

RESEARCH CENTRE

**Inria Paris Centre**

IN PARTNERSHIP WITH:

**Ecole des Ponts ParisTech**

2023

ACTIVITY REPORT

Project-Team

**MATHERIALS**

## **MATHEmatics for MatERIALS**

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

### **DOMAIN**

**Applied Mathematics, Computation and  
Simulation**

### **THEME**

**Numerical schemes and simulations**

*Inria*

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## Project-Team MATERIALS

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

### 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. – High performance computing
- A6.3.1. – Inverse problems
- A6.3.4. – Model reduction
- A6.4.1. – Deterministic control

#### Other research topics and application domains

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

# 1 Team 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 [ENPC, Senior Researcher, HDR]
- Frédéric Legoll [ENPC, Senior Researcher, HDR]
- Tony Lelièvre [ENPC, Senior Researcher, HDR]
- Gabriel Stoltz [ENPC, Senior Researcher, HDR]
- Urbain Vaes [INRIA, ISFP]

## Faculty Members

- Yves Achdou [UNIV PARIS, Professor Delegation, until Aug 2023, HDR]
- Arnaud Guyader [SORBONNE UNIVERSITE, Professor Delegation, HDR]
- Luca Nenna [UNIV PARIS SACLAY, Associate Professor Delegation]

## Post-Doctoral Fellows

- Amandine Boucart [ENPC, Post-Doctoral Fellow, from Apr 2023]
- Mathias Dus [ENPC, Post-Doctoral Fellow]
- Rodrigue Lelotte [ENPC, Post-Doctoral Fellow, from Nov 2023]
- Etienne Polack [ENPC, Post-Doctoral Fellow, from Feb 2023]
- Mohamad Rachid [ENPC, Post-Doctoral Fellow, until Aug 2023]
- Giulia Sambataro [ENPC, Post-Doctoral Fellow, from Feb 2023]
- Masaaki Tokieda [INRIA, Post-Doctoral Fellow, until Mar 2023]

## PhD Students

- Rutger Biezemans [ENPC, until Sep 2023]
- Noé Blassel [ENPC]
- Andrea Bordignon [ENPC]
- Jean Cauvin-Vila [ENPC & Inria, until Aug 2023]
- Shiva Darshan [ENPC]
- Renato Freitas Spacek [INRIA]
- Raphaël Gastaldello [ENPC, from Dec 2023]
- Clément Guillot [ENPC, from Nov 2023]
- Alfred Kirsch [ENPC]

- Albéric Lefort [ENPC]
- Eloïse Letournel [ENPC]
- Alicia Negre [INRIA, from Oct 2023]
- Solal Perrin-Roussel [ENPC]
- Thomas Pigeon [INRIA, until Oct 2023]
- Simon Ruget [INRIA]
- Régis Santet [ENPC]
- Laurent Vidal [ENPC]

### **Interns and Apprentices**

- Raphael Gastaldello [INRIA, Intern, from Mar 2023 until Jul 2023]
- Alicia Negre [INRIA, Intern, from Apr 2023 until Sep 2023]

### **Administrative Assistant**

- Julien Guieu [INRIA]

### **Visiting Scientist**

- Pierre Marmey [IFPEN]

### **External Collaborators**

- Antoine Levitt [UNIV PARIS SACLAY, HDR]
- Alexei Lozinski [UNIV FRANCHE-COMTE, HDR]

## **2 Overall objectives**

The MATERIALS project-team was created jointly by the École des Ponts ParisTech (ENPC) and Inria in 2015. It is the follow-up and an extension of the former project-team MICMAC originally created in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques et Calcul Scientifique) at École des Ponts. The permanent research scientists of the project-team have positions at CERMICS and at two other laboratories of École des Ponts: Institut Navier and Laboratoire Saint-Venant. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulation of computational chemistry at the microscopic level and to create simulations coupling this microscopic scale with meso- or macroscopic scales (possibly using parallel algorithms). Over the years, the project-team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the project-team is to have created a corpus of literature, authoring books and research monographs on the subject [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

- C. Le Bris held a Senior Zuse fellowship at the Zuse Institut Berlin.
- V. Ehrlacher was awarded the ERC Starting Grant HighLEAP (High-dimensional mathematical methods for Large Agent and Particle Systems).
- V. Ehrlacher was awarded the "Young Female Scientist" Irène Joliot-Curie prize.
- U. Vaes was awarded the ANR IPSO (Interacting Particle systems for Sampling and Optimization), as part of the programme "Jeunes Chercheuses et Jeunes Chercheurs".

## 6 New software, platforms, open data

### 6.1 New software

#### 6.1.1 DFTK

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

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

**Release Contributions:** In 2023 DFTK has gained support for phonon computations, nonlinear core correction and improved Wannier integration. It also received many other smaller improvements, and 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:** Andrea Bordignon, Eric Cancès, Virginie Ehrlacher, Alfred Kirsch, Claude Le Bris, Eloïse Letournel, Solal Perrin-Roussel, Etienne Polack, Laurent Vidal.

#### 7.1.1 Density functional theory

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

E. Cancès co-edited with G. Friesecke (TU Munich, Germany) a book on Density Functional Theory reviewing modeling aspects, mathematical and numerical analysis results, computational methods, and state-of-the-art applications (Springer 2023, [40]). In Chapter 7 of this book [41], E. Cancès, A. Levitt, Y. Maday (Sorbonne University), and C. Yang (LBNL, Berkeley, USA) discuss the main algorithms used to solve the Kohn–Sham models, as well as the recent numerical analysis of these models and algorithms.

Together with G. Kemlin (former PhD student in the project-team and now at University of Amiens) and A. Levitt (University Paris-Saclay), E. Cancès has studied the numerical analysis of linear and nonlinear Schrödinger equations with periodic analytic potentials [20]. They prove that, for linear equations, when the potential is analytic in a strip of width  $A$  of the complex plane, the solution is analytic in the same strip, ensuring an exponential convergence of the planewave discretization of the equation with rate  $A$ . On the other hand, for nonlinear equations such as the periodic Kohn–Sham equations with Goedecker–Teter–Hutter (GTH) pseudopotentials, they find that the solution may be analytic only in a strip of width smaller than  $A$ . This behavior is illustrated by two examples using a combination of numerical and analytical arguments.

Together with G. Dusson (CNRS and University of Besançon), B. Stamm (University of Stuttgart), and F. Lipparini, P. Mazzeo, and F. Pes (quantum chemists from the university of Pisa), E. Polack proposed a scheme based on Grassmann extrapolation of density matrices for an accurate calculation of initial guesses in Born–Oppenheimer Molecular Dynamics simulations [32]. The method shows excellent results on large quantum mechanics/molecular mechanics systems simulated with Kohn–Sham density functional theory.

Etienne Polack and Laurent Vidal developed new functionalities in DFTK, a Julia library implementing plane-wave density functional theory for the simulation of the electronic structure of molecules and materials, whose development was launched in 2019 within the Project-Team MATERIALS (main developers: M. Herbst, now at EPFL, and A. Levitt, now at Université Paris-Saclay).

#### 7.1.2 Quantum embedding methods

The treatment of strongly correlated quantum systems is a long-standing challenge in computational chemistry and physics. The application of high-accuracy first-principle methods that are able to capture the electronic correlation effects at chemical accuracy is commonly stymied by a steep computational scaling with respect to system size. A potential remedy is provided by quantum embedding theories, which can be somehow interpreted as domain decomposition methods for the quantum many-body problem in the Fock space. Such approaches include the dynamical mean-field theory (DMFT) and the density matrix embedding theory (DMET). Together with F. Faultsich (UC Berkeley, USA) and A. Levitt, E. Cancès, A. Kirsch and E. Letournel provided the first mathematical analysis of DMET [47]. They prove that, under certain assumptions, (i) the exact ground-state density matrix is a fixed-point of the DMET map

for non-interacting systems, (ii) there exists a unique physical solution in the weakly-interacting regime, and (iii) DMET is exact at first order in the coupling parameter. They provide numerical simulations to support their results and comment on the physical meaning of the assumptions under which they hold true. They show that the violation of these assumptions may yield multiple solutions of the DMET equations.

### 7.1.3 Moiré materials

Twisted bilayer graphene (TBG) is obtained by stacking two identical graphene sheets on top of one another and rotating them in opposite directions around the transverse direction by a relative, typically small, angle  $\theta$ . Seen from above, this gives rise to a moiré pattern whose diameter scales as  $\theta^{-1}$ . TBG is a controllable quantum system, in the sense that its properties can be finely tuned by playing with the twist angle (with, currently, an experimental accuracy of  $\sim 0.1^\circ$ ), the transverse external electric field generated by gating (which allows one to control the doping, that is the density of charge carriers), the in-plane external electric field, the external magnetic field, the temperature, the interlayer distance (which can be changed by applying a pressure field), etc. The theoretical and experimental study of TBG has been one of the hottest topics in condensed matter physics since notably, the experimental discovery of supposedly unconventional superconducting regions in the phase diagram of TBG at “magic” twist angle  $\theta \simeq 1.08^\circ$ . Together with L. Meng (Ecole des Ponts), E. Cancès has investigated the mathematical properties of independent-electron models for TBG by examining the density-of-states of corresponding single-particle Hamiltonians using tools from semiclassical analysis [48]. This study focuses on a specific atomic-scale Hamiltonian constructed from Density-Functional Theory, and a family of moiré-scale Hamiltonians containing the Bistritzer-MacDonald model. It is shown that the density-of-states of these Hamiltonians admit asymptotic expansions in the twist angle parameter  $\epsilon := \sin(\theta/2)$ . The proof relies on a twisted version of the Weyl calculus and a trace formula for an exotic class of pseudodifferential operators suitable for the study of twisted 2D materials.

### 7.1.4 Open quantum systems and quantum computing

In his post-doctoral work co-supervised by Claude Le Bris (MATERIALS) and Pierre Rouchon (Inria QUANTIC), Masaaki Tokieda has addressed various issues related to the numerical simulation and the fundamental understanding of several models of physical systems likely candidates to play a crucial role in quantum computing.

### 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.

On the one hand, appropriate modified Wasserstein barycenters have been used in order to design new reduced-order model reduction methods to accelerate electronic structure calculations of molecules. First, together with Geneviève Dusson and Nathalie Nouaime, V. Ehrlacher developed new types of mixture Wasserstein distances and barycenters adapted to electronic densities that can be written as squares of linear combination of Slater determinants of Gaussian functions in [55]. Second, in [53], V. Ehrlacher (together with M. Dalery, G. Dusson and A. Lozinski) worked on the design of new greedy algorithms using the latter mixture Wasserstein barycenters and on the proof of estimates on the decay of Kolmogorov  $n$ -widths related to these Wasserstein-type distances on some one-dimensional electronic structure calculations toy models.

On the other hand, V. Ehrlacher and L. Nenna proved in [57] that moment-constrained approximations of the Lieb functional (which may be seen as a particular instance of quantum optimal transport problems) enjoyed similar sparsity properties as moment-constrained approximation of classical optimal transport problems.

## 7.2 Computational statistical physics

**Participants:** Noé Blassel, Shiva Darshan, Raphaël Gastaldello, Arnaud Guyader, Tony Lelièvre, Thomas Pigeon, Mohamad Rachid, Régis Santet, Renato Spacek, Gabriel Stoltz, Urbain Vaes.

The aim of computational statistical physics is to compute macroscopic properties of materials starting from a microscopic description, using concepts of statistical physics (thermodynamic ensembles and molecular dynamics). The contributions of the team can be divided into four 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 use of particle methods for sampling and optimization.

Before presenting the contributions in more detail, let us first mention two recent reviews written by the members of the team, in a book entitled *Comprehensive Computational Chemistry*, namely [43] by T. Lelièvre with D. Perez (LANL, USA), and [42] by T. Lelièvre and G. Stoltz with C. Chipot (CNRS and Université de Lorraine, France) and P. Gkeka (Sanofi, France). They respectively review recent advances in Accelerated Molecular Dynamics methods, and on (non)equilibrium methods for free-energy calculations with molecular dynamics.

### 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. In [61], T. Lelièvre, R. Santet and G. Stoltz develop and study a new variant of the Hamiltonian Monte Carlo algorithm which can be used for nonseparable Hamiltonian. Such Hamiltonian functions naturally appear in many contexts, for numerical or physical reasons, for example when a position-dependent mass is considered. To get an unbiased sampling method, a reversibility check has to be enforced, because of the implicitness of the Störmer–Verlet integrator.

In order to improve the efficiency of sampling, variance reduction techniques should be used. In [50], T. Lelièvre, G. Stoltz and U. Vaes, together with M. Chak (Sorbonne Université, France) analyze an importance sampling approach for Markov chain Monte Carlo methods that relies on the overdamped Langevin dynamics. More precisely, they study an estimator based on an ergodic average along a realization of an overdamped Langevin process for a modified potential. An explicit expression for the biasing potential that minimizes the asymptotic variance of the estimator is obtained in dimension 1, and a general numerical approach for approximating the optimal potential in the multi-dimensional setting is proposed. The capabilities of the proposed method are demonstrated by means of numerical experiments.

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 (Université Paris Dauphine, France), G. Stoltz studied in [46] how to obtain constructive decay estimates for the semigroup corresponding to hypoelliptic generators associated with Langevin dynamics, using hypocoercive techniques based on space time averages and Lions' lemma.

Finally, let us mention that the stochastic dynamics used to sample probability measures in statistical physics can also be used to minimize functions when the temperature is sent to 0. This idea is used in the work [27] by G. Stoltz together with K. Karoni and B. Leimkuhler (University of Edinburgh, United-Kingdom), where variations of the adaptive Langevin dynamics (an underdamped Langevin dynamics where the friction is adjusted through some feedback term à la Nosé–Hoover) are considered to minimize high dimensional objectives.

### 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. R. Gastaldello is starting his PhD work on this topic. Let us next describe the efforts of the team done in the previous year.

In [35], R. Spacek and G. Stoltz proposed to add an additional perturbation to the system (so-called synthetic forcing), which preserves the invariant measure and hence does not change the linear response, but which allows to limit the nonlinearity of the response. This makes it possible to resort to larger forcings in practice, and hence more easily determine the response of the nonequilibrium system. Several classes of admissible synthetic forcings are systematically studied, and their performance is assessed on toy systems.

Another way to possibly reduce the variance of estimators of transport coefficients based on nonequilibrium molecular dynamics is to resort to a dual strategy. Whereas standard non-equilibrium approaches fix the forcing and measure the average flux induced in the system driven out of equilibrium, a dual philosophy consists in fixing the value of the flux, and measuring the average magnitude of the forcing needed to induce it. A deterministic version of this approach, named Norton dynamics, was studied in the 1980s by Evans and Morriss. In [45], N. Blassel and G. Stoltz introduce a stochastic version of this method, first developing a general formal theory for a broad class of diffusion processes, and then specializing it to underdamped Langevin dynamics, which are commonly used for molecular dynamics simulations. Numerical evidence demonstrates that the stochastic Norton method provides an equivalent measure of the linear response, and in fact that this equivalence extends well beyond the linear response regime. This work raises many intriguing questions, both from the theoretical and the numerical perspectives.

On the applicative side, G. Stoltz studied in [26] with T. Hoang Ngoc Minh and B. Rotenberg (Sorbonne Université, France) the effect of confinement, adsorption on surfaces, and ion-ion interactions on the response of confined electrolyte solutions to oscillating electric fields in the direction perpendicular to the confining walls. Nonequilibrium simulations allow to characterize the transitions between linear and nonlinear regimes when varying the magnitude and frequency of the applied field, but the linear response, characterized by the frequency-dependent conductivity, is more efficiently predicted from the equilibrium current fluctuations. To that end, a Green-Kubo relation appropriate for overdamped dynamics is rederived for time periodic forcings. The expression highlights the contributions of the underlying Brownian fluctuations and of the interactions of the particles between them and with external potentials. The frequency-dependent conductivity always decays from a bulk-like behavior at high frequency to a vanishing conductivity at low frequency due to the confinement of the charge carriers by the walls.

### 7.2.3 Sampling dynamical properties and rare events

Sampling transitions from one metastable state to another is a difficult task. In [33] T. Lelièvre, T. Pigeon and G. Stoltz, together with A. Anciaux-Sekadrian, M. Corral-Valero, M. Moreaud (collaborators at IFPEN, France) apply for the first time the Adaptive Multilevel Splitting (AMS) method to study catalytic reactions. Computing accurate rate constants for catalytic events occurring at the surface of a given material represents a challenging task with multiple potential applications in chemistry. The AMS method requires a one dimensional reaction coordinate to index the progress of the transition. To build such a reaction coordinate, various approaches are tested, including Support Vector Machine and path collective variables. The calculated rate constants and transition mechanisms are discussed and compared to those obtained by a conventional static approach based on the Eyring-Polanyi equation with harmonic approximation. The AMS method is able to better take into account entropic effects as well as complex transition mechanisms, e.g. those involving multiple pathways.

On the methodological side, A. Guyader and T. Lelièvre are currently exploring how AMS and Importance Sampling (IS) are affected by an importance function which is not exactly the committor  $\xi^*$  but a perturbation of it. AMS is expected to be less sensitive than IS, but IS to be better when the perturbation is small (zero variance principle). Specifically, one can think of an infinitesimal calculation and look at how the variance of AMS/IS degrades when considering an importance function of the form  $\xi_\eta(x) = \xi^*(x) + \eta\delta\xi(x)$ , in the limit  $\eta \rightarrow 0$ . In this respect, is it possible to combine AMS and IS in order to use "more IS" when the perturbation is small and "more AMS" when the perturbation is large?

More generally, finding collective variables to describe some important coarse-grained information on

physical systems, in particular metastable states, remains a key issue in molecular dynamics. Collective variables allow to compute free energy differences and/or bias the dynamics to observe transitions. In [59], T. Lelièvre, T. Pigeon and G. Stoltz, together with W. Zhang (FU Berlin, Germany) analyze the performances of autoencoders to construct collective variables. They study some relevant mathematical properties of the loss function considered for training autoencoders, and provide physical interpretations based on conditional variances and minimum energy paths. They also consider various extensions in order to better describe physical systems, by incorporating more information on transition states at saddle points, and/or allowing for multiple decoders in order to describe several transition paths. On the application side, T. Lelièvre and G. Stoltz, together with Z. Belkacemi, M. Bianciotto, P. Gkeka, H. Minoux (collaborators at Sanofi, France) characterize in [12] the dynamics of the N-terminal domain of the heat shock protein 90 (Hsp90) using an autoencoder-learned collective variable in conjunction with adaptive biasing force Langevin dynamics. Using this machine-learned collective variable is a crucial ingredient to generate transitions between native states.

#### 7.2.4 Interacting particle methods for sampling

In some situations, stochastic numerical methods can be made more efficient by using various replicas of the system. For algorithms based on interacting particle systems that admit a mean-field description, convergence analysis is often more accessible at the mean-field level. In order to transpose convergence results obtained at the mean-field level to the finite ensemble size setting, it is desirable to show that the particle dynamics converge in an appropriate sense to the corresponding mean-field dynamics. In [58], U. Vaes together with N. J. Gerber (Hausdorff Center for Mathematics, Germany) and F. Hoffmann (Caltech, USA) proved quantitative mean-field limit results for two related interacting particle systems: Consensus-Based Optimization and Consensus-Based Sampling. The approach employed to this end is based a generalization of Sznitman's classical argument: in order to circumvent issues related to the lack of global Lipschitz continuity of the coefficients, an event of small probability is discarded, the contribution of which is controlled using moment estimates for the particle systems. In addition, their work presents new results on the well-posedness of the particle systems and their mean-field limit, and provides novel stability estimates for the weighted mean and the weighted covariance.

### 7.3 Homogenization

**Participants:** Yves Achdou, Rutger Biezemans, Amandine Boucart, Virginie Ehrlicher, Claude Le Bris, Albéric Lefort, Frédéric Legoll, Alexei Lozinski, Simon Ruget.

#### 7.3.1 Deterministic non-periodic systems

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

In that direction, Y. Achdou (partially on leave at INRIA from Université Paris-Cité in 2022-2023) and C. Le Bris have studied in [10] the homogenization of a class of stationary Hamilton-Jacobi equations in which the Hamiltonian is obtained by perturbing near the origin an otherwise periodic Hamiltonian. Homogenization leads to an effective Hamilton-Jacobi equation supplemented with an effective Dirichlet boundary condition at the origin: this boundary value problem has to be understood in the sense of the stratified problems introduced by Bressan et al and later studied by Barles and Chasseigne. The effective Dirichlet data is obtained as the limit of a sequence of ergodic constants associated to truncated cell problems posed in balls with diameter tending to infinity. Several research directions stem from this work. In particular, an ongoing research deals with situations in which homogenization leads to stratified problems with more complex geometries, for example a stratification of the plane composed of three manifolds: an open half-line, the end-point of the latter and finally the complement of the closed half-line. Other open questions concern the rate of convergence to the solution of the effective problem and the behavior of the above-mentioned ergodic constants as the diameter of the truncated cell tends to infinity. These questions seem difficult and a sensible way to tackle them would be to carry out numerical simulations first.

Also in that direction of research, C. Le Bris has co-authored with X. Blanc two textbooks on Homogenization Theory, one in French [1] and one in English [2]. The two books mostly present the same material. The French version however dwells a bit more on the theoretical aspects while the English version is slightly more focused on computational issues. This action testifies to the wish of the team to reach the largest possible audience and introduce them to the challenging field of multiscale science. In addition, a short text that summarizes the major results obtained has been written by C. Le Bris and has been published in the "Séminaire Laurent Schwartz 2022-2023 volume" [28].

### 7.3.2 Inverse multiscale problems

In the context of the PhD of S. Ruget, C. Le Bris and F. Legoll have pursued their work on the question of how to determine the homogenized coefficient of a multiscale problem without explicitly performing an homogenization approach. This work is a follow-up on earlier works over the years in collaboration with K. Li, S. Lemaire and O. Gorynina. They have first extended their approach to the case of Schroedinger equations with rapidly oscillating potentials. Current efforts are focused on investigating the robustness of the approach with respect to the available data, which, in practice, may be noisy, blurred, incomplete, or only available in the form of averages over domains of large size (compared to the size of the microstructure).

### 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 when the homogenized problem is not known (e.g. in difficult nonlinear cases), or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as a sufficiently accurate approximation). The MsFEM approach uses a Galerkin approximation of the problem on a pre-computed basis, obtained by solving local problems mimicking the problem at hand at the scale of mesh elements.

In the context of the PhD of R. Biezemans, C. Le Bris and F. Legoll have addressed the question of how to design accurate MsFEM approaches for various types of equations, beyond the purely diffusive case, and in particular for the case of multiscale advection-diffusion problems, in the advection-dominated regime. Thin boundary layers are present in the exact solution, and numerical approaches should be carefully adapted to this situation, e.g. using stabilization. How stabilization and the multiscale nature of the problem interplay with one another is a challenging question, and several MsFEM variants have been compared by R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. The main results have been collected in Part II of the PhD manuscript of R. Biezemans (who defended his PhD thesis in September 2023) and a manuscript is about to be submitted for publication. It is shown there how MsFEM with weak continuity conditions of Crouzeix-Raviart type can be stabilized by adding specific bubble functions, satisfying the same type of weak boundary conditions.

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. From a numerical perspective, two difficulties are present in the time-dependent version of the problem. First, the coefficients of the equation (and therefore the solution) oscillate at a small spatial scale. In addition, the problem in time is stiff. In order to not address all difficulties at the same time, the associated eigenvalue problem has been considered, for which a promising MsFEM-type approach was introduced. The robustness of the method is currently being investigated.

In parallel to the exploration of advection-diffusion equations and reaction-diffusion equations, another direction of research is focused on hyperbolic multiscale conservation laws. The homogenized limit of a large class of such conservation laws has recently been established in the literature. As a preliminary work on this topic, A. Boucart (currently post-doc in the project-team), C. Le Bris and F. Legoll have put in action the classical homogenization approach, and numerically demonstrated that the two-scale approximation provided by homogenization theory is indeed an accurate approximation of the reference solution, however for a ratio between the macro and the micro scales which needs to be larger than for elliptic problems. A manuscript collecting their conclusions (on this topic as well as on related questions) is being prepared for publication.

### 7.3.4 Stochastic homogenization

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

In collaboration with B. Stamm and S. Xiang (both at Aachen University, Germany), V. Ehrlacher and F. Legoll have studied in [56] new alternatives for the approximation of the homogenized matrix in the case of the (vector-valued) linear elasticity equation. This work extends previous works dedicated to scalar-valued equations. These alternative definitions rely on the use of an embedded corrector problem, where a finite-size domain made of the highly oscillatory material is embedded in a homogeneous infinite medium whose diffusion coefficients have to be appropriately determined.

In collaboration with M. Bertin and S. Brisard (ENPC), F. Legoll has introduced in [16] a variance reduction approach for the computation of the homogenized coefficients. The method is based on concurrently using (in a control variate fashion) the reference computations (solving the corrector problem on a large but finite domain) together with some inexpensive mean-field approximations often used in the computational mechanics community, such as the ones stemming from the Hashin-Shtrikman principle. The numerical efficiency of the approach has been demonstrated on several examples, including cases with large contrasts.

## 7.4 Various topics

### 7.4.1 Complex fluids

**Participants:** Sébastien Boyaval.

In 2023, S. Boyaval has generalized the symmetric-hyperbolic system of conservation laws introduced in 2020 to a whole class of models for non-Newtonian fluids [15]. Precisely, a family of quasilinear PDEs is proved symmetric-hyperbolic and endowed with an additional dissipation inequality (a formulation of the second-principle) whatever the choice of a "stored energy functional"-"relaxation functional" couple within that class. This defines a framework for numerical methods.

### 7.4.2 Model-order reduction methods

**Participants:** Virginie Ehrlacher, Tony Lelièvre, Giulia Sambattaro.

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

In [62], V. Ehrlacher together with I. Niakh, G. Drouet (EDF) and A. Ern (SERENA) introduced a new model reduction method for parametrized linear variational inequalities of the first and second kind for mechanical contact and friction problems. The method relies on the use of a so-called Nitsche formulation of the problem. This avoids the use of dual variables, which are well-known not to be easily reducible for these types of problems.

In [52] and [51], V. Ehrlacher and T. Lelièvre, together with G. Dusson (Université de Besançon) and Y. Conjungo Taumhas, and F. Madiot (CEA) develop a reduced basis method for parametrized non-symmetric eigenvalue problems arising in the loading pattern optimization of a nuclear core in neutronics. This requires to derive a posteriori error estimates for the eigenvalue and left and right eigenvectors. A first implementation of the method in APOLLO3, the CEA/DES deterministic multi-purpose code for reactor physics analysis, is presented.

### 7.4.3 Cross-diffusion systems

**Participants:** Jean Cauvin-Vila, Virginie Ehrlacher.

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

In [49], J. Cauvin-Vila, V. Ehrlacher, G. Marino (Augsburg) and J.-F. Pietschmann (Augsburg) studied mathematically a model of a multicomponent mixture where cross-diffusion effects occur between the different species but only one species separates from the other. The evolution of the system is modeled by a gradient flow, in an appropriate metric, of a degenerate Ginzburg–Landau energy, which yields a system of coupled partial differential equations of Cahn–Hilliard type. Local minimizers of the energy functional are shown to exist and to qualify as classical stationary solutions of the system. Finally, the authors prove exponential convergence to a constant stationary solution in a particular parameter regime, and they introduce a novel structure-preserving finite volume scheme to approximate the evolution numerically.

In [37], C. Cancès, J. Cauvin-Vila, C. Chainais-Hillairet and V. Ehrlacher developed a new structure-preserving numerical scheme for a model of a physical vapor deposition process used for the fabrication of thin film layers. The model involves two different types of cross-diffusion systems coupled by an evolving interface. The moving interface is addressed with a cut-cell approach, where the mesh is locally deformed around the interface. The scheme is shown to preserve the structure of the continuous system, namely: mass conservation, nonnegativity, volume-filling constraints and decay of the free energy.

## 8 Bilateral contracts and grants with industry

Many research activities of the project-team are conducted in close collaboration with private or public companies: CEA, EDF, IFPEN, Sanofi, OSMOS Group, SAFRANTech. The project-team is also supported by the Office of Naval Research and the European Office of Aerospace Research and Development, for multiscale simulations of random materials. All these contracts are operated at and administrated by the École des Ponts, except the contracts with IFPEN, which are administrated by Inria.

## 9 Partnerships and cooperations

### 9.1 International initiatives

T. Lelièvre, G. Stoltz and F. Legoll participate in the Laboratoire International Associé (LIA) CNRS / University of Illinois at Urbana-Champaign on complex biological systems and their simulation by high performance computers. This LIA involves French research teams from Université de Nancy, Institut de Biologie Structurale (Grenoble) and Institut de Biologie Physico-Chimique (Paris). The LIA has been last renewed in January 1st, 2018.

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

### 9.2 International research visitors

#### 9.2.1 Visits to international teams

##### Research stays abroad

###### Claude Le Bris

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

**Country:** Germany

**Dates:** January-February

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

**Mobility program/type of mobility:** Research stay

### 9.3 European initiatives

#### 9.3.1 H2020 projects

##### EMC2

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

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

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

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

##### Partners:

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

**Inria contact:** Laura Grigori (Inria Alpines)

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

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

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

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

#### TIME-X

**Participants:** Frédéric Legoll, Tony Lelièvre.

[TIME-X project on openaire.eu](https://openaire.eu)

**Title:** TIME parallelisation: for eXascale computing and beyond

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

#### Partners:

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

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

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

- (i) provide software for parallel-in-time integration on current and future Exascale HPC architectures, delivering substantial improvements in parallel scaling;
- (ii) develop novel algorithmic concepts for parallel-in-time integration, deepening our mathematical understanding of their convergence behaviour and including advances in multi-scale methodology;
- (iii) demonstrate the impact of parallel-in-time integration, showcasing the potential on problems that, to date, cannot be tackled with full parallel efficiency in three diverse and challenging application fields with high societal impact: weather and climate, medicine and fusion.

To realise these ambitious, yet achievable goals, the inherently inter-disciplinary TIME-X Consortium unites top researchers from numerical analysis and applied mathematics, computer science and the selected application domains. Europe is leading research in parallel-in-time integration. TIME-X unites all relevant actors at the European level for the first time in a joint strategic research effort. A strategic investment from the European Commission would enable taking the necessary next step: advancing parallel-in-time integration from an academic/mathematical methodology into a widely available technology with a convincing proof of concept, maintaining European leadership in this rapidly advancing field and paving the way for industrial adoption.

## HighLEAP

**Participants:** Virginie Ehrlicher, Clément Guillot, Mathias Dus, Rodrigue Lelotte, Giulia Sambataro.

[EMC2 project on cordis.europa.eu](https://cordis.europa.eu/emc2)

**Title:** High-dimensional mathematical methods for Large Agent and Particle Systems

**Duration:** From December 1, 2023 to November 30, 2028

**Partners:**

- École Nationale des Ponts et Chaussées (ENPC), France

**Coordinators:** Virginie Ehrlicher (ENPC)

**Summary:** Interacting particle or agent-based systems are ubiquitous in science. They arise in an extremely wide variety of applications including materials science, biology, economics and social sciences. Several mathematical models exist to account for the evolution of such systems at different scales, among which stand optimal transport problems, Fokker-Planck equations, mean-field games systems or stochastic differential equations. However, all of them suffer from severe limitations when it comes to the simulation of high-dimensional problems, the high-dimensionality character coming either from the large number of particles or agents in the system, the high amount of features of each agent or particle, or the huge quantity of parameters entering the model. The objective of this project is to provide a new mathematical framework for the development and analysis of efficient and accurate numerical methods for the simulation of high-dimensional particle or agent systems, stemming from applications in materials science and stochastic game theory.

The main challenges which will be addressed in this project are:

- sparse optimization problems for multi-marginal optimal transport problems, using moment constraints;
- numerical resolution of high-dimensional partial differential equations, with randomized iterative algorithms;
- efficient approximation of parametric stochastic differential equations, by means of reduced-order modeling approaches.

The potential impacts of the project are huge: making possible such extreme-scale simulations will enable to gain precious insights on the predictive power of agent- or particle-based models, with applications in various fields, such as quantum chemistry, molecular dynamics, crowd motion or urban traffic.

#### 9.4 National initiatives

The project-team is involved in several ANR projects:

- V. Ehrlicher was the PI of the ANR project COMODO (2019-2023) which focuses on the development of efficient numerical methods to simulate cross-diffusion systems on moving domains, with application to the simulation of the fabrication process of thin film solar cells. It includes Inria project-teams from Lille and Sophia-Antipolis as well as research teams from Germany. This project ended this year due to the ERC Starting Grant Virginie Ehrlicher was awarded this year.
- V. Ehrlicher was the PI of the ANR Tremplin-ERC project HighDim (2022-2023) which focuses on the development of efficient numerical methods for the resolution of high-dimensional partial differential equations, using machine learning and neural networks. This project also ended this year due to the ERC Starting Grant Virginie Ehrlicher was awarded this year.
- T. Lelièvre is responsible of the node "Ecole des Ponts" of the ANR QuAMProcs (2019-2023), to which G. Stoltz also participates, PI: L. Michel, Université de Bordeaux.
- G. Stoltz is the PI of the ANR project SINEQ (2022-2025), whose aim is to improve the mathematical understanding and numerical simulation of nonequilibrium stochastic dynamics, in particular their linear response properties. This project involves researchers from CEREMADE, Université Paris-Dauphine and the SIMSART project-team of Inria Rennes.

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).

The project-team is involved in the Labex Bezout (2011-).

C. Le Bris is a participant to the Inria Challenge EQIP (Engineering for Quantum Information Processors), in particular in collaboration with P. Rouchon (QUANTIC project-team).

## 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), NBody (*N*-body quantum problem in chemistry and physics), and Rest (Theoretical spectroscopy);
- 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, June 5-7, 2023.

V. Ehrlacher

- is a member of the "Conseil d'Administration" of Ecole des Ponts;
- is a member of the "Conseil d'Administration" of the COMUE Paris-Est;
- is a member of the Cordi-S selection committee of INRIA;
- has co-organized a three-months research program at the Institute of Pure and Applied Mathematics (Los Angeles) on "New Mathematics for the Exascale: Applications to Materials Science";
- has been vice-president of the ANR selection committee CE 46 on "Modeling, simulation and scientific computing".

C. Le Bris

- is a member of the editorial boards of *Annales mathématiques du Québec* (2013-), *Archive for Rational Mechanics and Analysis* (2004-), *Calcolo* (2019-), *Communications in Partial Differential Equations* (2022-), *COCV (Control, Optimization and Calculus of Variations)* (2003-), *Mathematics in Action* (2008-), *Networks and Heterogeneous Media* (2007-), *Nonlinearity* (2005-), *Journal de Mathématiques Pures et Appliquées* (2009-), *Pure and Applied Analysis* (2018-);

- is a member of the editorial boards of the monograph series *Mathématiques & Applications*, Springer (2008-), *Modelling, Simulations and Applications*, Springer (2009-), *Springer Monographs in Mathematics*, Springer (2016-);
- is the president of the scientific advisory board of the Institut des Sciences du calcul et des données, Sorbonne Université, and a member of the Scientific Advisory Committee of the Institute for Mathematical and Statistical Innovation, University of Chicago;
- is a member of several scientific advisory boards in the industrial sector, in particular (since 2020) of the Energy Division of the Atomic Energy Council (CEA) and (since 2019) of *Framatome* senior management;
- holds a position of Visiting Professor at the University of Chicago, for one quarter a year;
- has been a 2023 MATH+ Distinguished Visiting Scholar at the Berlin Mathematics Research Center (Freie Universität, Humboldt-Universität, Technische Universität);
- holds a Senior Zuse fellowship at the Zuse Institut Berlin (2023-).

#### E. Legoll

- is a member of the editorial board of *SIAM MMS* (2012-) and of *ESAIM: Proceedings and Surveys* (2012-);
- has co-organized (with A. Lozinski) the minisymposium "Computational approaches for multiscale problems and their applications" within the SIAM CSE 2023 conference (Amsterdam), February 26 - March 3, 2023;
- has co-organized (with J. Zeman) the invited session "Computational approaches for heterogeneous materials" within the COMPLAS 2023 conference (Barcelona), September 5-7, 2023;
- was a member of the review panel for project proposals submitted to the Croatian Science Foundation.

#### 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-);
- T. Lelièvre co-edited with D. Picard the third volume of *Transitions, Les Nouvelles annales des Ponts et Chaussées*, on "Models and data for the environment";
- is the head of the applied mathematics department (CERMICS) at Ecole des Ponts (since 2020);
- has organized the conference *Analysis and simulation of metastable systems*, CIRM (Marseille) 3rd-7th April 2023 (with A. Bianchi and C. Landim);
- has organized the MCM 2023, 14th Monte Carlo Methods Conference, Paris, 26-30th June 2023 (with S. Allasonnière, J.-F. Chassagneux, F. Forbes, E. Gobet, B. Jourdain and G. Pagès);
- 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 a member of the "Bureau de Comités des équipes-Projets d'Inria Paris" (since 2022);
- is an external member of the *Conseil Scientifique et de Prospective* of the *Institut de Mathématiques de Toulouse* (since 2023).



G. Stoltz

- 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 and of the Faculty Board of EELISA (European Engineering Learning Innovation Science Alliance);
- has co-organized with Alessandra Iacobucci the research school "Sampling high dimensional probability measures" at Ecole des Ponts in September 2023, and the minisymposium "Numerical methods in statistical physics" at MCM2023 (Paris).

## 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):

- Analyse et équations aux dérivées partielles, 30h (M. Dus, V. Ehrlicher, A. Lefort, E. Letournel, S. Ruget, G. Sambataro)
- Équations aux dérivées partielles: approches variationnelles, 15h (S. Darshan, F. Legoll, S. Ruget, R. Santet)
- Initiation au travail en projet, 15h (R. Santet, R. Spacek, U. Vaes, L. Vidal)
- Introduction à l'optimisation (M. Dus)
- Mathématiques en action (R. Biezemans, N. Blassel, A. Bordignon, E. Cancès, S. Darshan, É. Polack, R. Santet, G. Stoltz, L. Vidal)
- Mécanique des milieux continus fluides, 25h (S. Boyaval)
- Mécanique quantique, 15h (E. Cancès, A. Kirsch)
- PAMS project, 16h (N. Blassel, R. Spacek)
- Pratique du calcul scientifique, 18h (N. Blassel, S. Darshan, R. Santet, R. Spacek, U. Vaes)
- Probabilités, 24h (N. Blassel, S. Darshan)
- Tutorats d'analyse et calcul scientifique, 18h (M. Rachid)

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

- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès)
- Problèmes d'évolution, 36h (V. Ehrlicher, F. Legoll)
- Projets Modéliser Programmer Simuler (T. Lelièvre)
- Statistics and data sciences, 30h (G. Stoltz)
- Techniques de développement logiciel, 32h30 (É. Polack)

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

- Équations aux dérivées partielles et modélisation, 24h (F. Legoll)
- Introduction to computational statistical physics, 20h (G. Stoltz)

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

At other institutions:

- Aléatoire (MAP361), 40h, Ecole Polytechnique (T. Lelièvre)
- 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)
- Modélisation, 40h, ENS Paris (S. Perrin-Roussel)
- Numerical Analysis, 56h, NYU Paris (U. Vaes)
- Réduction d'Endomorphismes (18h), Analyse numérique (18h), ESILV Paris (M. Rachid)
- Technologies for quantum computing: a mathematical perspective, 5 lectures, block course at Berlin Mathematical School, Winter 2022-2023 (C. Le Bris)
- Théorie spectrale et mécanique quantique, 30h, ENS Paris (S. Perrin-Roussel)

### 10.2.2 Supervision

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

- Rutger Biezemans, funding DIM Math Innov (Inria), Méthodes multi-échelles : approches non-intrusives, problèmes advection-dominés et questions reliées, co-supervised by C. Le Bris and A. Lozinski (University of Besançon), defended in September.
- Jean Cauvin-Vila, funding Ecole des Ponts, Cross-diffusion systems in moving-boundary domains, co-supervised by V. Ehrlacher and A. Hayat, defended in December.
- Yonah Conjugo-Taumhas, thèse CIFRE CEA, Criticality calculations in neutronics: model order reduction and a posteriori error estimators, co-supervised by T. Lelièvre and V. Ehrlacher together with G. Dusson (CNRS Besançon) and F. Madiot (CEA), defended in December.
- Maria Fuente-Ruiz, funding INRIA (COMMEDIA team), Adaptive tensor methods for high dimensional problems, co-supervised by D. Lombardi and V. Ehrlacher, defended in March.
- Thomas Pigeon, funding INRIA, Rare event sampling methods and machine learning to study catalytic reaction mechanisms, co-supervised by P. Raybaud (IFPEN) and T. Lelièvre, together with G. Stoltz and M. Corral-Vallero (IFPEN), defended in October.

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

- Hichem Belbal, thèse CIFRE EDF, Understanding suspended matter measures in Loire river, since September 2022, supervised by S. Boyaval (and O. Cerdan from BRGM)
- Elisa Beteille, thèse CIFRE EDF, Propagation of Urban Flood waves, since November 2021, supervised by S. Boyaval (and F. Larrarte from UGE)
- Noé Blassel, funding ERC Synergy EMC2, Approximation of the quasi-stationary distribution, Ecole des Ponts, since October 2022, co-supervised by T. Lelièvre and G. Stoltz

- Andrea Bordignon, Mathematical and numerical analysis for Density Functional Theory, funding ERC Synergy EMC2, co-supervised by E. Cancès and A. Levitt
- Thomas Brunel, funded by ANR Neptune, Paddle sports physics: Velocity–stroke rate and active drags, supervised by S. Boyaval (and R. Carmigniani from ENPC)
- Charlotte Chapellier, Generative methods for drug design, funding CIFRE Sanofi, since October 2023, co-supervised by T. Lelièvre and G. Stoltz
- Shiva Darshan, funding ANR SINEQ, Linear response of constrained stochastic dynamics, since October 2022, co-supervised by G. Stoltz and S. Olla (Université Paris-Dauphine)
- Raphaël Gastaldello, funding CNRS, Variance reduction methods for the computation of transport coefficients, since December 2023, co-supervised by G. Stoltz and U. Vaes
- Clément Guillot, funding ENPC, Space-time variational principles for the Schrödinger equation in large dimension, since November 2023, supervised by V. Ehrlacher and M. Dupuy (Sorbonne Université)
- Abbas Kabalan, thèse CIFRE SAFRANTech, Reduced-order models for problems with non-parametric geometrical variations, since November 2022, co-supervised by V. Ehrlacher and F. Casenave (SAFRANTech)
- Alfred Kirsch, funding Simons foundation, Mathematical and numerical analysis of interacting electrons models, École des Ponts, since September 2021, co-supervised by E. Cancès and D. Gontier (Paris-Dauphine CEREMADE)
- Albéric Lefort, funding CERMICS-ENPC, Multiscale numerical methods for reaction-diffusion equations and related problems, Ecole des Ponts, since November 2022, co-supervised by F. Legoll and C. Le Bris
- Eloïse Letournel, funding DIM Math Innov (Inria), Finite size effects in electronic structure, École des Ponts, since September 2021, supervised by A. Levitt
- 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 Octobre 2023, co-supervised by E. Cancès and T. Ayrat (Eviden)
- Solal Perrin-Roussel, funding École des Ponts, Mathematical analysis and numerical simulation of electronic transport in moiré materials, co-supervised by É. Cancès and by D. Gontier (CEREMADE, Université Paris-Dauphine PSL)
- 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-Saclay) and A. Lebée (Ecole des Ponts)
- Simon Ruget, funding Inria, Coarse approximation for a Schrödinger problem with highly oscillatory coefficients, Ecole des Ponts, since October 2022, co-supervised by F. Legoll and C. Le Bris
- Régis Santet, funding Ecole des Ponts, Enhancing the sampling efficiency of reversible and non-reversible dynamics, Ecole des Ponts, since October 2021, co-supervised by T. Lelièvre and G. Stoltz
- Lev-Arcady Sellem, funding Advanced ERC Q-Feedback (PI: P. Rouchon), Mathematical approaches for simulation and control of open quantum systems, Ecole des Mines de Paris, since October 2020, co-supervised by C. Le Bris and P. Rouchon (Inria QUANTIC)

- Renato Spacek, funding FSMP CoFund, Efficient computation of linear response of nonequilibrium stochastic dynamics, ED 386 Sorbonne-Université, since November 2021, co-supervised by G. Stoltz and P. Monmarché (Sorbonne Université)
- Jana Tarhini, funded by Inria-IFPEN, Fast simulation of CO<sub>2</sub>/H<sub>2</sub> storage in geological bassins, since November 2021, supervised by S. Boyaval (and G. Enchéry, H. Tran from IFPEN)
- Jean-Paul Traver, thèse CIFRE EDF, Data assimilation for flood predictions, since November 2022, supervised by S. Boyaval (and C. Goeury from EDF)
- Laurent Vidal, funding ERC Synergy EMC2, Model reduction in physics and quantum chemistry, since February 2021, supervised by E. Cancès and A. Levitt.

### 10.2.3 Juries

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

- E. Cancès, PhD of Thiago Carvalho Corso ("Mathematical contributions to static and time-dependent density functional theory") defended at TU Munich in July (referee)
- E. Cancès, PhD of Adechola Kouande ("Étude mathématique de l'instabilité de Peierls dans le modèle discret du polyacétylène"), defended at University Paris-Dauphine PSL in October (president)
- V. Ehrlicher, PhD of Yipeng Wang ("Estimation d'erreur a posteriori pour des calculs de structure électronique par des méthodes ab initio et son application pour diminuer le cout de calcul"), defended at Sorbonne University in December (president)
- V. Ehrlicher, PhD of Anatole Gallouët ("Problèmes inverses en optique anidolique et équations de jacobien généré"), defended at Grenoble University in October (president)
- V. Ehrlicher, PhD of Gong Chen ("Force Field Parameterization in Molecular Simulation by Machine Learning Methods"), defended at Sorbonne Université in September
- V. Ehrlicher, PhD of Rodrigue Lelotte ("Sur les gaz de Coulomb et le transport optimal multimarge"), defended at Dauphine University in October (referee)
- V. Ehrlicher, PhD of Hannes Vandecasteele ("Micro-Macro accelerated Markov Chain Monte Carlo Methods with Applications in Molecular Dynamics"), defended at Leuven University in June
- V. Ehrlicher, PhD of Matthieu Dolbeault ("Echantillonnage optimal et réduction de modèle"), defended at Sorbonne University in May (referee)
- V. Ehrlicher, PhD of Mathias Beaupère ("Algorithmes parallèles pour le calcul des décompositions de rang faible des matrices et tenseurs"), defended at INRIA in March
- C. Le Bris, PhD of Alexandre Girodroux-Lavigne ("Derivation and study of effective models for heterogeneous media and fluid suspensions"), defended at Université Paris-Cité in September
- C. Le Bris, PhD of Pierre Amenoagbadji ("Propagation des ondes dans des milieux quasi-périodiques"), defended at ENSTA Paris in December
- F. Legoll, PhD of Amandine Boucart ("Diffraction électromagnétique par une couche mince de nanoparticules réparties aléatoirement: développement asymptotique, conditions effectives et simulations"), defended at ENSTA Paris in April (referee)
- T. Lelièvre, PhD of Maksim Kaledin ("Development and Theoretical Analysis of the Algorithms for Optimal Control and Reinforcement Learning"), defended at National Research University Higher School of Economics in January (referee)
- T. Lelièvre, PhD of Kevin Fröhlicher ("Improving Monte Carlo reactor physics simulations using adaptive sampling of neutron histories"), defended at Université Paris Saclay in February (president)

- T. Lelièvre, PhD of Athina Monemvassitis ("Analysis and development of non-reversible samplers: Applications in Statistical and High-energy Physics"), defended at Université Clermont Auvergne in March (referee)
- T. Lelièvre, PhD of Claudia Fonte Sanchez ("Constructive and asymptotic estimates for the solutions of some linear and nonlinear PDEs"), defended at Université PSL in April (examiner)
- T. Lelièvre, PhD of Matthieu Dolbeault ("Optimal Sampling and Model Order Reduction"), defended at Sorbonne Université in June (examiner)
- T. Lelièvre, PhD of Iosif Lytras ("Solving sampling and optimization problems via Tamed Langevin MCMC algorithms in the presence of super-linearities"), defended at the University of Edinburgh, in September (referee)
- T. Lelièvre, PhD of Ashot Aleksian ("Exit-problem for Self-interacting and Self-stabilizing Diffusion Processes"), defended at Université Jean Monnet in November (referee)
- G. Stoltz, PhD of Thimotée Devergne ("Machine learning methods for computational studies in origins of life"), defended at Sorbonne Université in September
- G. Stoltz, PhD of Gong Chen ("Force Field Parameterization in Molecular Simulation by Machine Learning Methods"), defended at Sorbonne Université in September (referee)
- G. Stoltz, PhD of Théo Jaffrelot–Inizan ("Machine learning for new generation molecular dynamics"), defended at Sorbonne Université in October

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

- E. Cancès, HdR of Bérengère Delourme ("Quelques contributions à l'étude théorique et numérique des phénomènes de propagation des ondes dans des milieux périodiques"), defended at Université Sorbonne Paris Nord in October
- T. Lelièvre, HdR of Davide Mancusi ("Reactors, reactions, and random numbers"), defended at Université Paris Saclay in September

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

- E. Cancès, Poste de Professeur en mathématiques appliquées, Université de Rouen
- V. Ehrlacher, Chaire professeur junior, Ecole des Ponts
- V. Ehrlacher, Member of the INRIA-CordiS selection committee
- V. Ehrlacher, Poste de Maître de Conférences en mathématiques appliquées, Centrale Lyon
- V. Ehrlacher, Poste de Professeur en mathématiques appliquées, Université de Rennes
- V. Ehrlacher, Vice-president of the ANR project selection committee CE46
- T. Lelièvre, Poste de Professeur en mathématiques appliquées, Ecole Polytechnique
- T. Lelièvre, Postes CRCN et ISFP, Inria Paris
- L. Nenna, Poste MCF, Université Paris-Saclay
- G. Stoltz, Chaire professeur junior, Sorbonne Université
- G. Stoltz, Chaire professeur junior, Ecole des Ponts

### 10.3 Conference participation

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

- N. Blassel, Workshop “Nonequilibrium Molecular Dynamics”, University of Birmingham, May
- N. Blassel, GAMM 2023, Dresden, May
- N. Blassel, MCM 2023, Paris, June
- N. Blassel, ANR SINEQ Summer School 2023, September
- A. Boucart, CERMICS Young Researchers Seminar, Champs-sur-Marne, May
- S. Boyaval, ICIAM 2023, Symposium on hyperbolic models for complex fluids, Tokyo, August
- S. Boyaval, JMVPR 2023, Workshop on phase-resolved water wave modelling, October
- E. Cancès, GdT 2D materials, ENS Ulm, January
- E. Cancès, IPAM workshop on Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing, Los Angeles, March
- E. Cancès, Seminar (Lin’s group), Berkeley, April
- E. Cancès, CCQ workshop on Moiré Materials, Simons Foundation, New York, June
- E. Cancès, EMC2 seminar, Roscoff, July
- E. Cancès, Workshop on Mathematical Aspects of Condensed Matter Physics, ETH Zürich, July
- E. Cancès, BIRS workshop on The Mathematics and Physics of Moiré Superlattices, Banff, October
- E. Cancès, Colloquium CMAP, Ecole Polytechnique, November
- E. Cancès, IPAM workshop on Advancing Quantum Mechanics with Mathematics and Statistics, Lake Arrowhead, December
- J. Cauvin-Vila, Workshop “Energetic methods for multi-component reactive mixtures”, WIAS Berlin, September
- J. Cauvin-Vila, conference “Finite volume for complex applications 10”, Strasbourg, November
- S. Darshan, Journées de Physique Statistique, Paris, January
- S. Darshan, Workshop “Nonequilibrium Molecular Dynamics”, University of Birmingham, May
- S. Darshan, Journée des Doctorants d’ED MSTICS, Champs-sur-Marne, May
- S. Darshan, GAMM 2023, Dresden, May
- S. Darshan, Journées de Probabilités 2023, Angers, June
- S. Darshan, MCM 2023, Paris, June
- S. Darshan, ANR SINEQ Summer School 2023, September
- M. Dus, IPAM workshop on Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing, Los Angeles, March
- M. Dus, ENSTA seminar IDEFIX, May
- M. Dus, CEMRACS, Marseille, August

- M. Dus, New Monge Problems and Applications, Champs-sur-Marne, September
- M. Dus, LMJL seminar, Nantes, October
- V. Ehrlacher, GdR MANU, October
- V. Ehrlacher, CEMRACS 2023, Luminy, August
- V. Ehrlacher, ARIA, Bordeaux, May
- V. Ehrlacher, EMRM 2023, Berlin, September
- V. Ehrlacher, FOCM 2023, Paris, June
- V. Ehrlacher, GDT CALVA, Paris, January
- V. Ehrlacher, IPAM, Los Angeles, March
- V. Ehrlacher, Institut Pascal, Orsay, September
- V. Ehrlacher, ABPDE, Lille, June (plenary)
- V. Ehrlacher, MORTECH, Saclay, November
- V. Ehrlacher, SCALES, Mainz (Germany), June
- V. Ehrlacher, SIAM CSE, Amsterdam, March
- V. Ehrlacher, Séminaire du laboratoire de mathématiques appliquées, Université de Versailles-Saint Quentin, December
- C. Guillot, EMC2 seminar, Roscoff, July
- C. Guillot, CEMRACS, CIRM, Luminy, August
- C. Guillot, MOANSI annual meeting, Stuttgart, Germany, November
- A. Guyader, "Analysis and simulations of metastable systems", CIRM, Luminy, April
- A. Kirsch, Moiré materials workshop, CCQ Simons Foundation, New York, June
- A. Kirsch, GDR Rest annual meeting, Oléron, June
- A. Kirsch, EMC2 seminar, Roscoff, July
- A. Kirsch, Mathematics and Physics of Moiré Superlattices BIRS, Banff, October
- C. Le Bris, Max Planck Institute Leipzig Oberseminar "Analysis and Probability Theory", January
- C. Le Bris, Numerical Analysis Seminar of the University of Hong-Kong, online, February
- C. Le Bris, Weierstrass Institut Langenbach Seminar, February
- C. Le Bris, Séminaire Pierre-Louis Lions du Collège de France<sup>1</sup>, March
- F. Legoll, Colloquium of the CRC 1114 "Scaling Cascades in Complex Systems", Berlin, January
- F. Legoll, IPAM workshop "Scale-Bridging Materials Modeling at Extreme Computational Scales", Los Angeles, April
- F. Legoll, ADMOS conference, Goteborg, June
- F. Legoll, 12th Parallel-in-Time Integration workshop, Hamburg (invited speaker), July

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<sup>1</sup>video recording at [this link](#).

- F. Legoll, ICIAM 2023, Tokyo (online), August
- F. Legoll, EnuMath conference, Lisbon, September
- F. Legoll, Complas conference, Barcelona, September
- F. Legoll, IFPEN-Inria joint laboratory 2023 workshop, Rueil-Malmaison, November
- F. Legoll, International Workshop on Multiscale Model Reduction and Scientific Machine Learning, Hong Kong, December
- T. Lelièvre, Workshop "Rare Events: Analysis, Numerics, and Applications", Brin Mathematics Research Center, Washington, February
- T. Lelièvre, CRC 1114 "Scaling Cascades in Complex Systems" seminar, Berlin, February
- T. Lelièvre, Workshop STOCHNUM "Stochastic Numerics and Statistical Learning: Theory and Applications Workshop", KAUST, Saudi Arabia, online, May
- T. Lelièvre, Workshop "Stochastic processes, metastability and applications", Nancy, June
- T. Lelièvre, Foundations of Computational Mathematics conference, Paris, June
- T. Lelièvre, ELLIS theory workshop, Tübingen, June
- T. Lelièvre, ICIAM 2023, Tokyo (online) August
- T. Lelièvre, Workshop "Probabilistic sampling for physics", Institut Pascal, September
- T. Lelièvre, Seminar IMPMC Sorbonne University, September
- T. Lelièvre, Seminar "Modélisation Stochastique", LPSM, Université Paris Cité, October
- T. Lelièvre, Entretiens Jacques Cartier, Clermont-Ferrand, October
- T. Lelièvre, Seminar SANOFI, Vitry-sur-Seine, December
- T. Lelièvre, Colloquium LAMA, Université Paris Est Créteil, December
- R. Letotte, MOANSI annual meeting, Stuttgart, Germany, November
- E. Letournel, SIAM Conference on Computational Science and Engineering, Amsterdam, March
- E. Letournel, ICIAM 2023, Tokyo, August
- L. Nenna, Interpolations of Measures, Lagrange center, Paris, January
- L. Nenna, Journée transport optimal, Université de Évry, February
- L. Nenna, New Monge Problems seminar, Champs-sur-Marne, February
- L. Nenna, GFM seminar, University of Lisbon, April
- L. Nenna, Optimization and control in Burgundy, Université de Bourgogne, May
- L. Nenna Emerging topics in applied optimal transport, ETH, Zürich, June
- L. Nenna, Computational Optimal Transport, FOCM23, Paris, June
- L. Nenna, Numerical Analysis seminar, Université de Lille, October
- L. Nenna, PGM days, EDF Lab, Palaiseau, November
- T. Pigeon, Europacat 2023, Prague (Czech Republic), August
- T. Pigeon, ACS Fall 2023, USA, San Francisco (online), August



- T. Pigeon, LIA anual meeting, Hauteluce, January
- T. Pigeon, MCM2023, Paris, June
- M. Rachid, Fluctuations and First-Passage Problems, Stockholm, April
- M. Rachid, Groupe de travail GdT EDP et Théorie Spectrale, March
- M. Rachid, Groupe de travail EDP et Physique mathématique, March
- M. Rachid, Rencontre ANR QuAMProcs, March
- S. Ruget, Forum des jeunes mathématicien-nes, Bruxelles, October
- G. Sambataro, COUPLED 2023, Chania, June
- R. Santet, Workshop “Nonequilibrium Molecular Dynamics”, University of Birmingham, May
- R. Santet, GAMM 2023, Dresden, May
- R. Santet, MCM 2023, Paris, June
- R. Santet,  $d^2$  reading group, Oxford, October
- R. Spacek, Workshop “Nonequilibrium molecular dynamics”, University of Birmingham, May
- R. Spacek, GAMM 2023, Dresden, May
- R. Spacek, MCM 2023, Paris, June
- R. Spacek, Mathematics seminar, State University of Santa Cruz (online), Ilhéus, June
- R. Spacek, Data Science and Computational Statistics Seminar, University of Birmingham, December
- G. Stoltz, Materials Innovation Factory seminar (online), February
- G. Stoltz, Workshop “Rare event sampling”, BRIN center, University of Maryland, February
- G. Stoltz, Parisian seminar of statistics, March
- G. Stoltz, Workshop “Nonequilibrium molecular dynamics”, University of Birmingham, May
- G. Stoltz, Program “Probabilistic sampling for physics” at Institut Pascal, Orsay, September
- G. Stoltz, MOANSI annual meeting, Stuttgart, Germany, November
- G. Stoltz, CECAM workshop “Quantum2 on machine learning enhanced sampling”, Lausanne, Switzerland, November
- G. Stoltz, Sanofi, Vitry-sur-Seine, December
- U. Vaes, IRMAR probability seminar, Rennes, February
- U. Vaes, Lorentz Center Workshop “Purpose-driven particle systems”, Leiden, March
- U. Vaes, Workshop “Nonequilibrium Molecular Dynamics”, University of Birmingham, May
- U. Vaes, Mostly Monte Carlo seminar, Paris, December
- A. Bordignon, MOANSI annual meeting, Stuttgart, Germany, November
- L. Vidal, SIAM Conference on Computational Science and Engineering, Amsterdam, March

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

- N. Blassel and T. Lelièvre, "From Langevin dynamics to kinetic Monte Carlo: The quasi-stationary distribution approach to metastability", 1h30 lecture + 1h30 hands-on session, SINEQ summer school, September
- E. Cancès, "Mathematical methods for quantum chemistry", 3h lectures + 1h30 hands-on session, MWM summer school, Pisa, August
- S. Darshan, "Nonequilibrium systems and coupling methods", 1h30 hands-on session, SINEQ summer school, September
- A. Guyader, "Adaptive Multilevel Splitting Methods", 1h30 lecture + 1h30 hands-on session, SINEQ summer school, September
- L. Nenna, "An introduction to Optimal Transport", 3h lectures, Summer school on Optimal Transport, TU Dortmund, September
- R. Santet, "Discretization of Langevin dynamics and its metropolization", 1h30 hands-on session, SINEQ summer school, Marne-la-Vallée, France, September
- R. Spacek, "Computing transport coefficients with Molly", 1h30 hands-on session, SINEQ summer school, September
- U. Vaes, "Nonequilibrium systems and computation of transport coefficients", 1h lecture, SINEQ summer school, September

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

- S. Darshan, Stochastic Processes and Applications 2023, Lisbon, July
- S. Darshan, Particle Systems and Partial Differential Equations XI, Lisbon, November
- A. Kirsch, Precision Many-Body Physics 2023, Paris, June
- T. Pigeon, CECAM workshop "Soft matter and machine learning", online, January
- S. Ruget, Congrès des Jeunes Chercheurs en Mathématiques et Applications, Gif-sur-Yvette, September
- G. Sambataro, ARIA 1st Workshop, Bordeaux, March
- G. Sambataro, IMPDE 2023, Paris, May
- G. Sambataro, MORTech 2023, Paris, November
- R. Santet, MASCOT-NUM 2023, Le Croisic, April

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

- N. Blassel, Analysis and simulations of metastable systems, CIRM, Marseille, April
- N. Blassel, ELLIS theory workshop, Tübingen, June
- N. Blassel, EMC2 Workshop, Roscoff, July
- N. Blassel, CEMRACS 2023, Marseille, July
- N. Blassel, Probabilistic Sampling for Physics (Institut Pascal research program), Orsay, September
- E. Cancès, IPAM program on Mathematical and Computational Challenges in Quantum Computing, October-November
- J. Cauvin-Vila, conference "Cross-diffusion systems: analysis and stochastics", Konstanz, February

- S. Darshan, Analysis and simulations of metastable systems, CIRM, Marseille, April
- S. Darshan, CEMRACS 2023, Marseille, July
- S. Darshan, Probabilistic Sampling for Physics workshop, Orsay, September
- S. Darshan, GAMM MOANSI 2023, Stuttgart, November
- A. Lefort, SIAM Conference on Computational Science and Engineering, Amsterdam, March
- E. Letournel, GDR NBODY minischool 2023, Jussieu, June
- E. Letournel, GDR REST General Meeting, Oleron, June
- E. Letournel, EMC2 Workshop, Roscoff, July
- A. Bordignon, GDR NBODY minischool 2023, Jussieu, June
- A. Bordignon, GDR REST General Meeting, Oleron, June
- A. Bordignon, EMC2 Workshop, Roscoff, July
- A. Negre, IPAM program on Mathematical and Computational Challenges in Quantum Computing, September-November
- S. Ruget, SIAM Conference on Computational Science and Engineering, Amsterdam, March
- S. Perrin-Roussel, REST General meeting, Saint-Pierre-d'Oléron, June
- S. Perrin-Roussel, EMC2 Workshop, Roscoff, July
- S. Perrin-Roussel, Masterclass Angers 2023, Angers, December
- É. Polack, EMC2 Workshop, Roscoff, July
- R. Spacek, CEMRACS 2023 (online attendance), Marseille, July
- U. Vaes, EMC2 Workshop, Roscoff, July
- L. Vidal, Wannier Developer Meeting 2023, Daresbury Laboratory Chester, May
- L. Vidal, GDR NBODY minischool 2023, Jussieu, June
- L. Vidal, REST General meeting, Saint-Pierre-d'Oléron, June
- L. Vidal, EMC2 Workshop, Roscoff, July

#### 10.4 Popularization

- Interviews of V. Ehrlicher have been published in several journals (Madame Figaro, Paris Match, La Montagne, A Priori) following her Joliot-Curie prize, in particular on the recent results of France at the PISA evaluation.
- V. Ehrlicher was interviewed on several radio channels (France Inter, France Bleu, Radio Campus France) on the same topics as above.
- V. Ehrlicher was interviewed on the television channel BFMTV Business on the results of France in the PISA evaluation.
- V. Ehrlicher did one session of CHICHE (presentation of research in numerical sciences for high school students) in December at Lycée Montaigne in Paris.

- V. Ehrlicher, Réduction de modèles et jumeaux numériques pour la transition énergétique, *Revue Transitions, Les nouvelles Annales des ponts et chaussées*, 2023, pp 84-89<sup>2</sup>
- V. Ehrlicher participated to a speedmeeting of the RJMI (Rendez-vous des Jeunes Mathématiciennes et Informatiennes) organized in December 2023 at the Ulm Ecole Normale Supérieure.
- C. Le Bris, Campus de l'Innovation, video "Maths & Industrie"<sup>3</sup>
- C. Le Bris, Sciences du numérique et énergie nucléaire, *Revue Transitions, Les nouvelles Annales des ponts et chaussées*, pp 84-89<sup>4</sup>
- S. Perrin-Roussel is one of the organizers of the 2023 Rendez-vous des Jeunes Mathématiciennes et Informatiennes at Inria Paris
- R. Santet presented the subject of his PhD in 3 minutes for the "Ma Thèse en 180 secondes" competition in March 2023
- G. Stoltz did 4 sessions of CHICHE in December at Mantes-la-Jolie
- G. Stoltz presented a booth on "Predicting trajectories – from atom to galaxies" at the Science feast of Ecole des Ponts in October 2023

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

<sup>2</sup>see [this link](#).

<sup>3</sup>video recording at [this link](#).

<sup>4</sup>see [this link](#).

## 11.2 Publications of the year

### International journals

- [10] Y. Achdou and C. Le Bris. ‘Homogenization of some periodic Hamilton-Jacobi equations with defects’. In: *Communications in Partial Differential Equations* 48.6 (4th Aug. 2023). DOI: [10.1080/03605302.2023.2238953](https://doi.org/10.1080/03605302.2023.2238953). URL: <https://cnrs.hal.science/hal-03870614>.
- [11] M. Baudel, A. Guyader and T. Lelièvre. ‘On the Hill relation and the mean reaction time for meta-stable processes’. In: *Stochastic Processes and their Applications* 155 (Jan. 2023), pp. 393–436. DOI: [10.1016/j.spa.2022.10.014](https://doi.org/10.1016/j.spa.2022.10.014). URL: <https://hal.science/hal-02921281>.
- [12] Z. Belkacemi, M. Bianciotto, H. Minoux, T. Lelièvre, G. Stoltz and P. Gkeka. ‘Autoencoders for dimensionality reduction in molecular dynamics: collective variable dimension, biasing and transition states’. In: *Journal of Chemical Physics* 159 (11th July 2023), p. 024122. DOI: [10.1063/5.0151053](https://doi.org/10.1063/5.0151053). URL: <https://hal.science/hal-04118079>.
- [13] R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. ‘Non-intrusive implementation of Multiscale Finite Element Methods: an illustrative example’. In: *Journal of Computational Physics* 477 (2023), p. 111914. DOI: [10.1016/j.jcp.2023.111914](https://doi.org/10.1016/j.jcp.2023.111914). URL: <https://hal.science/hal-03643103>.
- [14] R. A. Biezemans, C. Le Bris, F. Legoll and A. Lozinski. ‘Non-intrusive implementation of a wide variety of Multiscale Finite Element Methods’. In: *Comptes Rendus. Mécanique* 351.1 (2023). DOI: [10.5802/crmeca.178](https://doi.org/10.5802/crmeca.178). URL: <https://hal.science/hal-03884721>.
- [15] S. Boyaval. ‘A class of symmetric-hyperbolic PDEs modelling fluid and solid continua’. In: *ESAIM: Proceedings and Surveys* (2023). URL: <https://enpc.hal.science/hal-04223434>.
- [16] S. Brisard, M. Bertin and F. Legoll. ‘A variance reduction strategy for numerical random homogenization based on the equivalent inclusion method’. In: *Computer Methods in Applied Mechanics and Engineering* 417 (2023), p. 116389. DOI: [10.1016/j.cma.2023.116389](https://doi.org/10.1016/j.cma.2023.116389). URL: <https://hal.science/hal-04058543>.
- [17] C. Cancès, V. Ehrlicher and L. Monasse. ‘Finite Volumes for the Stefan-Maxwell Cross-Diffusion System’. In: *IMA Journal of Numerical Analysis* (5th June 2023). DOI: [10.1093/imanum/drad032](https://doi.org/10.1093/imanum/drad032). URL: <https://hal.science/hal-02902672>.
- [18] E. Cancès, G. Dusson, G. Kemlin and L. Vidal. ‘On basis set optimisation in quantum chemistry’. In: *ESAIM: Proceedings and Surveys* 73 (30th Aug. 2023), pp. 107–129. DOI: [10.1051/proc/202373107](https://doi.org/10.1051/proc/202373107). URL: <https://inria.hal.science/hal-03736412>.
- [19] E. Cancès, M. F. Herbst, G. Kemlin, A. Levitt and B. Stamm. ‘Numerical stability and efficiency of response property calculations in density functional theory’. In: *Letters in Mathematical Physics* 113.1 (16th Feb. 2023). DOI: [10.1007/s11005-023-01645-3](https://doi.org/10.1007/s11005-023-01645-3). URL: <https://inria.hal.science/hal-03797450>.
- [20] E. Cancès, G. Kemlin and A. Levitt. ‘A priori error analysis of linear and nonlinear periodic Schrödinger equations with analytic potentials’. In: *Journal of Scientific Computing* 98.1 (19th Dec. 2023), p. 25. DOI: [10.1007/s10915-023-02421-0](https://doi.org/10.1007/s10915-023-02421-0). URL: <https://inria.hal.science/hal-03692851>.
- [21] É. Cancès, L. Garrigue and D. Gontier. ‘Simple derivation of moiré-scale continuous models for twisted bilayer graphene’. In: *Physical Review B* 107.15 (Apr. 2023), p. 155403. DOI: [10.1103/PhysRevB.107.155403](https://doi.org/10.1103/PhysRevB.107.155403). URL: <https://hal.science/hal-03859731>.
- [22] F.-B. Cartiaux, A. Ehrlicher, F. Legoll, A. Libal and J. Reygner. ‘Probabilistic formulation of Miner’s rule and application to structural fatigue’. In: *Probabilistic Engineering Mechanics* 74 (2023), p. 103500. DOI: [10.1016/j.probengmech.2023.103500](https://doi.org/10.1016/j.probengmech.2023.103500). URL: <https://hal.science/hal-04050871>.
- [23] J. Cauvin-Vila, V. Ehrlicher and A. Hayat. ‘Boundary stabilization of one-dimensional cross-diffusion systems in a moving domain: linearized system’. In: *Journal of Differential Equations* 350 (Mar. 2023), pp. 251–307. DOI: [10.1016/j.jde.2022.12.021](https://doi.org/10.1016/j.jde.2022.12.021). URL: <https://hal.science/hal-03706841>.

- [24] L. Chamoin and F. Legoll. ‘An introductory review on a posteriori error estimation in Finite Element computations’. In: *SIAM Review* 65.4 (2023), pp. 963–1028. DOI: [10.1137/21M1464841](https://doi.org/10.1137/21M1464841). URL: <https://hal.science/hal-03368356>.
- [25] O. Gorynina, F. Legoll, T. Lelièvre and D. Perez. ‘Combining machine-learned and empirical force fields with the parareal algorithm: application to the diffusion of atomistic defects’. In: *Comptes Rendus. Mécanique* 351.1 (2023). DOI: [10.5802/crmeca.220](https://doi.org/10.5802/crmeca.220). URL: <https://hal.science/hal-03909092>.
- [26] T. Hoang Ngoc Minh, G. Stoltz and B. Rotenberg. ‘Frequency and field-dependent response of confined electrolytes from Brownian dynamics simulations’. In: *Journal of Chemical Physics* 158.10 (14th Mar. 2023), p. 104103. DOI: [10.1063/5.0139258](https://doi.org/10.1063/5.0139258). URL: <https://hal.science/hal-04019763>.
- [27] A. Karoni, B. Leimkuhler and G. Stoltz. ‘Friction-adaptive descent: a family of dynamics-based optimization methods’. In: *Journal of Computational Dynamics* 10.4 (1st Oct. 2023), pp. 450–484. DOI: [10.3934/jcd.2023007](https://doi.org/10.3934/jcd.2023007). URL: <https://hal.science/hal-04185134>.
- [28] C. Le Bris. ‘Defects in homogenization theory’. In: *Séminaire Laurent Schwartz - EDP et applications* (12th July 2023), pp. 1–17. DOI: [10.5802/slsedp.157](https://doi.org/10.5802/slsedp.157). URL: <https://hal.science/hal-04368333>.
- [29] T. Lelièvre, G. Robin, I. Sekkat, G. Stoltz and G. Victorino Cardoso. ‘Generative methods for sampling transition paths in molecular dynamics’. In: *ESAIM: Proceedings* 73 (30th Aug. 2023), pp. 238–256. DOI: [10.1051/proc/202373238](https://doi.org/10.1051/proc/202373238). URL: <https://hal.science/hal-03661671>.
- [30] T. Lelièvre, G. Stoltz and W. Zhang. ‘Multiple projection MCMC algorithms on submanifolds’. In: *IMA Journal of Numerical Analysis* 43.2 (3rd Mar. 2023), pp. 737–788. DOI: [10.1093/imanum/drac006](https://doi.org/10.1093/imanum/drac006). URL: <https://hal.science/hal-02515267>.
- [31] I. Niakh, G. Drouet, V. Ehrlicher and A. Ern. ‘Stable model reduction for linear variational inequalities with parameter-dependent constraints’. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 57.1 (2023), pp. 167–189. URL: <https://hal.science/hal-03611982>.
- [32] F. Pes, É. Polack, P. Mazzeo, G. Dusson, B. Stamm and F. Lipparini. ‘A Quasi Time-Reversible scheme based on density matrix extrapolation on the Grassmann manifold for Born-Oppenheimer Molecular Dynamics’. In: *Journal of Physical Chemistry Letters* 14.43 (11th July 2023), pp. 9720–9726. DOI: [10.1021/acs.jpcllett.3c02098](https://doi.org/10.1021/acs.jpcllett.3c02098). URL: <https://hal.science/hal-04161077>.
- [33] T. Pigeon, G. Stoltz, M. Corral-Valero, A. Anciaux-Sedrakian, M. Moreaud, T. Lelièvre and P. Raybaud. ‘Computing Surface Reaction Rates by Adaptive Multilevel Splitting Combined with Machine Learning and Ab Initio Molecular Dynamics’. In: *Journal of Chemical Theory and Computation* 19.12 (27th June 2023), pp. 3538–3550. DOI: [10.1021/acs.jctc.3c00280](https://doi.org/10.1021/acs.jctc.3c00280). URL: <https://ifp.hal.science/hal-04190303>.
- [34] I. Sekkat and G. Stoltz. ‘Removing the mini-batching error in Bayesian inference using Adaptive Langevin dynamics’. In: *Journal of Machine Learning Research* 24.329 (20th Dec. 2023), pp. 1–58. URL: <https://hal.science/hal-03386488>.
- [35] R. Spacek and G. Stoltz. ‘Extending the regime of linear response with synthetic forcings’. In: *Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal* 21.4 (14th Nov. 2023), pp. 1602–1643. DOI: [10.1137/23M1557611](https://doi.org/10.1137/23M1557611). URL: <https://hal.science/hal-04019027>.

#### Invited conferences

- [36] D. Lombardi, V. Ehrlicher and M. Fuente-Ruiz. ‘SoTT: a greedy construction of a sum of Tensor Trains’. In: ICOSAHOM 2023 - International Conference on Spectral and High Order Methods. Seoul, South Korea, 14th Aug. 2023. URL: <https://inria.hal.science/hal-04392369>.

### International peer-reviewed conferences

- [37] C. Cancès, J. Cauvin-Vila, C. Chainais-Hillairet and V. Ehrlacher. ‘Structure Preserving Finite Volume Approximation of Cross-Diffusion Systems Coupled by a Free Interface’. In: *Finite Volume for Complex Applications X – Volume 1, Elliptic and parabolic problems*. Finite Volumes for Complex Applications X. Vol. 432. Springer Proceedings in Mathematics & Statistics. Strasbourg, France: Springer Nature Switzerland, 1st Oct. 2023, pp. 205–213. DOI: [10.1007/978-3-031-40864-9\\_15](https://doi.org/10.1007/978-3-031-40864-9_15). URL: <https://hal.science/hal-04050166>.
- [38] L.-A. Sellem, R. Robin, P. Campagne-Ibarcq and P. Rouchon. ‘Stability and decoherence rates of a GKP qubit protected by dissipation’. In: *22nd World Congress of the International Federation of Automatic Control*. IFAC 2023 - 22nd World Congress of the International Federation of Automatic Control. Yokohama, Japan, 7th Apr. 2023. DOI: [10.48550/arXiv.2304.03806](https://doi.org/10.48550/arXiv.2304.03806). URL: <https://inria.hal.science/hal-04071008>.

### Scientific books

- [39] X. Blanc and C. Le Bris. *Homogenization Theory for Multiscale Problems: An introduction*. 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>.
- [40] E. Cancès and G. Friesecke (eds.) *Density Functional Theory*. Springer International Publishing, 2023. DOI: [10.1007/978-3-031-22340-2](https://doi.org/10.1007/978-3-031-22340-2). URL: <https://hal.science/hal-04371921>.

### Scientific book chapters

- [41] E. Cancès, A. Levitt, Y. Maday and C. Yang. ‘Numerical Methods for Kohn–Sham Models: Discretization, Algorithms, and Error Analysis’. In: *Density Functional Theory*. Springer International Publishing, 19th Dec. 2023, pp. 333–400. DOI: [10.1007/978-3-031-22340-2\\_7](https://doi.org/10.1007/978-3-031-22340-2_7). URL: <https://hal.science/hal-04412352>.
- [42] C. Chipot, P. Gkeka, T. Lelièvre and G. Stoltz. ‘Equilibrium and Nonequilibrium Methods for Free-Energy Calculations With Molecular Dynamics’. In: *Comprehensive Computational Chemistry*. Vol. 3. Elsevier; Elsevier, 2024, pp. 384–400. DOI: [10.1016/B978-0-12-821978-2.00112-4](https://doi.org/10.1016/B978-0-12-821978-2.00112-4). URL: <https://hal.science/hal-04178827>.
- [43] D. Perez and T. Lelièvre. ‘Recent advances in Accelerated Molecular Dynamics Methods: Theory and Applications’. In: *Comprehensive Computational Chemistry*. Vol. 3. Elsevier, 2024, pp. 360–383. DOI: [10.1016/B978-0-12-821978-2.00116-1](https://doi.org/10.1016/B978-0-12-821978-2.00116-1). URL: <https://hal.science/hal-04361720>.

### Edition (books, proceedings, special issue of a journal)

- [44] B. Battisti, T. Blickhan, G. Enchery, V. Ehrlacher, D. Lombardi and O. Mula, eds. *Wasserstein model reduction approach for parametrized flow problems in porous media*. CEMRACS 2021 - Data Assimilation and Reduced Modeling for High Dimensional Problems. Vol. 73. EDP Sciences, 30th Aug. 2023, pp. 28–47. DOI: [10.1051/proc/202373028](https://doi.org/10.1051/proc/202373028). URL: <https://hal.science/hal-04390131>.

### Reports & preprints

- [45] N. Blassel and G. Stoltz. *Fixing the flux: A dual approach to computing transport coefficients*. 14th May 2023. URL: <https://hal.science/hal-04099515>.
- [46] G. Brigati and G. Stoltz. *How to construct decay rates for kinetic Fokker–Planck equations?* 28th Feb. 2023. URL: <https://hal.science/hal-04334470>.
- [47] E. Cancès, F. M. Faulstich, A. Kirsch, E. Letournel and A. Levitt. *Some mathematical insights on Density Matrix Embedding Theory*. 2nd Oct. 2023. URL: <https://hal.science/hal-04371915>.
- [48] E. Cancès and L. Meng. *Semiclassical analysis of two-scale electronic Hamiltonians for twisted bilayer graphene*. 23rd Nov. 2023. URL: <https://hal.science/hal-04371908>.

- [49] J. Cauvin-Vila, V. Ehrlacher, G. Marino and J.-F. Pietschmann. *Stationary solutions and large time asymptotics to a cross-diffusion-Cahn-Hilliard system*. 6th July 2023. URL: <https://hal.science/hal-04152908>.
- [50] M. Chak, T. Lelièvre, G. Stoltz and U. Vaes. *Optimal importance sampling for overdamped Langevin dynamics*. 11th July 2023. URL: <https://hal.science/hal-04169540>.
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