IN PARTNERSHIP WITH:
Ecole des Ponts ParisTech

Activity Report 2019

Project-Team MATHERIALS

MATHematics for MatERIALS

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

RESEARCH CENTER
Paris

THEME
Numerical schemes and simulations

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Project-Team MATHERIALS

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

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1. Team, Visitors, External Collaborators

Research Scientists

Claude Le Bris [Team leader, Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Sébastien Boyaval [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Éric Cancès [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Virginie Ehrlacher [Ecole Nationale des Ponts et Chaussées, Researcher]
Frédéric Legoll [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Tony Lelièvre [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]
Antoine Levitt [Inria, Researcher]
Gabriel Stoltz [Ecole Nationale des Ponts et Chaussées, Senior Researcher, HDR]

Faculty Member

Xavier Blanc [Univ Denis Diderot, Professor, *en délégation* from Sep 2019, HDR]

Post-Doctoral Fellows

Manon Baudel [Ecole Nationale des Ponts et Chaussées, until Jun 2019]
Olga Gorynina [Ecole Nationale des Ponts et Chaussées]
Michael Herbst [Sorbonne Université]
Geneviève Robin [Inria, from Oct 2019]

PhD Students

Robert Benda [Ecole Nationale des Ponts et Chaussées]
Qiming Du [Inria, from Oct 2019]
Grégoire Ferré [Ecole Nationale des Ponts et Chaussées, until Sep 2019]
Rémi Goudey [Ecole Nationale des Ponts et Chaussées, from Sep 2019]
Gaspard Kemlin [Ecole Nationale des Ponts et Chaussées, from Sep 2019]
Adrien Lesage [Ecole Nationale des Ponts et Chaussées]
Mouad Ramil [Ecole Nationale des Ponts et Chaussées]
Pierre-Loïk Rothé [Ecole Nationale des Ponts et Chaussées]
Laura Silva Lopes [Ecole Nationale des Ponts et Chaussées until Sep 2019, Inria Oct-Dec 2019]
Sami Siraj-Dine [Univ Paris-Est Marne La Vallée]

Interns and Apprentices

Luca Gorini [Inria, from Mar 2019 until Sep 2019]
Gaspard Kemlin [Inria, from Apr 2019 until Aug 2019]

2. Overall Objectives

2.1. Overall Objectives

The MATHERIALS project-team has been created jointly by the École des Ponts ParisTech (ENPC) and Inria in 2015. It is the follow-up and an extension of the former project-team MICMAC originally created in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques et Calcul Scientifique) at École des Ponts. The permanent research scientists of the project-team have positions at CERMICS and at two other laboratories of École des Ponts: Institut Navier and Laboratoire Saint-Venant. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulation of computational chemistry at the microscopic level and to create simulations coupling this microscopic scale with meso- or macroscopic scales (possibly using parallel algorithms). Over the years, the project-team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the project-team is to have created a corpus of literature, authoring books and research monographs on the subject [1], [2], [3], [4], [5], [6], [7] that other scientists may consult in order to enter the field.

3. Research Program

3.1. 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.

3.1.1. Electronic structure of large systems

Quantum Chemistry aims at understanding the properties of matter through the modelling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström (10^{-10} meters), and the size of the nucleus embedded in it is 10^{-15} meters; the typical vibration period of a molecular bond is the femtosecond (10^{-15} seconds), and the characteristic relaxation time for an electron is 10^{-18} seconds. Consequently, Quantum Chemistry calculations concern very short time (say 10^{-12} seconds) behaviors of very small size (say 10^{-27} m^3) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability of minerals to naturally split along crystal surfaces (e.g. mica yields to thin flakes), is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time-dependent form or in its time-independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its L^2 norm is set to one.

The time-dependent equation is a first-order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of $L^2(\mathbb{R}^d)$, with $d = 3(M + N)$, M and N respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter

d is already 39 for a single water molecule and rapidly reaches 10^6 for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is 10^4 times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on $L^2(\mathbb{R}^3)$. The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales.

As the size of the systems one wants to study increases, more efficient numerical techniques need to be resorted to. In computational chemistry, the typical scaling law for the complexity of computations with respect to the size of the system under study is N^3, N being for instance the number of electrons. The Holy Grail in this respect is to reach a linear scaling, so as to make possible simulations of systems of practical interest in biology or material science. Efforts in this direction must address a large variety of questions such as

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

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

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

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

3.1.2. 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 $k_{\mathrm{B}}T \simeq 4 \times 10^{-21}$ J at room temperature, and the typical times are of the order of 10^{-15} s.

To give some insight into such a large number of particles contained in a macroscopic sample, it is helpful to compute the number of moles of water on earth. Recall that one mole of water corresponds to 18 mL, so that a standard glass of water contains roughly 10 moles, and a typical bathtub contains 10^5 mol. On the other hand, there are approximately 10^{18} m^3 of water in the oceans, *i.e.* 7×10^{22} mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating $\mathcal{N}_A$ atoms and performing $\mathrm{O}(10^{15})$ time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of a few microseconds.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of N particles correctly approximate the macroscopic property, formally obtained in the thermodynamic limit $N \to +\infty$ (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

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

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

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

3.1.3. Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on how to couple models written at the atomistic scale with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

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

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

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to provide a good description of the materials;
- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

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

4. Highlights of the Year

4.1. Highlights of the Year

4.1.1. Grants

- Eric Cancès, Laura Grigori (ALPINES, Inria Paris), Yvon Maday (Sorbonne Université), and Jean-Philip Piquemal (Sorbonne Université) are the PIs of the ERC Synergy project EMC2 (Extreme-scale Mathematically-based Computational Chemistry) launched in September 2019 (grant agreement No 810367).

- Virginie Ehrlacher is the PI of the ANR JCJC COMODO (CrOss-diffusion systems on MOving DOmains) project, to start in January 2020.

4.1.2. Awards

- C. Le Bris was a plenary speaker at ICIAM 2019, July 2019, Valencia, Spain.
- T. Lelièvre has received a Visiting professorship from the Leverhulme Trust, for his sabbatical leave at Imperial College London (Sep 2019-Jul 2020).

5. New Software and Platforms

5.1. 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.

- Contact: Antoine Levitt
- URL: http://dftk.org

5.2. gen.parRep

KEYWORDS: Molecular simulation - MPI - HPC - C++

SCIENTIFIC DESCRIPTION: Metastability is one of the major encountered obstacle when performing long molecular dynamics simulations, and many methods were developed to address this challenge. The "Parallel Replica" (ParRep) dynamics is known for allowing to simulate very long trajectories of metastable Langevin dynamics in the materials science community, but it relies on assumptions that can hardly be transposed to the world of biochemical simulations. The later developed "Generalized ParRep" variant solves those issues, but it was not applied to significant systems of interest so far.

In a recent article article, we presented the program gen.parRep, the first publicly available implementation of the Generalized Parallel Replica method (BSD 3-Clause license), targeting frequently encountered metastable biochemical systems, such as conformational equilibria or dissociation of protein-ligand complexes. It was shown that the resulting C++ implementation exhibits a strong linear scalability, providing up to 70 % of the maximum possible speedup on several hundreds of CPUs.

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

RELEASE FUNCTIONAL DESCRIPTION: The software was modified in order to allow reproducibility in some cases (the limiting factor is OpenMM which does not always provides deterministic output even when using the same seeds (!), see http://docs.openmm.org/latest/userguide/library.html#determinism).

The main executable now has 2 more command line options, '–inp-seeds [fname]' or '–out-seeds [fname]' for respectively loading seeds or writing seeds from/to a unique binary file. See rand.hpp/rand.cpp, od the Doxygen doc for more details.

These modifications now allow Continuous Integration (CI) on the infrastructure provided by Inria : in mol/ci a small test case will be executed at each commit to the repository and compared to reference results.

The two other minor modifications concern the Lua scripts:

"get_minimised_energy_crdvels" was added to the set of functions that the user can call from the Lua script : it simply combines in one call what "get_minimised_energy" and "get_minimised_crdvels" already provided.

a extra optional parameter is available for the "simulation" parameters block when "simulation.algorithm" is "PARREP_FV" , this parameter is "simulation.minAccumulatedObs" : it will enforce that at least minAccumulatedObs observations of an observable have already been accumulated before the convergence test is performed , this may be useful if there is a risk of early pseudo-convergence for some of the observables when only a few samples have been accumulated.

Download sources:

https://gitlab.inria.fr/parallel-replica/gen.parRep/tags/v1.2.0

or

https://github.com/FHedin/gen.parRep/releases/tag/v1.2.0

NEWS OF THE YEAR: Corresponding publication : https://hal.archives-ouvertes.fr/hal-01832823

- Participants: Florent Hedin and Tony Lelièvre
- Partner: Ecole des Ponts ParisTech
- Contact: Florent Hedin
- Publication: gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems
- URL: https://gitlab.inria.fr/parallel-replica/gen.parRep

6. New Results

6.1. Electronic structure calculations and related problems

Participants: Robert Benda, Éric Cancès, Virginie Ehrlacher, Luca Gorini, Gaspard Kemlin, Claude Le Bris, Antoine Levitt, Sami Siraj-Dine, Gabriel Stoltz.

6.1.1. Mathematical analysis

The members of the team have continued their systematic study of the properties of materials in the reduced Hartree-Fock (rHF) approximation, a model striking a good balance between mathematical tractability and the ability to reproduce qualitatively complex effects.

In collaboration with L. Cao, E. Cancès and G. Stoltz have studied the nuclear dynamics of infinite crystals with local defects within the Born-Oppenheimer approximation, using the reduced Hartree-Fock model to compute the electronic ground state. In this model, nuclei obey an autonomous classical Hamiltonian dynamics on a potential energy surface obtained by rHF electronic ground-state calculations. One of the main motivations for this work is to study the *nonlinear* collective excitations of nuclei in a crystal, in order to go beyond the simple harmonic approximation of non-interacting phonons. rHF ground states associated with generic nuclear displacements with respect to the periodic configuration are not mathematically well-defined at the time of writing. However, by relying on results by Cancès, Deleurence and Lewin for the rHF ground states of crystals with local defects, it is possible to study the fully nonlinear rHF Born-Oppenheimer dynamics of nuclei in the neighborhood of an equilibrium periodic configuration of a crystal. A Hilbert space of admissible nuclear displacements, and an infinite-dimensional Hamiltonian describing the dynamics of nuclei can then be defined. For small initial data, it is proved that the Cauchy problem associated with this Hamiltonian dynamics is well posed for short times (see the PhD thesis of Lingling Cao). The existence and uniqueness for arbitrary initial data, and/or long times requires a perturbation analysis of the rHF model when the Fermi level is occupied, which is work in progress.

6.1.2. Numerical analysis

E. Cancès has pursued his long-term collaboration with Y. Maday (Sorbonne Université) on the numerical analysis of linear and nonlinear eigenvalue problems. Together with G. Dusson (Besançon), B. Stamm (Aachen, Germany), and M. Vohralìk (Inria SERENA), they have designed *a posteriori* error estimates for conforming numerical approximation of eigenvalue clusters of second-order self-adjoint operators on bounded domains [44]. Given a cluster of eigenvalues, they have estimated the error in the sum of the eigenvalues, as well as the error in the eigenvectors represented through the density matrix, i.e. the orthogonal projector on the associated eigenspace. This allows them to deal with degenerate (multiple) eigenvalues within this framework. The bounds are guaranteed and converge at the same rate as the exact error. They can be turned into fully computable bounds as soon as an estimate on the dual norm of the residual is available, which is notably the case (i) for the Laplace eigenvalue problem discretized with conforming finite elements, and (ii) for a Schrödinger operator with periodic boundary conditions discretized with plane waves.

R. Benda, E. Cancès and B. Lebental (Ecole Polytechnique) have initiated the design and analysis of multiscale models for the electrical conductivity of networks of functionalized carbon nanotubes. Such devices are used as nanosensors, for instance to monitor the quality of water. In [11], they study by means of Monte-Carlo numerical simulations the resistance of two-dimensional random percolating networks of stick, widthless nanowires. They use the multi-nodal representation (MNR) to model a nanowire network as a graph. They derive numerically from this model the expression of the total resistance as a function of all meaningful parameters, geometrical and physical, over a wide range of variation for each. They justify their choice of non-dimensional variables applying Buckingham π-theorem. The effective resistance of 2D random percolating networks of nanowires is found to have a nice expression in terms of the geometrical parameters (number of wires, aspect ratio of electrode separation over wire length) and the physical parameters (nanowire linear resistance per unit length, nanowire/nanowire contact resistance, metallic electrode/nanowire contact resistance). The dependence of the resistance on the geometry of the network, on the one hand, and on the physical parameters (values of the resistances), on the other hand, is thus clearly separated thanks to this expression, much simpler than the previously reported analytical expressions. In parallel, atomic scale models based on electronic structure theory are being developed to parameterize these mesoscale models (PhD thesis of R. Benda).

C. Le Bris has pursued his long term collaboration with Pierre Rouchon (Ecole des Mines de Paris and Inria QUANTIC) on the study of high dimensional Lindblad type equations at play in the modelling of open quantum systems. They have co-supervised the M2 internship of Luca Gorini, that was focused on the simulation of some simple quantum gates, and has investigated several discretization strategies based upon the choice of suitable basis sets.

V. Ehrlacher, L. Grigori (Inria ALPINES), D. Lombardi (Inria COMMEDIA) and H. Song (Inria ALPINES) have designed a new numerical method for the compression of high-order tensors [49]. The principle of the algorithm consists in constructing an optimal partition of the set of indices of the tensor, and construct an approximation of the tensor on each indices subdomain by means of an adapted High-Order Singular Value Decomposition. This method was used, among other examples, for the reduction of the solution of the Vlasov-Poisson system, and enabled to reach very significant compression factors. They also obtained very encouraging results on the compression of the Coulomb potential, which could be very interesting with a view to the resolution of the time-dependent Schrödinger equation in high dimension, which is currently work in progress.

A. Alfonsi, R. Coyaud (Ecole des Ponts), V. Ehrlacher and D. Lombardi (Inria COMMEDIA) studied a different approach for discretizing optimal transport problems, which relies in relaxing the marginal constraints in a finite number of marginal moment constraints, while keeping an infinite state space [40]. The advantage of such an approach is that the approximate solution of the multi-marginal optimal transport problem with Coulomb cost, which is the semi-classical limit of the so-called Lévy-Lieb functional, can be represented as a discrete measure charging a low number of points, thus avoiding the curse of dimensionality when the number of electrons is large.

M. Herbst and his collaborators have developed the `adcc` Python/C++ software package for performing excited state calculations based on algebraic-diagrammatic construction methods. It connects to four SCF packages (pyscf, psifour, molsturm and veloxchem), allows the inclusion of environmental effects through implicit or explicit solvent models, and implements methods up to third order in perturbation theory. Its features are summarized in [54].

6.2. Computational Statistical Physics

Participants: Manon Baudel, Qiming Du, Grégoire Ferré, Frédéric Legoll, Tony Lelièvre, Mouad Ramil, Geneviève Robin, Laura Silva Lopes, Gabriel Stoltz.

The objective 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 development of methods for sampling the configuration space; (ii) the efficient computation of dynamical properties which requires to sample metastable trajectories; (iii) the simulation of nonequilibrium systems and the computation of transport coefficients; (iv) coarse-graining techniques to reduce the computational cost of molecular dynamic simulations and gain some insights on the models.

6.2.1. Sampling of the configuration space: new algorithms and applications

The work [52] by G. Ferré and G. Stoltz considers fluctuations of empirical averages for stochastic differential equations. Such averages are commonly used to compute ergodic averages in statistical physics in order to estimate macroscopic quantities, but they are subject to fluctuations. If small deviations are described by the central limit theorem, important fluctuations enter the large deviations framework. This theory is well understood when considering bounded observables of a stochastic differential equation, but quantities of interest are generally unbounded. The authors identify the class of unbounded functions which enter the "usual" regime of large deviations. The answer is not trivial, and suggests that many physical observables satisfy another type of large deviations, which leads to further works. Additionally, the influence of irreversibility on the fluctuations was studied by providing a mathematical illustration of the second law of thermodynamics, stating that irreversible dynamics generate more entropy, or more disorder, than reversible ones.

The team also pursued its endeavour to study and improve free energy biasing techniques, such as adaptive biasing force or metadynamics. The gist of these techniques is to bias the original metastable dynamics used to sample the target probability measure in the configuration space by an approximation of the free energy along well-chosen reaction coordinates. This approximation is built on the fly, using empirical measures over replicas, or occupations measures over the trajectories of the replicas. Two works have been performed on such methods

- First, in [50], V. Ehrlacher, T. Lelièvre and P. Monmarché (Sorbonne Université) have developed a new numerical method in order to compute the free energy and the biased potential given by the Adaptive Biasing Force method in the case where the number of reaction cordinates in the system is too large to apply standard grid-based approximation techniques. The algorithm uses a greedy algorithm and a tensor product approximation. Convergence proofs of both the underlying ABF technique (which uses an unbiased occupation measure) and the greedy tensor-product approximation are provided.
- Second, in [55], T. Lelièvre together with B. Jourdain (Ecole des Ponts) and P.-A. Zitt (Université Paris Est) have used a parallel between metadynamics and self interacting models for polymers to study the longtime convergence of the original metadynamics algorithm in the adiabatic setting, namely when the dynamics along the collective variables decouple from the dynamics along the other degrees of freedom. The bias which is introduced when the adiabatic assumption does not hold is also discussed.

The team has also considered new applications in terms of sampling, and the analysis of related sampling methods:

- For large scale Bayesian inference, B. Leimkuhler (Edinburgh, United Kingdom), M. Sachs (Duke, USA) and G. Stoltz have studied in [57] the convergence of Adaptive Langevin dynamics, which is a method for sampling the Boltzmann-Gibbs distribution at a prescribed temperature in cases where the potential gradient is subject to stochastic perturbation of unknown magnitude. The method replaces the friction in underdamped Langevin dynamics with a dynamical variable, updated according to a negative feedback loop control law as in the Nose-Hoover thermostat. Hypocoercive techniques allow to show that the law of Adaptive Langevin dynamics converges exponentially rapidly to the stationary distribution, with a rate that can be quantified in terms of the key parameters of the dynamics. This implies in particular that a central limit theorem holds for the time averages computed along a stochastic path.
- For the simulation of log-gases, G. Ferré and G. Stoltz have studied in [46] with D. Chafaï (Université Paris Dauphine) a follow up to a former project on the efficient simulation of Coulomb and logarithmic gases. A previous work has demonstrated the usefulness of Hybrid Monte Carlo techniques for sampling the invariant measure of such gases. Gases under constraint are now considered. First, the algorithm proposed in [31] was used to numerically explore the situation. Then, large deviations techniques were employed to study the limiting behaviour of the conditioned gas when the number of particles gets large. For a class of constraints, the equation solved by the limiting empirical density shows in particular cases a spectacular behaviour. This work suggests to further explore some research paths, such as the limiting distribution for large constraints.

6.2.2. Sampling of dynamical properties and rare events

In the preprint [48], T. Lelièvre uses the quasi-stationary distribution approach to study the first exit point distribution from a bounded domain of the overdamped Langevin dynamics, in collaboration with G. Di Gesù (TU Wien, Austria), B. Nectoux (Université Blaise Pascal) and D. Le Peutrec (Université Paris-Sud). The quasi-stationary distribution approach has been developed by T. Lelièvre and collaborators over the past years in order to rigorously model the exit event from a metastable state by a jump Markov process, and to study this exit event in the small temperature regime. In [48], the authors prove that in the small temperature regime and under rather general assumptions on the initial conditions and on the potential function, the support of the distribution of the first exit point concentrates on some points realizing the minimum of the potential on the boundary. The proof relies on tools to study tunnelling effects in semi-classical analysis. This preprint has been divided into two separate articles for publication: the first one [22] has been accepted for publication; the second one is currently under review.

6.2.3. Nonequilibrium systems and computation of transport coefficients

Stemming from the IHP trimester "Stochastic Dynamics Out of Equilibrium" held at Institut Henri Poincare in April-July 2017, a collection of contributions has been grouped in a volume of proceedings [38], focusing on aspects of nonequilibrium dynamics and its ongoing developments. This volume has been edited by G. Giacomin (Universite Paris Diderot), S. Olla (Université Paris Dauphine), E. Saada (CNRS and Université Paris Descartes), H. Sophn (TU Munich, Germany) and G. Stoltz. It includes contributions from various events relating to three domains: (i) transport in non-equilibrium statistical mechanics; (ii) the design of more efficient simulation methods; (iii) life sciences.

In addition, P. Plechac (University of Delaware, USA), T. Wang (Army Research Lab, USA) and G. Stoltz have considered in [61] numerical schemes for computing the linear response of steady-state averages of stochastic dynamics with respect to a perturbation of the drift part of the stochastic differential equation. The schemes are based on Girsanov's change-of-measure theory to reweight trajectories with factors derived from a linearization of the Girsanov weights. Both the discretization error and the finite time approximation error have been investigated. The designed numerical schemes have been shown to be of bounded variance with respect to the integration time, which is a desirable feature for long time simulation. The discretization error has been shown to be improved to second order accuracy in the time step by modifying the weight process in an appropriate way.

6.2.4. Coarse-graining

Two works have been done to explore new methods to define "good" reaction coordinates:

- The estimation of the Poincaré constant of a given probability measure allows to quantify the typical convergence rate of reversible diffusions to their equilibrium measure. Loucas Pillaud-Vivien, F. Bach and A. Rudi (Inria SIERRA), together with T. Lelièvre and G. Stoltz, have shown in [58], both theoretically and experimentally how to estimate the Poincaré constant given sufficiently many samples of the probability measure under consideration, using reproducing Hilbert kernel spaces. As a by-product of this estimation, they have also derived an algorithm that captures a low dimensional representation of the data by finding directions which are difficult to sample – reaction coordinates in the language of molecular dynamics. This amounts to finding the marginal of the high dimensional sampled measure for which the Poincaré constant is the largest possible.
- In [60], T. Lelièvre together with B. Leimkuhler and Z. Trstanova (University of Edinburgh, Scotland) has explored numerically the interest of using diffusion maps to define reaction coordinates or metastable states. Diffusion maps approximate the generator of Langevin dynamics from simulation data, and the idea is thus to use the eigenvalues and eigenvectors to build coarse-grained variables. They have also discussed the use of diffusion maps to define local reaction coordinates within the metastable sets, formalising the locality via the concept of quasi-stationary distribution and justifying the convergence of diffusion maps applied to samples within a metastable set.

Another coarse-graining procedure was considered to justify the approximation of an infinite system of ordinary differential equations (the Becker-Doring equations, describing coagulation/fragmentation processes of species of integer sizes) in terms of a partial differential equation. Formal Taylor expansions motivate that the dynamics at large sizes should be dictated by an advection-diffusion equation, called Fokker-Planck equation. P. Terrier and G. Stoltz rigorously proved in [59] the link between these two descriptions for evolutions on finite times rather than in some hydrodynamic limit, motivated by the results of numerical simulations and the construction of dedicated algorithms based on splitting strategies. In fact, the Becker-Doring equations and the Fokker-Planck equation are related through some pure diffusion with unbounded diffusion coefficient. The crucial point in the analysis is to obtain decay estimates for the solution of this pure diffusion and its derivates to control remainders in the Taylor expansions. The small parameter in this analysis is the inverse of the minimal size of the species.

6.3. Homogenization

Participants: Xavier Blanc, Virginie Ehrlacher, Olga Gorynina, Rémi Goudey, Claude Le Bris, Frédéric Legoll, Adrien Lesage, Pierre-Loïk Rothé.

In homogenization theory, members of the project-team have pursued their ongoing systematic study of perturbations of periodic problems (by local and nonlocal defects). This has been done in several different directions.

6.3.1. Deterministic non-periodic systems

For linear elliptic equations with highly oscillating coefficients, X. Blanc and C. Le Bris have recently developed, in collaboration with P.-L. Lions (Collège de France), a theory in the case of periodic problems with local defects. In particular, the existence of a corrector function for such problems has been shown. More details on the quality of approximation achieved by their theory have been recently provided. The fact that a corrector exists with suitable properties indeed allows one to quantify the rate of convergence of the two-scale expansion (which uses that corrector) to the actual exact solution, as the small homogenization parameter ε vanishes. In that spirit, some of these works by X. Blanc and C. Le Bris, in collaboration with M. Josien (former PhD student in the team, now at MPI Leipzig, Germany), have been presented in [12], [13].

Also in the context of homogenization theory, O. Gorynina, C. Le Bris and F. Legoll have explored the question of how to determine the homogenized coefficient of heterogeneous media without explicitly performing an homogenization approach. This work is a follow-up on earlier works by C. Le Bris and F. Legoll in collaboration with K. Li and next S. Lemaire over the years. During the year, O. Gorynina, C. Le Bris and F. Legoll have mathematically studied a computational approach initially introduced by R. Cottereau (CNRS Marseille). This approach combines, in the Arlequin framework, the original fine-scale description of the medium (modelled by an oscillatory coefficient) with an effective description (modelled by a constant coefficient) and optimizes upon the coefficient of the effective medium to best fit the response of a purely homogeneous medium. In the limit of asymptotically infinitely fine structures, the approach yields the value of the homogenized coefficient. The aim is to mathematically study the problem and to investigate how to improve on the practical algorithm, in order to obtain a procedure as efficient as possible. Results will be presented in a couple of manuscripts in preparation.

6.3.2. Stochastic homogenization

The project-team has pursued its efforts in the field of stochastic homogenization of elliptic equations, aiming at designing numerical approaches that are practically relevant and keep the computational workload limited.

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, and the team has proposed, over the past years, many approaches to improve on the computation of the homogenized tensor.

Besides the averaged behavior of the oscillatory solution u_ε on large space scales (which is given by its homogenized limit), a question of interest is to describe how u_ε fluctuates. This question has been investigated in the PhD thesis of P.-L. Rothé, both from a theoretical and a numerical viewpoints. First, theoretical results have been obtained for a weakly stochastic setting (where the coefficient is the sum of a periodic coefficient and a small random perturbation). It has been shown that, at the first order and when ε is small, the localized fluctuations (characterized by a test function g) of u_ε are Gaussian. The corresponding variance depends on the localization function g, on the right-hand side f of the problem satisfied by u_ε, and on a fourth order tensor Q which is defined in terms of the corrector. Since the corrector function is challenging to compute, so is Q. A numerical approach (based on using the standard truncated corrector problem) has been designed to approximate Q and its convergence has been proven, again in a weakly stochastic setting. All these theoretical results critically depend on detailed properties of the Green function associated to the periodic operator. Second, numerical experiments in more general settings (i.e. full stochastic case) following the same approach have been performed, in order to investigate the generality of the obtained results. First, the convergence of the approximation of Q has been monitored. Second, it has been checked that the localized fluctuations of u_ε indeed become Gaussian when ε decreases, and that their variance can be related to Q. These promising numerical results, which are consistent with the theoretical results obtained in the weakly stochastic setting, are presented in a manuscript in preparation.

6.3.3. Multiscale Finite Element approaches

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

During the year, several research tracks have been pursued in this general direction.

The MsFEM approach uses a Galerkin approximation on a pre-computed basis, obtained by solving local problems mimicking the problem at hand at the scale of mesh elements, with carefully chosen right-hand sides and boundary conditions. The initially proposed version of MsFEM uses as basis functions the solutions to these local problems, posed on each mesh element, with null right-hand sides and with the coarse P1 elements as Dirichlet boundary conditions. Various improvements have next been proposed, such as the *oversampling* variant, which solves local problems on larger domains and restricts their solutions to the considered element.

In collaboration with U. Hetmaniuk (University of Washington in Seattle, USA), C. Le Bris, F. Legoll and P.-L. Rothé have completed the study of a MsFEM method improved differently. They have considered a variant of the classical MsFEM approach with enrichments based on Legendre polynomials, both in the bulk of the mesh elements and on their interfaces. A convergence analysis of this new variant has been performed. In addition, residue type a posteriori error estimators have been proposed and certified, leading to a numerical strategy where the degree of enrichment is *locally* adapted in order to reach, at the smallest computational cost, a given error. The promising numerical results are currently being collected in a manuscript in preparation.

Many numerical analysis studies of the MsFEM are focused on obtaining a priori error bounds. In collaboration with L. Chamoin, who was on leave in the project-team a few years ago from ENS Cachan, members of the project-team have been working on a posteriori error analysis for MsFEM approaches, with the aim of developing error estimation and adaptation tools. They have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution u_h has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux $k\nabla u$. In the context of the MsFEM, it is important to be able to perform all expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach has thus been adapted to that context. In the recent work [47], the approach has also been adapted towards the design of adaptive algorithms for specific quantities of interest (in the so-called "goal-oriented" setting). It provides an accurate estimation of the error, and leads to a discretization which is efficiently tailored to the specific quantity under consideration.

One of the perspectives of the team, through the PhD thesis of A. Lesage, is the development of Multiscale Finite Element Methods for thin heterogeneous plates. The fact that one of the dimension of the domain of interest scales as the typical size of the heterogeneities within the material induces theoretical and practical difficulties that have to be carefully taken into account (see [37]). The first steps of the work of V. Ehrlacher, F. Legoll and A. Lesage, in collaboration with A. Lebée (Ecole des Ponts) have consisted in studying the homogenized limit (and the two-scale expansion) of problems posed on thin heterogeneous plates. After having considered the case of a diffusion equation, the more challenging case of elasticity has been studied. In the so-called membrane case (that is, when the loading is in the in-plane directions), an approximation result for the two-scale expansion has been obtained. Several MsFEM variants have been proposed and compared numerically. The results will be presented in a forthcoming manuscript.

6.4. Various topics

Participants: Sébastien Boyaval, Virginie Ehrlacher.

A new mathematical framework has been identified for the modelling of complex fluids in [42]. It allows one to incorporate rheological features of a real (non-ideal, visous and compressible) fluid and, at the same time, to compute flows as solution to a *hyperbolic system of conservation laws* complemented by an initial value. In [42], the framework is specified for 2D hydrostatic flows of *Maxwell fluids*, with a numerical finite-volume scheme preserving the positivity of mass and a Clausius-Duem inequality. Formally, the (macroscopic) model has a (microscopic) molecular justification using a generalized Langevin equation for the distortion of the fluid texture.

On the other hand, recall that stochastic models are also used for the numerical simulation of hydrodynamical turbulence. In particular, a generalized Langevin equation can be used to model the "thermostated" velocity fluctuations in a "stationary" turbulent flow modelled as an invariant measure. But the interest for the effective numerical simulation of turbulent flows is not fully understood yet. In [43], S. Boyaval with S. Martel and J. Reygner (Ecole des Ponts) have studied the convergence of a discretization of a 1D stochastic scalar viscous conservation laws (a toy-model), for the numerical simulation of its invariant measure.

A. Benaceur (EDF), V. Ehrlacher and A. Ern (École des Ponts and Inria SERENA) developped a new EIM/reduced-basis method [10] for the reduction of parametrized variational inequalities with nonlinear constraints, and applied this method to the reduction of contact mechanics problems with non-coincident meshes.

V. Ehrlacher, D. Lombardi (Inria COMMEDIA), O. Mula (Université Paris-Dauphine) and F-X. Vialard (Université Paris-Est) developped new model-order reduction techniques based on the use of Wasserstein spaces for transport-dominated problems [51], which gives very encouraging results on several classes of conservative transport problems like the Burger's equation. Theoretical convergence rates are proved on some particular test cases.

J. Berendsen (Chemnitz, Germany), Martin Burger (Erlangen, Germany), V. Ehrlacher, J-F. Pietschmann (Chemnitz, Germany) proved the existence and uniqueness of strong solutions and weak-strong stability in a particular system of cross-diffusion equations [41]. It is in general very difficult to obtain such kind of results for general cross-diffusion systems. The proof for the particular system studied here relies on the fact that, when all the cross-diffusion coefficients of the system are equal to the same constant, the system boils down to a set of independent heat equations, for which uniqueness of strong solutions is trivial. The uniqueness of strong solutions was proved under the assumption that the cross-diffusion coefficients should not be close enough to one another.

7. Bilateral Contracts and Grants with Industry

7.1. Contracts and grants with Industry

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

8. Partnerships and Cooperations

8.1. National Initiatives

The project-team is involved in several ANR projects:

- S. Boyaval is the PI of the ANR JCJC project SEDIFLO (2016-2021) to investigate new numerical models of solid transport in rivers.
- V. Ehrlacher is the PI of the ANR project COMODO (2020-2024) which focuses on the development of efficient numerical methods to simulate cross-diffusion systems on moving domains, with application to the simulation of the fabrication process of thin film solar cells. It includes research teams from Inria Lille, Inria Sophia-Antipolis and Germany.
- V. Ehrlacher is a member of the ANR project ADAPT (2018-2022), PI: D. Lombardi, Inria REO team-project. This project is concerned with the parallelization of tensor methods for high-dimensional problems.
- F. Legoll is a member of the ANR project CINE-PARA (2015-2020), PI: Y. Maday, Sorbonne Université. This project is concerned with parallel-in-time algorithms.
- T. Lelièvre is responsible of the node "Ecole des Ponts" of the ANR QuAMProcs (2019-2023), to which G. Stoltz also participates, PI: L. Michel, Université de Bordeaux.
- G. Stoltz is the PI of the ANR project COSMOS (2014-2019) which focuses on the development of efficient numerical techniques to simulate high-dimensional systems in molecular dynamics and computational statistics. It includes research teams from Institut Mines-Telecom, Inria Rennes and IBPC Paris.

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

- AMORE (Advanced Model Order REduction),
- CORREL (correlated methods in electronic structure computations),
- DYNQUA (time evolution of quantum systems, with applications to transport problems, nonequilibrium systems, etc.),
- EGRIN (gravity flows),
- MANU (MAthematics for NUclear applications),
- MASCOT-NUM (stochastic methods for the analysis of numerical codes),
- MEPHY (multiphase flows),
- NBODY (electronic structure),
- REST (theoretical spectroscopy),
- CHOCOLAS (experimental and numerical study of shock waves).

The project-team is involved in two Labex: the Labex Bezout (2011-) and the Labex MMCD (2012-).

We have invited the following national researchers to visit our team:

- A. Lozinski (University of Besançon): repeated visits during the year 2019.

8.2. European Initiatives

The ERC consolidator Grant MSMATH (ERC Grant Agreement number 614492, PI T. Lelièvre) ended in June 2019.

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

8.3. International Initiatives

T. Lelièvre, G. Stoltz and F. Legoll participate in the Laboratoire International Associé (LIA) CNRS / University of Illinois at Urbana-Champaign on complex biological systems and their simulation by high performance computers. This LIA involves French research teams from Université de Nancy, Institut de Biologie Structurale (Grenoble) and Institut de Biologie Physico-Chimique (Paris). The LIA has been renewed for 4 years, starting January 1st, 2018.

9. Dissemination

9.1. Promoting Scientific Activities

E. Cancès

- has been director (until August 2019) and is now co-director (starting September 2019) of CERMICS, the Applied Mathematics department at École des Ponts,
- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-), SIAM Journal of Scientific Computing (2008-), SIAM Multiscale Modeling and Simulation (2012-), and the Journal of Computational Mathematics (2017-),
- has co-organized the 4th international conference on Mathematical and Numerical Analysis of Electronic Structure Models (Suzhou, China, June), an interdisciplinary summer school on Mathematical Methods for Molecular Simulation at Jussieu (Paris, June), a series of minisymposia at ICIAM 2019 (Valencia, Spain, July), and the FSMP Horizon Maths 2019 conference (Paris, December).

V. Ehrlacher

- is a member of the “Conseil d’Enseignement et de Recherche” of Ecole des Ponts,
- co-organizes the colloquium of the CERMICS lab,
- co-organized a minisymposium at the ICIAM conference in Valencia, July.

C. Le Bris is a managing editor of Networks and Heterogeneous Media. He is a member of the editorial boards of Annales mathématiques du Québec (2013-), Archive for Rational Mechanics and Analysis (2004-), Calcolo (2019-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Nonlinearity (2005-), Journal de Mathématiques Pures et Appliquées (2009-), Pure and Applied Analysis (2018-). He is a member of the editorial boards of the monograph series Mathématiques & Applications, Series, Springer (2008-), Modelling, Simulations and Applications, Series, Springer (2009-), Springer Monographs in Mathematics, Springer (2016-). He is a member of

- the “Conseil de la Faculté des sciences et ingénierie”, Sorbonne Université,
- the “Conseil scientifique” of SMAI.

He is the president of the scientific advisory board of the Institut des Sciences du calcul et des données, Sorbonne Université. He holds a regular position of Visiting Professor at the University of Chicago.

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings and Surveys (with D. Chafai, C. Imbert and P. Lafitte),
- is a member of the editorial boards of IMA: Journal of Numerical Analysis, SIAM/ASA Journal of Uncertainty Quantification, Communications in Mathematical Sciences and Journal of Computational Physics,
- is a member of the “Conseil d’Administration” of SMAI and École des Ponts,
- has co-organized the CECAM workshop "Learning the collective variables of biomolecular processes" at Inria Paris July 10-12th 2019 (with L. Delemotte, J. Hénin and G. Stock),
- has co-organized the ICL/CNRS workshop on "Interacting Particle Systems and applications" at Imperial College of London, December 9-10th 2019 (with G. Pavliotis),
- holds a visiting professorship position at Imperial College of London (from August 2019).

F. Legoll

- is a member of the editorial board of SIAM MMS (2012-) and of ESAIM: Proceedings and Surveys (2012-),
- is a member of the ANR committee CES-40 "Mathématiques et informatique",
- has co-organized, with U. Hetmaniuk (U. of Washington, USA), the mini-symposium "Multiscale and domain decomposition approaches for PDEs with rough coefficients" within the SIAM CSE 2019 conference (Spokane, USA, February),
- has co-organized, with C. Le Bris, the mini-symposium "Computational approaches for multiscale, possibly random problems" within the ICIAM 2019 conference (Valencia, Spain, July).

A. Levitt co-organises the applied mathematics seminar of the CERMICS lab.

G. Robin

- co-organizes the working group “Machine learning and optimization” of the Labex Bezout (with G. Stoltz, as well as W. Hachel and R. Elie),
- is the president of the group "Jeunes de la Société Française de Statistique" (SFdS).

G. Stoltz

- is a member of the scientific council of UNIT (Université Numérique Ingénierie et Technologie),
- is a member of the "Conseil d’Enseignement et de Recherche" of Ecole des Ponts.

9.2. Teaching - Supervision - Juries

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

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

- Analyse et calcul scientifique, 30h (V. Ehrlacher, O. Gorynina, R. Goudey, A. Lesage, S. Siraj-Dine, G. Stoltz),
- Équations aux dérivées partielles et éléments finis, 15h (F. Legoll, P.-L. Rothé),
- Hydraulique numérique, 15h (S. Boyaval),
- Mécanique quantique, 10h (E. Cancès, A. Levitt),
- Méthodes numériques pour les problèmes en grande dimension, 17h30 (V. Ehrlacher, S. Boyaval),
- Optimisation, 15h, L3 (G. Kemlin, A. Lesage), Outils mathématiques pour l'ingénieur, 15h (E. Cancès, G. Ferré, F. Legoll, T. Lelièvre, P-L. Rothé),
- Projet de première année, 15h (G. Ferré).

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

- Analyse de Fourier, 15h (A. Levitt),
- Problèmes d'évolution, 36h (F. Legoll, V. Ehrlacher),
- Contrôle de systèmes dynamiques et équations aux dérivées partielles, 18h (E. Cancès),
- Projet du département IMI, 12h (G. Ferré, M. Ramil, J. Roussel, L. Silva Lopes),
- Projets Modéliser Programmer Simuler (V. Ehrlacher, G. Robin),
- Statistics and data sciences, 24h (G. Stoltz),
- Techniques de développement logiciel, 18h (M. Herbst).

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

- Méthodes de quantification des incertitudes en ingénierie, 18h (V. Ehrlacher),
- Remise à niveau: outils mathématiques, 9h (A. Lesage).

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

- Introduction à la physique statistique computationnelle, 20h (G. Stoltz),
- Méthodes numériques probabilistes, 24h (T. Lelièvre),
- Problèmes multiéchelles, aspects théoriques et numériques, 24h (F. Legoll),
- Théorie spectrale et variationnelle, 10h (E. Cancès).

At other institutions:

- Homogenization theory and multiscale problems, 21h, University of Chicago (C. Le Bris).
- Maths 2, 3h, L3, École des Mines (G. Stoltz),
- Probabilités de 1ère année, 27h, L3, Ecole des Mines (M. Ramil),
- Supervision of M2 projects, Master Mathématiques pour les sciences du vivant (MathSV) Université Paris-Saclay (G. Robin).

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

- Ling-Ling Cao, Mathematical analysis of models of electronic structure for defected materials, Université Paris-Est, École des Ponts, defended on October 29th, 2019, supervised by E. Cancès and G. Stoltz,
- Grégoire Ferré, Large deviations theory in statistical physics: some theoretical and numerical aspects, Université Paris-Est, École des Ponts, defended on November 27th, 2019, supervised by G. Stoltz,
- Pierre-Loik Rothé, Numerical methods for the estimation of fluctuations in multi-scale materials and related problems, Université Paris-Est, École des Ponts, defended on December 12th, 2019, supervised by F. Legoll,
- Laura Silva Lopes, Rare event simulation and applications to biological systems, Université Paris-Est, Ecole des Ponts, defended on December 19th, 2019, supervised by J. Hénin (IBPC) and T. Lelièvre.

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

- Zineb Belkacemi, thèse CIFRE SANOFI, Machine learning for reaction coordinates in molecular dynamics, Université Paris-Est, since November 2018, supervised by T. Lelièvre and G. Stoltz,
- Robert Benda, Multiscale modeling of functionalized nanotube networks for sensor applications, École Polytechnique, started September 1st, 2018, supervised by E. Cancès and B. Lebental (École Polytechnique),
- Raed Blel, Monte Carlo methods and model reduction, started October 1st, 2018, supervised by V. Ehrlacher and T. Lelièvre,
- Rafaël Coyaud, Méthodes déterministes et stochastiques pour le transport optimal, Université Paris-Est, École des Ponts, started october 2017, supervised by A. Alfonsi (CERMICS), co-supervised by V. Ehrlacher,
- Qiming Du, Mathematical analysis of splitting methods, Ecole Doctorale Sciences Mathématiques de Paris Centre, started September 1st, 2016, supervised by A. Guyader (UPMC) and T. Lelièvre,
- Rémi Goudey, Problèmes d'homogénéisation en présence de défauts, Université Paris-Est, started in September 2019, supervised by C. Le Bris.
- Gaspard Kemlin, Mathematical and numerical analysis for electronic structures, École des Ponts, started September 1st, 2019, supervised by E. Cancès and co-supervised by A. Levitt.
- Adrien Lesage, Multi-scale methods for calculation and optimization of thin structures, started October 1st, 2017, supervised by F. Legoll, co-supervised by V. Ehrlacher and A. Lebée (Ecole des Ponts),
- Mouad Ramil, Metastability for interacting particle systems, started October 1st 2017, supervised by T. Lelièvre and J. Reygner (CERMICS),
- Lise Maurin, Non reversible and adaptive biasing processes for sampling, started 1st October 2018, supervised by T. Lelièvre and J.-P. Piquemal (Sorbonne Université), together with P. Monmarché (Sorbonne Université),
- Idrissa Niakh, Réduction de modèles pour les inégalités variationnelles, Université Paris-Est, École des Ponts, thèse CIFRE EDF, started november 2019, supervised by A. Ern (CERMICS), co-supervised by V. Ehrlacher,
- Inass Sekkat, Large scale Bayesian inference, Université Paris-Est, since March 2018, supervised by G. Stoltz,
- Sami Siraj-Dine, Modélisation mathématique des matériaux 2D, École des Ponts, started October 1st, 2017, supervised by E. Cancès, C. Fermanian and co-supervised by A. Levitt.

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

- S. Boyaval, PhD of Olivier Ozenda ("Continuous modelisation of suspension rheology and migration processes"), defended at Université Grenoble Alpes in Mars 2019,
- S. Boyaval, PhD of Sofiane Martel ("Numerical and theoretical analysis of invariant measures of scalar stochastic viscous conservation laws"), defended at Ecole des Ponts in December 2019,
- E. Cancès, PhD of Amaury Hayat ("Stabilisation de systèmes hyperboliques non-linéaires en dimension un d'espace"), defended at Sorbonne University in May 2019,
- V. Ehrlacher, PhD of Nadia Jbili ("Design and analysis of optimization schemes for nuclear magnetic resonance"), defended at Université Paris-Dauphine in December 2019,
- V. Ehrlacher, PhD of Charles Paillet ("Nouvelles démarches de réduction de modèles pour le traitement des problèmes à très grand nombre de paramètres"), defended at Ecole Normale Supérieure Paris-Saclay in June 2019,
- F. Legoll, referee for the PhD of Qingqing Feng ("Développement d'une méthode d'éléments finis multi-échelles pour les écoulements incompressibles dans un milieu hétérogène"), defended at École Polytechnique in September 2019,

- T. Lelièvre, referee for the PhD of Augustin Chevallier ("Random walks for estimating densities of states and the volume of convex bodies in high dimensional spaces"), defended at Université Côte d'Azur in April 2019,
- T. Lelièvre, referee for the PhD of Oleg Balabanov ("Randomized linear algebra for model order reduction"), defended at Université Bretagne Loire in October 2019,
- T. Lelièvre, referee for the PhD of Lara Neureither ("Irreversible multi-scale diffusions: time scales and model reduction"), defended at Brandenburgische Technische Universität in November 2019,
- G. Stoltz, referee for the PhD of Nicolas Brosse ("Around the Langevin algorithm in high dimension: extensions and applications"), defended at Ecole polytechnique in June 2019,
- G. Stoltz, PhD thesis of Laurent Laflèche ("Large particle dynamical systems"), defended at Université Paris-Dauphine Université Paris-Dauphine in June 2019,
- G. Stoltz, referee for the PhD of Nada Cvtekovic ("Convergent discretization schemes for transition path theory for diffusion processes"), defended at FU Berlin in Fall 2019,
- G. Stoltz, referee for the PhD of Nadia Jbili ("Design and analysis of optimization schemes for nuclear magnetic resonance"), defended at Université Paris-Dauphine in December 2019.

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

- S. Boyaval, HdR of Sophie Ricci (“Uncertainties quantification and reduction in the computational geosciences – Application to free-surface hydraulics”), defended at CERFACS in April 2019,
- T. Lelièvre, president of the HDR jury of Denis Villemonais ("Exponential convergence to quasistationary distributions and applications"), defended at Université de Lorraine in November 2019.

9.3. Conference participation

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

- R. Benda, Informal Scientific Discussion (ISD) seminar of LSI laboratory, Ecole Polytechnique, Palaiseau, March,
- S. Boyaval, ICIAM minisymposia, Valencia (Spain), July,
- S. Boyaval, Workshop in computational hydraulics at UM6P, Ben Guerir (Morocco), September,
- S. Boyaval, 19th day of scientific computing and mathematical modelling in Amiens (France), June,
- E. Cancès University of Strasbourg, colloquium of the mathematics department, January,
- E. Cancès, WONAPDE, Conception, Chile, January (plenary lecture),
- E. Cancès, BIRS workhop, Banff, Canada, January,
- E. Cancès, Sorbonne Université, EMC2 seminar, Paris, February,
- E. Cancès, University of Chicago, Computational and applied mathematics seminar, USA, March,
- E. Cancès, ICMS workshop, Edinburgh, United Kingdom, March,
- E. Cancès, Fields Institute workshop, Toronto, Canada, April,
- E. Cancès, CECAM workshop, Lausanne, Switzerland, May,
- E. Cancès, AMMCS, Waterloo, Canada, August (plenary lecture),
- E. Cancès, IMS workshop, Singapore, September,
- E. Cancès, Sorbonne University, ERC EMC2 kick-off meeting, October,
- E. Cancès, Campus des Cordeliers, laboratoire J.-L. Lions 50th anniversary, Paris, November,
- V. Ehrlacher, GAMM meeting (keynote lecture), Vienna, February,
- V. Ehrlacher, Inria-LJLL seminar, Paris, April,
- V. Ehrlacher, Laboratoire Paul Painlevé seminar, Lille, April,
- V. Ehrlacher, Workshop Cambridge-MMCD, Marne-la-Vallée, April,

- V. Ehrlacher, workshop on “Optimal Transport: from Geometry to Numerics“, Erwin Schrödinger Institut, Vienna, April,
- V. Ehrlacher, workshop on “Scientific Computing Across Scales: Quantum Systems in Cold-matter Physics and Chemistry”, Fields Institut, Toronto, April,
- V. Ehrlacher, ICIAM, Valencia, July,
- V. Ehrlacher, MFO workshop: “Computational Multiscale Methods”, Oberwolfach, August,
- V. Ehrlacher, MORTECH, Paris, November,
- G. Ferré, Young researchers’ seminar, Université Paris-Dauphine, France, February,
- G. Ferré, Probability seminar at Lille University, France, March,
- G. Ferré, Probability seminar at Marseille University, France, May,
- G. Ferré, Congrès SMAI 2019, Lorient, France, May,
- G. Ferré, Journées de Probabilités, Dourdan, France, June,
- G. Ferré, ICIAM 2019, Valencia, Spain, July,
- G. Ferré, SciCADE 2019, Innsbruck, Austria, July
- G. Ferré, GAMM MoAnSi 2019 meeting, Munich, Germany, September,
- G. Ferré, Probability seminar, University Saint-Quentin en Yvelines, France, November,
- O. Gorynina, Congrès SMAI, Guidel, France, May,
- O. Gorynina, ICIAM 2019 conference, Valencia, Spain, July,
- O. Gorynina, Applied Mathematics Seminar, Surgut State University, Russia, December,
- M. Herbst, Université de Lorraine Laboratoire de Physique et Chimie Théoriques seminar, Metz, May,
- M. Herbst, Université de Lille, Laboratoire de Physique des Lasers, Atomes et Molécules seminar, Lille, May,
- M. Herbst, Technische Universität München, seminar Domcke group, München, September,
- M. Herbst, GAMM moansi annual meeting, München, September,
- M. Herbst, Université Paul Sabatier Toulouse, Laboratoire de Chimie et Physique Quantiques seminar, Toulouse, November,
- G. Kemlin, GAMM - MOANSI meeting, München, Germany, September
- C. Le Bris, ICIAM 2019 Invited speaker, July 2019, Valencia, Spain,
- F. Legoll, University of Chicago, CAMP seminar, Chicago, USA, February,
- F. Legoll, SIAM CSE 2019 conference, Spokane, USA, February,
- F. Legoll, Séminaire "Probabilités, Statistiques, Contrôle", ENSTA, Palaiseau, March,
- F. Legoll, CECAM workshop on "Big data and Uncertainty Quantification", Lausanne, Switzerland, March,
- F. Legoll, Colloque national en calcul des structures 2019, Giens, May,
- F. Legoll, ADMOS 2019 conference, Alicante, Spain, May,
- F. Legoll, Coupled problems 2019 conference, Barcelona, Spain, June,
- F. Legoll, MAFELAP (Mathematics of Finite Elements and Applications) 2019 conference, London, United Kingdom, June,
- F. Legoll, Séminaire du Laboratoire de Mécanique et d’Acoustique, Marseille, June,
- F. Legoll, ICIAM 2019 conference, Valencia, Spain, July,
- F. Legoll, Complas 2019 conference, Barcelona, Spain, September,

- F. Legoll, Workshop on "New trends in asymptotic methods for multiscale PDEs", Karlstad, Sweden, October,
- F. Legoll, MORTech 2019 workshop, Paris, November,
- T. Lelièvre, LIA CNRS - UIUC Meeting, Hauteluce, January,
- T. Lelièvre, Séminaire LPCT, Nancy, February,
- T. Lelièvre, Computational and Applied Mathematics / PDE seminar, University of Chicago, February,
- T. Lelièvre, CECAM Workshop, CIB-EPFL, Lausanne, Switzerland, March,
- T. Lelièvre, CECAM Workshop, CIB-EPFL, Lausanne, Switzerland, May,
- T. Lelièvre, CNLS Seminar, Los Alamos National Laboratory, USA, June,
- T. Lelièvre, IPAM, Lake Arrowhead, USA, June,
- T. Lelièvre, CECAM Workshop, Paris, July,
- T. Lelièvre, ICIAM, Valencia, Spain, July,
- T. Lelièvre, HetSys launch event, Warwick, England, September,
- T. Lelièvre, Numerical analysis in Bielefeld, Germany, September,
- T. Lelièvre, ANR QuAMProcs, Bordeaux, November,
- T. Lelièvre, AMMP Colloquium, Imperial College London, November,
- T. Lelièvre, "Fluids and Materials" seminar, Bristol, England, November,
- T. Lelièvre, Newton Institute, Cambridge, England, November,
- T. Lelièvre, Materials Research Society Fall Meeting, Boston, USA, December,
- A. Lesage, Congrès SMAI, Guidel, France, May,
- A. Lesage, ICIAM 2019 conference, Valencia, Spain, July,
- A. Levitt, BIRS workhop, Banff, Canada, January,
- A. Levitt, mathematical physics seminar, Copenhagen, February
- A. Levitt, Workshop Cambridge-MMCD, Marne-la-Vallée, April,
- A. Levitt, Congrès SMAI, Guidel, France, May,
- A. Levitt, Precision quantification in density functional theory, Louvain, Belgique, May,
- A. Levitt, Numerical Analysis of Electronic Structure Models, Suzhou, China, June,
- A. Levitt, ICIAM 2019 conference, Valencia, Spain, July,
- A. Levitt, GAMM - MOANSI meeting, München, Germany, September ,
- A. Levitt, weekly seminar, Aachen, Germany, October,
- A. Levitt, lunchtime seminar, Warwick UK, November,
- A. Levitt, Julia Meetup, Paris, December,
- G. Robin, seminar IACM, FORTH, Heraklion, October,
- G. Robin, seminar "Systèmes Complexes", CAMS, EHESS, November,
- P.-L. Rothé, Arbeitsgemeinschaft Applied Analysis, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany, April,
- P.-L. Rothé, Groupe de travail des thésards du Laboratoire Jacques-Louis Lions, Paris, May,
- P.-L. Rothé, Congrès SMAI, Guidel, France, May,
- P.-L. Rothé, ADMOS 2019 conference, Alicante, Spain, May,
- P.-L. Rothé, ICIAM 2019 conference, Valencia, Spain, July,
- P.-L. Rothé, Journée "Approches probabilistes en mécanique" de la Fédération Francilienne de Mécanique (F2M), Paris, November,

- L. Silva Lopes, LIA CNRS - UIUC annual Meeting, Hauteluce, France, January,
- L. Silva Lopes, Lorentz Workshop, Leiden, Netherlands, March,
- L. Silva Lopes, IPAM, Lakearrowhead, USA, June,
- L. Silva Lopes, ICIAM, Valencia, Spain, July,
- L. Silva Lopes, MOANSI annual meeting, Munich, Germany, October,
- G. Stoltz, Mathematical Physics Seminar, Institut Henri Poincaré, March,
- G. Stoltz, CECAM workshop "Microscopic simulations: forecasting the next two decades", Toulouse, France, April,
- G. Stoltz, Workshop Cambridge/Labex MMCD, Champs-sur-Marne, France, April,
- G. Stoltz, CIB workshop "Computational mathematics for model reduction and predictive modelling in molecular and complex systems", Lausanne, Switzerland, May,
- G. Stoltz, MAP5 Colloquium, Université Paris Descartes, June,
- G. Stoltz, Rencontres prospectives RFCT, Nantes, France, June,
- G. Stoltz, Maths/chemistry seminar EMC2, Sorbonne-Université, June,
- G. Stoltz, DEFI/MEDISIM/POEMS seminar, Inria Saclay, July,
- G. Stoltz, ICIAM 2019, Valencia, Spain, July,
- G. Stoltz, SciCADE 2019, Innsbruck, Austria, July,
- G. Stoltz, seminar CEREMADE, Université Paris-Dauphine, October,
- G. Stoltz, Applied PDEs seminar, Imperial College London, October,
- G. Stoltz, QuAMProcs meeting, Bordeaux, France, November.

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

- M. Herbst, Introduction to the Julia programming language, 6h, Julia Day, Paris, December,
- A. Levitt, Complex analysis and applications in quantum physics and chemistry, 9h, GDR CORREL spring school, Paris, April,
- G. Stoltz, Sampling high-dimensional probability distributions and Bayesian learning, 6h, doctoral school UM6P, Morocco, November,

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

- R. Benda, Ab Init School, CEA Bruyères-Le-Châtel (DAM), January.
- R. Benda, Journées Théorie, Modélisation et Simulations (JTMS) , Institut de Biologie Physico-chimique (IBPC), Paris, June.
- R. Benda, PhD day LPICM, Ecole Polytechnique, Palaiseau, April.
- R. Benda, LPICM Congress, Cap Ferret, October.
- R. Benda, GDR Graphene, Graphene & Co Meeting 2019, Bad Herrenalb, Germany, October.
- M. Herbst, 9th Molecular Quantum Mechanics Conference, Heidelberg, Germany, July,
- G. Ferré, CIB-CECAM meeting, Lausanne, Switzerland, May
- A. Lesage, Workshop "New trends and challenges in the mathematics of optimal design", Cambridge, United Kingdom, June,
- G. Robin, doctoral school UM6P, Morocco, November,
- L. Silva Lopes, GRC Liquids in Complex Environments, Driving Reactions, Assembling and Pushed to Their Limits, Holderness, USA, August,

Members of the team have benefited from long-term stays in institutions abroad:

- T. Lelièvre, University of Chicago, USA, February 2019 (three weeks),

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

- R. Benda, Mini-school on mathematics for theoretical chemistry and physics, Paris, June,
- O. Gorynina, Oberwolfach summer school "Beyond Numerical Homogenization", Oberwolfach, Germany, June,
- M. Herbst, Mini-school on mathematics for theoretical chemistry and physics, Paris, June
- M. Herbst, Kick-off meeting extreme-scale mathematically-based computational chemistry, Paris, October,
- G. Kemlin, Mini-school on mathematics for theoretical chemistry and physics, Paris, June,
- G. Kemlin, Une giornata con Alessio - Quelques mathématiques autour d'Alessio Figali, Saclay, July,
- G. Kemlin, Kick-off meeting of the ERC project EMC2, Paris, October,
- G. Kemlin, Laboratoire J.-L. Lions 50th anniversary, Paris, November,
- G. Kemlin, Horizon Maths 2019 - Mathématiques et Chimie, Paris, December
- M. Ramil, ANR QuAMProcs, Bordeaux, November 2019,
- P.-L. Rothé, Workshop "Industrial problems solving", Montréal, Canada, August,
- L. Silva Lopes, CECAM Workshop, Paris, France July 2019,
- S. Siraj-Dine, Quantum Transport and Universality, Accademia Nazionale dei Lincei, September,

9.4. Popularization

9.4.1. Internal or external Inria responsibilities

- A. Levitt is a member of the editorial board of Interstices, Inria's popularization website,
- C. Le Bris has presented the project-team at "Mon équipe en 180 secondes", on November 7, 2019.

9.4.2. Articles and contents

- V. Ehrlacher has been interviewed for the online magazine "DigiSchool"
- G. Robin has been interviewed for the online magazine "Usbek et Rica" following her "L'Oréal-UNESCO For Women in Science" prize

9.4.3. Internal actions

- C. Le Bris has organized a research day for the students at École des Ponts on November 6, 2019.
- V. Ehrlacher has participated to a meeting "Mathématiques, nom féminin?" organized at Ecole des Ponts with pupils from middle school.

10. Bibliography

Major publications by the team in recent years

[1] E. CANCÈS, M. DEFRANCESCHI, W. KUTZELNIGG, C. LE BRIS, Y. MADAY. *Computational Quantum Chemistry: A Primer*, 2003, Le Bris, Claude (ed.), Special Volume: Computational Chemistry. Amsterdam: North-Holland. Handb. Numer. Anal. 10, 3-270 (2003)

[2] E. CANCÈS, C. LE BRIS, Y. MADAY. *Mathematical Methods in Quantum Chemistry. An Introduction. (Méthodes mathématiques en chimie quantique. Une introduction.)*, Mathématiques et Applications (Berlin) 53. Berlin: Springer. xvi, 409 p. , 2006

[3] I. CATTO, C. LE BRIS, P.-L. LIONS. *The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models*, Oxford Mathematical Monographs. Oxford: Clarendon Press. xiii, 277 p., 1998

[4] J.-F. GERBEAU, C. LE BRIS, T. LELIÈVRE. *Mathematical Methods for the Magnetohydrodynamics of Liquid Metals*, Numerical Mathematics and Scientific Computation. Oxford: Oxford University Press., 324 p., 2006

[5] C. LE BRIS. *Multi-scale Analysis. Modeling and Simulation. (Systèmes multi-échelles. Modélisation et simulation.)*, Mathématiques et Applications (Berlin) 47. Berlin: Springer. xi, 212 p., 2005

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

[7] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Free Energy Computations: A Mathematical Perspective*, Imperial College Press, 458 p., 2010

Publications of the year

Doctoral Dissertations and Habilitation Theses

[8] G. FERRÉ. *Large Deviations Theory in Statistical Physics: Some Theoretical and Numerical Aspects*, Université Marne La Vallée, November 2019, https://hal.archives-ouvertes.fr/tel-02441535

[9] P.-L. ROTHÉ. *Numerical methods for the study of fluctuations in multi-scale materials and related problems*, Université Paris-Est Marne la Vallée, December 2019, https://tel.archives-ouvertes.fr/tel-02447725

Articles in International Peer-Reviewed Journals

[10] A. BENACEUR, A. ERN, V. EHRLACHER. *A reduced basis method for parametrized variational inequalities applied to contact mechanics*, in "International Journal for Numerical Methods in Engineering", October 2019 [*DOI :* 10.1002/NME.6261], https://hal.archives-ouvertes.fr/hal-02081485

[11] R. BENDA, E. CANCÈS, B. LEBENTAL. *Effective resistance of random percolating networks of stick nanowires: Functional dependence on elementary physical parameters*, in "Journal of Applied Physics", July 2019, vol. 126, n^{o} 4, 044306 p. [*DOI :* 10.1063/1.5108575], https://hal.archives-ouvertes.fr/hal-02281362

[12] X. BLANC, M. JOSIEN, C. LE BRIS. *Local precised approximation in multiscale problems with local defects*, in "Comptes Rendus Mathématique", 2019, https://arxiv.org/abs/1901.09669 [*DOI :* 10.1016/J.CRMA.2018.12.005], https://hal.archives-ouvertes.fr/hal-01893991

[13] X. BLANC, M. JOSIEN, C. LE BRIS. *Precised approximations in elliptic homogenization beyond the periodic setting*, in "Asymptotic Analysis", January 2020, vol. 116, n^{o} 2, pp. 93-137, https://arxiv.org/abs/1812.07220 [*DOI :* 10.3233/ASY-191537], https://hal.archives-ouvertes.fr/hal-01958207

[14] T. BOIVEAU, V. EHRLACHER, A. ERN, A. NOUY. *Low-rank approximation of linear parabolic equations by space-time tensor Galerkin methods*, in "ESAIM: Mathematical Modelling and Numerical Analysis", May 2019, vol. 53, n^{o} 2, pp. 635-658, https://arxiv.org/abs/1712.07256 [*DOI :* 10.1051/M2AN/2018073], https://hal.archives-ouvertes.fr/hal-01668316

[15] C.-E. BRÉHIER, T. LELIÈVRE. *On a new class of score functions to estimate tail probabilities of some stochastic processes with Adaptive Multilevel Splitting*, in "Chaos", 2019, vol. 29, 033126 p. [*DOI :* 10.1063/1.5081440], https://hal.archives-ouvertes.fr/hal-01923385

[16] E. CANCÈS, L.-L. CAO, G. STOLTZ. *A reduced Hartree–Fock model of slice-like defects in the Fermi sea*, in "Nonlinearity", January 2020, vol. 33, n^{o} 1, pp. 156-195, https://arxiv.org/abs/1807.06960 [*DOI :* 10.1088/1361-6544/AB4C7D/META], https://hal.archives-ouvertes.fr/hal-01891488

[17] E. CANCÈS, V. EHRLACHER, F. LEGOLL, B. STAMM, S. XIANG. *An embedded corrector problem for homogenization. Part II: Algorithms and discretization*, in "Journal of Computational Physics", 2020, vol. 407, 109254 p. , https://arxiv.org/abs/1810.09885 [*DOI :* 10.1016/J.JCP.2020.109254], https://hal.archives-ouvertes.fr/hal-01903486

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[19] D. CHAFAÏ, G. FERRÉ. *Simulating Coulomb gases and log-gases with hybrid Monte Carlo algorithms*, in "Journal of Statistical Physics", February 2019, vol. 174, n^{o} 3, pp. 692–714, https://arxiv.org/abs/1806.05985 [*DOI :* 10.1007/S10955-018-2195-6], https://hal.archives-ouvertes.fr/hal-01818268

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[21] G. DI GESÙ, T. LELIÈVRE, D. LE PEUTREC, B. NECTOUX. *Sharp asymptotics of the first exit point density*, in "Annals of PDE", June 2019, vol. 5, n^{o} 1, 5 p. , https://arxiv.org/abs/1706.08728 - 146 pages [*DOI :* 10.1007/S40818-019-0059-2], https://hal.archives-ouvertes.fr/hal-01548737

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