encoding the fine-scale structure of the flux. Based on that observation, C. Le Bris, F. Legoll and G. Merlini have considered a strategy aiming at efficiently computing an approximation of the numerical solution given by a fine-scale finite volume scheme applied to the original hyperbolic multiscale conservation law. The idea is to homogenize the numerical scheme discretizing the PDE, rather than the PDE itself, by exploiting the numerical viscosity naturally present in the numerical scheme. This strategy has been first put in practice for the classical Lax–Friedrichs scheme. Numerical results demonstrate that the resulting homogenized model provides an accurate and computationally efficient approximation of the reference solution in one and two space dimensions for a broad class of multiscale conservation laws. Current and future works include extending this strategy to higher-order numerical schemes and investigating specific regimes or examples (such as shear flows), for which the asymptotic homogenized model is *not* of the form of a (standard) conservation law.

## 7.4 Various topics

### 7.4.1 Complex fluids

**Participants:** Sébastien Boyaval.

In 2025, S. Boyaval has pursued the modelling of viscoelastic flows using symmetric-hyperbolic balance laws consistent with polyconvex elastodynamics. In [63], he proved with Na Wang and Yuxi Hu that for one-dimensional flows, the symmetric-hyperbolic conservation laws are asymptotically consistent with the standard viscous compressible Navier-Stokes equations, when the viscoelastic stress relaxes infinitely fast. In [36], he investigated, with Emmanuel Audusse, Virgile Dubos and Minh Hoang Le, the construction of kinetic schemes for the numerical simulation of (linear) elastodynamics, formulated as a symmetric-hyperbolic system of PDEs.

In [61], S. Boyaval and his co-authors Jean-Paul Travert, Cédric Goeury, Vito Bacchi and Fabrice Zaoui study numerically, for various metrics, the sensitivity to post-processing parameters of the SAR (images) data used for flood mapping.

### 7.4.2 Model-order reduction methods

**Participants:** Sébastien Boyaval, Virginie Ehrlicher, Tony Lelièvre, Giulia Sambattaro.

The objective of a model-order 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 that 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 obtain an accurate approximation of the solution of the model for any other values of the parameters.

In [12], R. Blel, T. Lelièvre and V. Ehrlicher perform a numerical analysis of a variance reduction technique for the computation of parameter-dependent expectations using a reduced basis paradigm. The idea is to build online a control variate using expectations computed precisely in an offline stage, with a greedy procedure to select the parameters where those expectations are evaluated. Using concentration inequalities, they provide sufficient conditions on the number of samples used for the computation of empirical variances at each iteration of the greedy procedure to guarantee that the resulting method algorithm is a weak greedy algorithm with high probability.

#### 7.4.3 Numerical approaches for SPDEs

**Participants:** Claude Le Bris.

In collaboration with Ana Djurdjevac (FU Berlin) and Endre Suli (Oxford University), C. Le Bris has considered some dedicated numerical approaches for a large class of parabolic SPDEs with multiplicative noise. The specificity of the class considered is that it preserves positivity at the continuous level. Inspired by well-established techniques for the deterministic case, a FEM discretization was introduced that both is accurate and, unconditionally in the discretization parameters, also preserves positivity. Besides the numerical analysis of the semi-discrete algorithm, some numerical experiments were provided, which illustrate the added value with respect to other approaches in the literature. The work has been submitted to *Stochastics and Partial Differential Equations: Analysis and Computations*. A follow-up, devoted to the analysis of the fully discrete scheme and presenting other numerical experiments, has been concluded in collaboration with Ana Djurdjevac and Owen Hearder (FU Berlin). It is submitted to *Communications in Applied Mathematics and Computational Science*.

#### 7.4.4 Quantum optimal transport and applications

**Participants:** Thomas Borsoni, Virginie Ehrlicher.

In [40], T. Borsoni has contributed to the current development of quantum optimal transport formulations, by introducing the framework of folded optimal transport, which relies on Choquet theory of boundary representations. This framework encompasses classical and entanglement-free quantum optimal transport Kantorovich formulations. Also recovered is the semi-classical optimal transport cost, used in [41] by T. Borsoni and V. Ehrlicher to obtain an observability-type result for the von Neumann equation in a crystal setting. In this work, various concepts are also developed to fit the periodic case, such as the Husimi and Töplitz transforms.

## 8 Bilateral contracts and grants with industry

**Participants:** Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Gabriel Stoltz.

Many research activities of the project-team are conducted in close collaboration with private or public companies: CEA, EDF, IFPEN, Sanofi, 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.

## 9 Partnerships and cooperations

### 9.1 International initiatives

#### Other international visits to the team

**Wei Zhang**

**Status** Researcher

**Institution of origin:** FU Berlin

**Country:** Germany

**Dates:** Feb. 17th to April 17th

**Context of the visit:** work with Frédéric Legoll, Tony Lelièvre and Gabriel Stoltz on the derivation of effective dynamics for underdamped Langevin equations; as well as on deep generative and clustering methods, to be used to sample multimodal probability measures as the ones arising in molecular dynamics (with Tony Lelièvre and Gabriel Stoltz).

**Mobility program/type of mobility:** research stay, funded by Inria Paris

#### 9.1.1 Visits to international teams

##### Research stays abroad

- In February 2025, Antonin Della Noce and Urbain Vaes visited the group of Prof. Franca Hoffmann (Caltech, USA) for 10 days.

### 9.2 European initiatives

#### 9.2.1 H2020 projects

**EMC2** [EMC2 project on cordis.europa.eu](https://cordis.europa.eu)

**Title:** Extreme-scale Mathematically-based Computational Chemistry

**Duration:** From September 1, 2019 to August 31, 2026

##### Partners:

- INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France
- ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL), Switzerland
- ECOLE NATIONALE DES PONTS ET CHAUSSEES (ENPC), France

- CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS), France
- SORBONNE UNIVERSITE, France

**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.

### 9.3 National initiatives

The project-team is involved in several ANR projects:

- F. Legoll is a member of the ANR Anohona (2024-2028), on Advanced nonlinear homogenization for structural analysis. PI: N. Lahellec (LMA Marseille).
- 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.
- U. Vaes is the PI of the ANR project ISPO (2024-2025). The main objectives of this project are to improve, implement and mathematically analyze sampling and optimisation methods based on interacting particle systems.

The project-team is a partner of the **DIM QuantIP**. It is also involved in the Projet CNRS Recherche à risque et à impact (RI)2 “Nouvelles approches mathématiques pour des systèmes quantiques en interaction (MAQUI)”, lead PI: M. Lewin (CEREMADE, CNRS and University Paris-Dauphine PSL), co-PI: E. Cancès, J. Toulouse (LCT, SU).

The project-team is also involved in PEPR projects:

- T. Lelièvre is responsible of the node "Ecole des Ponts" of the project MAMABIO of PEPR B-BEST (Biomass, Biotechnologies & Environmentally Sustainable Technologies for chemicals and fuels; 2023-2028), to which G. Stoltz also participates.
- E. Cancès, C. Le Bris, T. Lelièvre and G. Stoltz are part of the node "MATERIALS" of the project EpiQ of PEPR Quantique, which is part of Plan France 2030.

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

- AMORE (Advanced Model Order REduction),

- DYNQUA (time evolution of quantum systems),
- MathGeoPhy (MATHematics for GeoPhysics), now RT Terre et Energies,
- MANU (MATHematics for NUclear applications), now RT Terre et Energies,
- GDM (Geometry and Mechanics),
- IAMAT (Artificial Intelligence for MATerials),
- MASCOT-NUM (stochastic methods for the analysis of numerical codes),
- MEPHY (multiphase flows),
- NBODY (electronic structure),
- REST (theoretical spectroscopy).

## 10 Dissemination

### 10.1 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 editorial boards of Mathematical Modelling and Numerical Analysis (2006- ), SIAM Multiscale Modeling and Simulation (2012-), the Journal of Computational Mathematics (2017-), and the Journal of Computational Physics (2023-);
- is a member of the Scientific Committee of the MFO (*Mathematisches Forschungsinstitut Oberwolfach*);
- is a member of the Scientific Committees of the GdR DynQua (quantum dynamics) and NBody (*N-body quantum problem in chemistry and physics*);
- has co-organized (with E. Fromager, E. Giner, P.-F. Loos, and J. Toulouse) a summer school on Mathematics for theoretical chemistry and physics, Paris, May 19-21, 2025;
- has been a member of the 2025 John Todd Award election committee.

V. Ehrlicher

- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2024- ), Acta Applicandae Mathematicae (2024-) and Mathematics of Computation (2024-);
- is head of the Modelisation, Analysis and Simulation team of the applied mathematics department (CERMICS) at Ecole des Ponts (since Sep. 2024);
- is member of the board of the SMAI-SIGMA group;
- is co-chair of the European Mathematical Society Topic Activity Group on "Scientific Machine Learning";
- is an expert for the Scientific Committee of IFPEN (since 2024);

- is a member of the Programme INRIA Quadrant (PIQ) (since 2024);
- 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;
- was a member of the evaluation committee of the Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, Germany;
- is a member of the scientific committee of the SMAI 2025 conference;
- has been a member of the SMAI-GAMNI PhD prize selection committee.

#### C. Le Bris

- is co-editor in chief (2024-) of *Journal de Mathématiques Pures et Appliquées*;
- 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-), *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 (2016-2024) of the scientific advisory board of the Institut des Sciences du calcul et des données, Sorbonne Université, and a member (2020-) of the Scientific Advisory Committee of the Institute for Mathematical and Statistical Innovation, University of Chicago;
- is a member (2019-) of the scientific advisory board of Framatome;
- is the Vice-director of the French Education Committee for the China-France Mathematics Talents Class, Université Paris Cité, 2024-2029.

#### F. Legoll

- is a member of the editorial boards of *SIAM MMS* (2012-), *ESAIM: Proceedings and Surveys* (2012-) and the *Journal of Machine Learning for Modeling and Computing* (2024-);
- has co-organized (with A. Lozinski) a winter school and a workshop on *Reduced-Order Modeling for Complex Engineering Problems* within the IMSI institute in Chicago, January 29 – February 7, 2025.

#### T. Lelièvre

- is a member of the editorial boards of *SIAM/ASA Journal of Uncertainty Quantification* (2017-), *IMA: Journal of Numerical Analysis* (2018-), *Communications in Mathematical Sciences* (2019-), *Journal of Computational Physics* (2019-), *ESAIM:M2AN* (2020-), and *Foundations of Computational Mathematics* (2022-);
- is an expert for the Scientific Committee of IFPEN (since 2022);
- is the Chair of the External Advisory Board, *Mathematical Theory of Radiation Transport: Nuclear Technology Frontiers (MaThRad)* (since 2023);
- is an external member of the *Conseil Scientifique et de Prospective* of the *Institut de Mathématiques de Toulouse* (since 2023).
- is an external member of the scientific committee of *ComplexCité (Université Paris Cité)* (since 2025).

- co-organized the 4-week program *New trends and applications around generalized Fokker-Planck operators*, Bernoulli Center, 16th June-11th July 2025 (with Omar Mohsen, Francis Nier, and Shu Shen).
- co-organized and was the head of the scientific committee for the IP Paris Research Day, Telecom Paris, 1st December 2025 (with Philippe Ciblat, Fabien Leurent, Catherine Lepers, Nathanaëlle Schneider, Marieke Stein, and Gauthier Vermandel).

### G. Stoltz

- is the head of the applied mathematics department (CERMICS) at Ecole des Ponts (since Sep. 2024);
- is a member of the editorial board of *Journal of Computational Dynamics*;
- is a member of the Executive Board of GdR IAMAT (Artificial Intelligence and Materials Science);
- is a member of the "Conseil d'Enseignement et de Recherche" of Ecole des Ponts;
- co-organized in June the workshop "Dimensionality reduction techniques for molecular dynamics" at ICMS, Edinburgh, together with Lucie Delemotte (KTH), Andrew Ferguson (Univ. Chicago), Stefan Klus (Heriott Watt), Ben Leimkuhler (Univ. Edinburgh) and Edina Rosta (UCL);
- co-organized in July the CECAM research school "Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics" at Birmingham, UK, together with Xiaocheng Shang (Birmingham);
- co-organized in October the closing workshop of ANR SINEQ at GSSI, L'Aquila, together with Alessandra Iacobucci (CEREMADE), Elisa Marini (CERMADE), Stefano Olla (CEREMADE) and Lu XU (GSSI);

## 10.2 Teaching - Supervision - Juries

### 10.2.1 Teaching

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

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

- Équations aux dérivées partielles: approches variationnelles, 15h (S. Darshan, T. Duez, F. Legoll)
- Mécanique des milieux continus fluides, 25h (S. Boyaval)
- Mécanique quantique, 15h (E. Cancès, A. Negre)
- Mise à niveau en mathématiques, 16h (E. Cancès)
- Modèles et équations aux dérivées partielles, 18h (L. Carillo, T. Duez, T. Lelièvre, G. Merlini)
- Pratique du calcul scientifique, 18h (L. Carillo, U. Vaes)
- Programmation en Python, 24h (L. Carillo, G. Sambataro)
- Projets de première année, 15h (L. Carillo, T. Duez, R. Gastaldello, A. Negre, S. Ruget)

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

- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès)
- Problèmes d'évolution, 10h (F. Legoll)

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

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

- Méthodes de tenseurs par la résolution d'équations aux dérivées partielles en grande dimension, 20h (V. Ehrlacher)
- Principes de modélisation, 30h (F. Legoll)
- Théorie spectrale et méthodes variationnelles, 10h (E. Cancès)

At other institutions:

- Aléatoire (MAP361), 40h, Ecole Polytechnique (V. Ehrlacher)
- Calcul Différentiel et Optimisation, 36h, Université Paris-Dauphine, PSL (D. Gontier)
- Gestion des incertitudes et analyse de risque (MAP568), 20h, Ecole Polytechnique (T. Lelièvre)
- Introduction to Machine Learning, 64h, Institut polytechnique Paris, M1 Applied mathematics and statistics (G. Stoltz)
- Modal de Mathématiques Appliquées (MAP473D), 15h, Ecole Polytechnique (T. Lelièvre)
- Modélisation de phénomènes aléatoires (MAP432), 40h, Ecole Polytechnique (V. Ehrlacher, T. Lelièvre)
- Optimisation et Transport Optimal, 38h, ENS Paris (S. Perrin-Roussel)
- Numerical Analysis, 56h, NYU Paris (U. Vaes)

### 10.2.2 Supervision

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

- Noé Blassel, funding ERC Synergy EMC2, Analysis and sampling of metastable and nonequilibrium stochastic dynamics, Ecole des Ponts, co-supervised by T. Lelièvre and G. Stoltz, defended in December.
- Shiva Darshan, funding ANR SINEQ, Linear response of constrained stochastic dynamics, co-supervised by G. Stoltz and S. Olla (Université Paris-Dauphine), defended in December.
- Arthur Guillot – Le Goff, funding ENPC, Hydrodynamic and microbiological modelling of urban water bodies for the prevention of health risks in open water bathing, Ecole des Ponts, co-supervised by B. Vinçon Leite, R. Carmigniani and S. Boyaval, defended in December.
- Abbas Kabalan, thèse CIFRE SAFRANTech, Reduced-order models for problems with non-parametric geometrical variations, co-supervised by V. Ehrlacher and F. Casenave (SAFRANTech), defended in December.
- Albéric Lefort, funding CERMICS-ENPC, Multiscale approaches for reaction-diffusion equations and applications, Ecole des Ponts, co-supervised by F. Legoll and C. Le Bris, defended in December.
- Simon Ruget, funding Inria, Effective approximations for multiscale PDEs based on limited information, Ecole des Ponts, co-supervised by F. Legoll and C. Le Bris, defended in December.
- Jean-Paul Travert, funding CIFRE EDF, Data assimilation for flood predictions, since November 2022, supervised by S. Boyaval (and C. Goeury, F. Zaoui and V. Bacchi from EDF), defended in October.

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

- Yann Bouchereau, funding ENPC, Multiscale approaches in neutronics, and related problems, Institut Polytechnique de Paris, since September 2025, co-supervised by F. Legoll and C. Le Bris
- Thomas Brunel, funded by ANR Neptune, Paddle sports physics: Velocity–stroke rate and active drags, supervised by S. Boyaval (and R. Carmigniani from ENPC)

- Louis Carillo, funded by a CDSN fellowship with additional funding from ENPC, Mathematical analysis and numerical methods for metastable systems in statistical physics, since September 2024, co-supervised by T. Lelièvre and U. Vaes
- Charlotte Chapellier, funding CIFRE Sanofi, Generative methods for drug design, since October 2023, co-supervised by T. Lelièvre and G. Stoltz
- Antonin Coatantiec, funding AMX, Mathematical and numerical analysis for sampling metastable dynamics, since October 2025, co-supervised by T. Lelièvre and G. Stoltz
- Théo Duez, funding CNRS, Contributions to the development of new approximations and numerical methods for Time-Dependent Density-Functional Theory (TDDFT) for molecules and materials, since October 2024, co-supervised by E. Cancès and M. Lewin (CEREMADE, CNRS and Université Paris-Dauphine PSL)
- François Escolan, funding ERC HighLEAP, Stochastic particle methods for optimal transport, since November 2024, co-supervised by V. Ehrlacher, J. Reygner (CERMICS) and A. Alfonsi (MATHRISK).
- Sofiane Ezzehi, funding Région Île-de-France and IFPEN, Nonlinear reduced-order modeling techniques for underground CO2 storage applications, since November 2024, co-supervised with G. Enchéry (IFPEN).
- Raphaël Gastaldello, funding CNRS, Variance reduction methods for the computation of transport coefficients, since December 2023, co-supervised by G. Stoltz and U. Vaes
- Baptiste Guilbery, funding Inria, Applications of model reduction techniques to thermo-hydro-mechanical simulations in porous media, since November 2025, co-supervised by S. Boyaval and G. Enchéry (IFPEN)
- Clément Guillot, funding ENPC, Space-time variational principles for the Schrödinger equation in large dimension, since November 2023, co-supervised by V. Ehrlacher and M. Dupuy (Sorbonne Université)
- Jean-Baptiste Himbert, funding Ministry of Ecology, Machine learning for molecular dynamics in materials science, since September 2025, co-supervised by T. Lelièvre and G. Stoltz
- Pierre Marmey, funding IFPEN, Evaluation of reaction constants using approaches coupling machine learning and quantum chemistry, since October 2023, co-supervised by T. Lelièvre and P. Raybaud (IFPEN), together with G. Stoltz and M. Corral-Valero (IFPEN)
- Alicia Negre, funding Inria, Quantum computing for quantum embedding methods, since October 2023, co-supervised by E. Cancès and T. Ayrat (Ecole Polytechnique)
- Solal Perrin-Roussel, funding ENPC and ERC Synergy EMC2, Mathematical analysis and numerical simulation of electronic transport in moiré materials, since September 2022, co-supervised by É. Cancès and by D. Gontier
- Henri Pinsolle, funding Onera, Calcul quantique appliqué à la résolution d'équations aux dérivées partielles linéaires et non linéaires, since November 2024, co-supervised by E. Cancès and F. Renac (Onera)
- Thaddeus Roussigne, funding Université Paris-Dauphine, Etude mathématique des distorsions dans le graphène, since Septembre 2023, co-supervised by D. Gontier and E. Séré (Université Paris-Dauphine).
- Jean Ruel, funding ENS-Saclay, Certified and robust reduced models for the simulation of elongated structures, Ecole des Ponts, since October 2023, co-supervised by F. Legoll, L. Chamoin (ENS Paris-Saclay) and A. Lebée (Ecole des Ponts)
- Jonte Weixler, funding Studienstiftung scholarship, New spectral methods for eigenvalue optimization, since Septembre 2025, co-supervised by D. Gontier and J. Dolbeault (Université Paris-Dauphine).

### 10.2.3 Juries

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

- T. Lelièvre, PhD of Nicolai Gouraud ("Stochastic algorithms for high-dimensional sampling in molecular dynamics: mathematical analysis and scalable implementation"), defended at Sorbonne Université in June (examiner)
- T. Lelièvre, PhD of Loïs Delande ("Hypocoercivité semiclassique et loi d'Eyring-Kramers pour des opérateurs de Fokker-Planck dégénérés") defended at Université de Bordeaux in June (examiner)

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

- E. Cancès, HdR of Ivan Duchemin ("Algorithms and Methodologies for Large Scale Simulations in Many Body Perturbation Theory"), defended at Université Grenoble Alpes in June (referee)

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

- T. Lelièvre, professor position at Ecole Polytechnique

## 10.3 Conference participation

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

- N. Blassel, "QSD and applications" workshop, CERMICS, May
- N. Blassel, SMAI 2025, Carcans-Maubuisson, June
- N. Blassel, "New trends and applications around generalized Fokker-Planck operators" program, Bernoulli center (Lausanne), July
- N. Blassel, "Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics" CECAM Summer School, Birmingham, July
- N. Blassel, ANR SINEQ final conference, l'Aquila, October
- T. Borsoni, OxPDE seminar, Oxford, December
- T. Borsoni, Séminaire d'Analyse Numérique, Rennes (IRMAR), November
- T. Borsoni, Workshop NewOT, Orsay (IMO), November
- T. Borsoni, Conference ArpiLYSM2, Arpino (Roma), November
- T. Borsoni, Workshop LYSacadémie, Allumiere (Roma), June
- T. Borsoni, Séminaire ANCS, Besançon (LMB), June
- T. Borsoni, Conference WASCOM, Parma, June
- T. Borsoni, Seminar at the University of Novi Sad, Serbia, April
- S. Boyaval, Groupe de travail "Schémas de Boltzmann sur réseau", Orsay, February
- S. Boyaval, GT CalVa, Orsay, March
- S. Boyaval, 7th ECCOMAS Conference MSF 2025, Split (Croatia), June
- S. Boyaval, 6th IAHR Conference ISSF 2025, Torino (Italy), September
- E. Cancès, Oberwolfach workshop on Mathematical Methods in Quantum Chemistry, March
- E. Cancès, PTEROSOR workshop on emerging electronic structure methods for excited states, Toulouse, April

- E. Cancès, Moiré Materials Magic workshop, Flatiron Institute, New York, USA, May
- E. Cancès, WATOC 2025 (invited lecture), Oslo, Norway, June
- E. Cancès, IHP seminar on Spectral problems in mathematical physics, Institut Henri Poincaré, Paris, December
- L. Carillo, Journée de la physique statistique, ENS, January
- L. Carillo, Stochastic processes: Inferences in complex systems, Cecam HQ, Lausanne, May
- L. Carillo, QSD and related field, ENPC, June
- L. Carillo, Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics, CECAM Summer School, Birmingham, July
- L. Carillo, CECAM Moser grant day, ESPCI, December
- L. Delande, Séminaire d'analyse, LMJL, November
- L. Delande, Séminaire PM-EDP, LAGA, December
- A. Della Noce, CMX Seminar, Caltech, USA, February
- D. Gontier, Topological Transport and Magnetic Matter Conference, Roma, June
- R. Gastaldello, SMAI 2025, Carcans-Maubuisson, June
- R. Gastaldello, "Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics" CECAM Summer School, Birmingham, July
- R. Gastaldello, ANR SINEQ final conference, l'Aquila, October
- L. Grazioli, Oberwolfach workshop on Mathematical Methods in Quantum Chemistry, March
- L. Grazioli, WATOC 2025, Oslo, Norway, June
- L. Grazioli, STC 2025, Berlin, Germany, September
- C. Guillot, Interdisciplinary conference on many-body theory, Faculté des Sciences et Technologies, Nancy, June
- C. Guillot, OMG-DMV-2025, Johannes Kepler University Linz (JKU), Linz
- C. Le Bris, Workshop in honor of Anders Szepessy 65th birthday, KTH Stockholm, Sweden, August
- C. Le Bris, 8th Najman conference, Centre for Advanced Academic Studies, Dubrovnik, Croatia, September
- A. Lefort, SMAI biannual meeting, Carcans-Maubuisson, June
- F. Legoll, 8th ENPC – U. Tokyo workshop on Multiscale Analysis of Materials (online), March
- F. Legoll, Workshop "Computational Multiscale Methods", Oberwolfach, 28 April – 2 May
- F. Legoll, ADMOS conference, Barcelona, June
- F. Legoll, CM3P conference, Porto, July
- F. Legoll, ENUMATH conference, Heidelberg, September
- F. Legoll, SIAM GS25 conference, Baton Rouge, October
- F. Legoll, MORTech workshop, Zaragoza, November
- T. Lelièvre, LIA CNRS - UIUC Meeting, Hauteluce, January

- T. Lelièvre, BCAM seminar, Bilbao, January
- T. Lelièvre, Colloquium, Université d'Evry, January
- T. Lelièvre, Recent Advances in Modelling Rare Events, RARE 2025, Khajuraho, India, March
- T. Lelièvre, GAMM Annual Meeting, Poznań, Poland, April
- T. Lelièvre, Groupe de travail  $a^3$ , Sorbonne Université, May
- T. Lelièvre, CECAM workshop, University of Chicago Center in Paris, June
- T. Lelièvre, Plenary speaker at the SMAI biannual meeting, Carcans-Maubuisson, June
- T. Lelièvre, H2020 ENGAGE conference, ESRF Grenoble, June
- T. Lelièvre, Bernoulli program "New trends and applications around generalized Fokker-Planck operators", Bernoulli center (Lausanne), June
- T. Lelièvre, Conference in honor of Anders Szepessy, KTH, August
- T. Lelièvre, ANR SINEQ final conference, Aquila, October
- T. Lelièvre, Bernoulli conference, "Particles, Flows & Maps for Sampling Complex Distributions", Bernoulli center (Lausanne), November
- T. Lelièvre, Conference "Navigating Rugged Landscape", JNCASR, Bengaluru, November
- T. Lelièvre, Conference "Mesures de Gibbs, Turbulence d'onde et EDP stochastiques", Université Evry-Paris Saclay, December
- G. Merlini, Conference SIMAI, Trieste, September
- S. Perrin-Roussel, GAMM Annual Meeting, Poznań, Poland, April
- S. Perrin-Roussel, Journées du DMA, Guerlédan, June
- S. Ruget, SMAI biannual meeting, Carcans-Maubuisson, June
- S. Ruget, Seminar of the Navier laboratory multiscale team, ENPC, November
- G. Stoltz, CECAM workshop "Data-driven, low-dimensional, and generative models for molecular and materials discovery and design", UChicago Center in Paris, Paris, June
- G. Stoltz, Bernoulli program "New trends and applications around generalized Fokker-Planck operators", Lausanne (Bernoulli center), Switzerland, July
- G. Stoltz, CECAM summer school "Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics", Birmingham, UK, July
- G. Stoltz, SCALES Conference, Mainz, Germany, September
- G. Stoltz, workshop "CoMPASs: computational materials science and mathematics at the particle and atomistic scales", ICMS, Edinburgh, UK, November
- U. Vaes, CMX Seminar, Caltech, USA, February
- U. Vaes, Ulm University Mathematics Seminar, Ulm, Germany, June
- U. Vaes, "Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics" CECAM Summer School, Birmingham, UK, July
- U. Vaes, ENUMATH conference, Heidelberg, Germany, September
- U. Vaes, Groupe de travail "Algorithmes stochastiques", Champs-sur-Marne, December

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

- E. Cancès, Numerical methods for the quantum many-body problem, Spring School on Sparsity and Singular Structures (4h), Rolduc, The Netherlands, May
- E. Cancès, Mathematical foundations of electronic structure calculation, Modern Wavefunction Methods in Electronic Structure Theory (MWM 2025) Summer School, Pisa, Italy, September
- D. Gontier, Eigenvalue optimization, online lecture at School of Mathematics & Statistics, Central China Normal University, Wuhan, China, November.
- T. Lelièvre, Programme New trends and applications around generalized Fokker-Planck operators, "Metastability and partial differential equations" (6h), Bernoulli Center, June
- G. Stoltz, (Un)supervised learning with applications to molecular dynamics, 9h lecture, 7th edition of the Mini-school on mathematics for theoretical chemistry and physics, Sorbonne Université, Paris, France, May

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

- S. Ruget, Workshop "Reduced-Order Modeling for Complex Engineering Problems", Chicago, USA, February

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

- T. Borsoni, Conference Kinetic theory and fluid mechanics, CIRM, April
- S. Boyaval, IVth ECCOMAS Conference CMCS 2025, Champs-sur-Marne, May
- A. Coataniec, Bernoulli conference, "Particles, Flows & Maps for Sampling Complex Distributions", Bernoulli center (Lausanne), November
- J.-B. Himbert, AdONE Summer School, Heilbronn, June
- J.-B. Himbert, LIA CNRS - UIUC Meeting, Hauteluce, January
- C. Le Bris, Workshop "Computational Multiscale Methods", Oberwolfach, 28 April – 2 May
- G. Merlini, Workshop HyBOX, ENSTA, December

## 10.4 Popularization

- A. Della Noce, Parole de Chercheuses et Chercheurs, Lycée Jean-Pierre Vernant, Sèvres, February
- D. Gontier gave a talk on "Puzzles" for secondary school students visiting CERMICS, ENPC, February
- D. Gontier animated several sessions on "Puzzles" for "Fête de la Science", ENPC, October
- T. Lelièvre did 1 session of CHICHE at Lycée Louise Michel (Champigny-sur-Marne)
- G. Stoltz did 10 sessions of CHICHE at lycées international Palaiseau, Hélène Boucher (Paris), Turgot (Paris) and Montesquieu (Herblay-sur-Seine)
- G. Stoltz did "AI improv sessions" at the Science feast of Ecole des Ponts (Marne-la-Vallée, October 2025)
- G. Stoltz chaired with Adèle Mazurek the "Flash science" session at the Double Science festival (Ground Control, Paris, June 2025)
- G. Stoltz did presentation sessions for high school interns (Inria and Ecole des Ponts, June 2025)
- S. Perrin-Roussel did presentation sessions for primary school pupils at Groupe scolaire Irène and Frédéric Joliot (Champs-sur-Marne)

## 11 Scientific production

### 11.1 Major publications

- [1] X. Blanc and C. Le Bris. *Homogénéisation en milieu périodique... ou non*. Vol. 88. Mathématiques et Applications. Springer International Publishing, 2022. DOI: [10.1007/978-3-031-12801-1](https://doi.org/10.1007/978-3-031-12801-1). URL: <https://hal.science/hal-04368339> (cit. on p. 10).
- [2] X. Blanc and C. Le Bris. *Homogenization Theory for Multiscale Problems*. Vol. 21. MS&A. Springer Nature Switzerland, 2023. DOI: [10.1007/978-3-031-21833-0](https://doi.org/10.1007/978-3-031-21833-0). URL: <https://hal.science/hal-04368342> (cit. on p. 10).
- [3] 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 (cit. on p. 6).
- [4] 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 (cit. on p. 6).
- [5] 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 (cit. on p. 6).
- [6] 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 (cit. on p. 6).
- [7] 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 (cit. on p. 6).
- [8] 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 (cit. on p. 6).
- [9] T. Lelièvre, M. Rousset and G. Stoltz. *Free Energy Computations: A Mathematical Perspective*. Imperial College Press, 458~p., 2010 (cit. on p. 6).

### 11.2 Publications of the year

#### International journals

- [10] E. Beteille, F. Larrarte, S. Boyaval, E. Demay and M.-H. Le. ‘Dam-break flow over various obstacles configurations’. In: *Journal of Ecohydraulics* 63 (3rd Mar. 2025), pp. 156–170. DOI: [10.1080/00221686.2025.2460020](https://doi.org/10.1080/00221686.2025.2460020). URL: <https://hal.science/hal-05035422>.
- [11] R. A. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. ‘MsFEM for advection-dominated problems in heterogeneous media: Stabilization via nonconforming variants’. In: *Computer Methods in Applied Mechanics and Engineering* 433 (2025), p. 117496. DOI: [10.1016/j.cma.2024.117496](https://doi.org/10.1016/j.cma.2024.117496). URL: <https://hal.science/hal-04620050>.
- [12] M.-R. Blel, V. Ehrlacher and T. Lelièvre. ‘Influence of sampling on the convergence rates of greedy algorithms for parameter-dependent random variables’. In: *Mathematics of Computation* (2025). DOI: [10.1090/mcom/3979](https://doi.org/10.1090/mcom/3979). URL: <https://hal.science/hal-03238244> (cit. on p. 18).
- [13] A. Bordignon, É. Cancès, G. Dusson, G. Kemlin, R. A. L. Reyes and B. Stamm. ‘Fully guaranteed and computable error bounds on the energy for periodic Kohn-Sham equations with convex density functionals’. In: *SIAM Journal on Scientific Computing* 47.5 (10th Oct. 2025), A2881–A2905. DOI: [10.1137/25M1735676](https://doi.org/10.1137/25M1735676). URL: <https://hal.science/hal-04699502>.
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