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ACTIVITY REPORT

Project-Team

RAPSODI

Reliable numerical approximations of dissipative systems

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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2 Overall objectives

Together with the diffusion of scientific computing, there has been a recent and impressive increase of the demand for numerical methods. The problems to be addressed are everyday more complex and require specific numerical algorithms. The quality of the results has to be accurately assessed, so that in-silico experiments results can be trusted. Nowadays, producing such reliable numerical results goes way beyond the abilities of isolated researchers, and must be carried out by structured teams.

The topics addressed by the RAPSODI project-team belong to the broad theme of numerical methods for the approximation of the solutions to systems of partial differential equations (PDEs). Besides standard convergence properties, a good numerical method for approximating a physical problem has to satisfy at least the following three criteria:

(a) preservation at the discrete level of some crucial features of the solution, such as positivity of solutions, conservation of prescribed quantities (e.g., mass), decay of physically motivated entropies, free energies, etc;

(b) provide accurate numerical approximations at a reasonable computational cost (and ultimately maximize the accuracy at a fixed computational effort);

(c) robustness with respect to physical conditions: the computational cost for a given accuracy should be essentially insensitive to a change in physical parameters.

We contribute to the development of methods fulfilling the above quality criteria for physical models which display, in their vast majority, a dissipative behavior, and that are motivated by industrial collaborations or multidisciplinary projects.

Ideally, we should allow ourselves to design entirely new numerical methods. For some applications however (often in the context of industrial collaborations), the members of the team have to work with existing codes. The numerical algorithms have thus to be optimized under this constraint.

Some technological bottlenecks related to points (a)–(c) mentioned above are well identified. In particular, it appears that a good numerical method should handle general meshes, so that dynamic mesh adaptation strategies can be used in order to achieve (b). But it should also be of the highest

possible order while remaining stable in the sense of (a), and robust in the sense of (c). There have been numerous research contributions on each point of (a)–(c) in the last decades, in particular for solving each difficulty separately, but combining them still leads to unsolved problems of crucial interest. Yet, before addressing the above points (a)–(c) concerning the design of nice numerical methods, one has to identify the structural properties of (and possibly modify) the continuous model to be discretized.

In a nutshell, our goal is to take advantage of and extend the most recent breakthroughs of the mathematical community to tackle in an efficient way some application-guided problems coming either from academics or from industrial partners. To this end, we focus on the following objectives, which are necessary for the applications we work on and which define the three research axes of our project:

1. Study of the structural properties of continuous PDE models.
2. Design and numerical analysis of structure-preserving numerical methods.
3. Computational optimization of the numerical methods.

The originality of the RAPSODI research team is its holistic approach as illustrated on Figure 1.

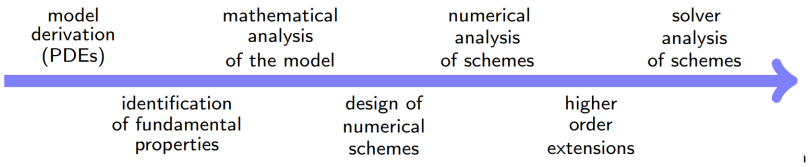

Figure 1: We consider the problem resolution in a global manner, starting from the model derivation (for instance based on physical principles) to the practical development of efficient numerical methods.

The study of the structural properties of the models under consideration helps in designing robust and accurate numerical schemes. It also helps in the design of efficient solvers. Our research program in these three axes, which constitute the core of the RAPSODI research project, is now going to be further detailed.

3 Research program

3.1 Axis 1: Study of the structural properties of continuous models

A well-behaved continuous (PDE based) model is a requisite to a reliable numerical approximation. The fine understanding of a continuous model is indeed a prior to the design of a numerical scheme in order to identify the structural properties to be preserved at the discrete level. Further, the mathematical analysis carried out on the continuous model often paves the way for the theoretical foundations of the numerical methods, hence our strong interest in this first research axis. Analyzing time-dependent PDE systems relying on their mathematical (Hamiltonian, gradient flow, ...) structure is very natural and unsurprisingly not new. However, the interest in this domain strongly increased in the last two decades. The focus of the RAPSODI project-team encompasses kinetic models, fluid mechanics, electromagnetism, multicomponent systems and applied calculus of variations. While carrying out theoretical analyses, we bear in mind that our results should be transposed to the discrete setting.

3.1.1 Thermodynamically consistent models for multi-component systems

Mathematical tools for the derivation and the mathematical analysis of models which are compatible with the second principle of thermodynamics and more specifically with Onsager's reciprocal principle [148] widely developed in the last decade. The general setting proposed in [141, 151] offers a powerful and robust framework for obtaining such models in configurations where inertia can be neglected.

This situation is typical of porous media flows in the Darcy regime. When rich physics are considered, like in presence of multiple phases and components within deformable and fractured matrices, the

derivation of such thermodynamically consistent models is a timely problem [157, 158, 160]. One of the goals of the RAPSODI project-team is to contribute to the mathematical understanding of such models [4].

Inertia is also commonly neglected in models for semi-conductors of van Roosbroeck type, as for instance in models for the corrosion of iron [81]. In the latter framework, the geometry of the domain varies along time and is one of the unknowns of the problem. The reference model proposed in [81] is not built from thermodynamical considerations. The design, the simulation and the calibration of a mathematical model which is consistent with the second principle is an ongoing task addressed by our team (see [101] for preliminary results).

3.1.2 Variational models and optimal transport

Optimal transport has a long history. In Monge's seminal work "Théorie des déblais et des remblais" dating back to 1781 [159], the problem was roughly stated the following way: how should one proceed to move piles of sand from one point to another in order to minimize the workload? This problem is now often referred to as "Monge problem". It has stayed with no solution in the general case until the 1940s, when Kantorovich inserted it into a proper framework [134], which allowed eventually to tackle it and provide solutions. A major breakthrough was obtained by Brenier [91], who showed that under very broad assumptions, the general solution to the optimal transport problem had a very specific form and could be linked with the famous Monge–Ampère equation.

In recent years, optimal transport has become a very active field of research, due to the discovery of new and efficient algorithms [119] and to its wide range of applications, to economy, image processing, analysis of partial differential equations or data sciences (see e.g. references in [153]).

One of the focus of our team is the use of optimal transport for understanding the formation of bi-layer cellular membranes thanks to a model introduced in [152]. In this model, the global shape of micelles or liposomes should be the result of competing forces: a short-range attractive force given by the area of the boundary, and a non-local repulsive force of Wasserstein-type (that is, an optimal transport cost). Our aim is to explore numerically this problem and obtain theoretically the shape of the solutions in some asymptotic regimes.

3.1.3 Kinetic models of large particle systems and their asymptotic regimes

Nearly 150 years after Boltzmann paved the way to the kinetic representation of complex phenomena [89], this approach for modeling is more than ever active. This increasing interest is partially due to the development of computational facilities that make the numerical approximation of such models possible, but also to the great flexibility of the approach which can be applied in biology [156], economics [121] or social sciences [93], way beyond its original scope in physics of gases.

One focus of our team is the asymptotic analysis of these equations. The large-time limit of kinetic equations has been dealt with thanks to hypocoercivity techniques in [76] and new hydrodynamic limits have been derived from kinetic models for gases composed of macroscopic particles interacting via energy dissipative collisions [132, 109] and plasmas [130]. A future concern will be the study of the long time dynamics of a kinetic model for relativistic electron bunches in storage rings [154] (see Section 4.6).

3.2 Axis 2: Design and analysis of structure-preserving numerical methods

The more complex is the PDE system to be discretized, the smaller is the chance that a naive discretization preserves at the discrete level its mathematical structure. Since this structure was the cornerstone of the mathematical analysis (typically by providing the well-posedness and the stability of the continuous system under consideration), its preservation at the discrete level will be key to get well-behaved and theoretically certified numerical methods. Our team concentrates a large part of its research effort on the design of provably convergent numerical methods, either based on the popular two-point flux approximation finite volume method, or on more flexible yet less natural structure preserving methods. We also pay attention to the fact that our schemes are robust with respect to the parameters and in the long time limit. The numerical approximation of complex (inhomogeneous or with low compressibility) flows is one of the topics we address.

3.2.1 Structure-preserving methods for systems of dissipative PDEs and variational models

A very important part of the activity of our team concerns the design of structure-preserving numerical methods for dissipative PDEs.

In this regard, two-point flux approximation (TPFA) finite volume schemes are very popular in industrial codes since they enjoy remarkable stability properties at a moderate computational price. Our team has a strong experience in the design of provably convergent entropy stable TPFA finite volume schemes for complex problems [68, 98, 104, 127, 107, 18, 97, 113, 102, 105, 107]. Ongoing [103, 146] and future research directions are based on the discretization of some action functionals and their optimization to obtain so-called variational schemes based on TPFA finite volumes. We also mention the Lagrangian approach [125], for which the computation of some optimal tessellation based on semi-discrete optimal transportation shows subtle but deep similarities with Eulerian TPFA based methods.

The main drawback of TPFA finite volume schemes is that they (essentially) restrict to isotropic diffusion problems and to regular grids [124, 126]. The strong constraints on the meshes and on the isotropic nature of the problems under consideration for TPFA schemes motivated in the last decades the development of more robust finite volume schemes, see for instance [122] for a review on this topic. These developments were particularly motivated by applications in geosciences, where anisotropic porous media are common and where (possibly poorly regular) meshes are often prescribed by data. Tuning such advanced methods, which do not enjoy monotonicity properties in general, to make them thermodynamically consistent is a key challenge for our team. An active research topic of our team is to propose new structure-preserving numerical schemes beyond TPFA. Our team has made important preliminary contributions on this topic through the design of structure-preserving control volume finite elements schemes [69, 70], vertex centered finite volume schemes [5], discrete duality finite volume schemes [100], finite element schemes [106] and hybrid finite volume schemes [112]. The latter numerical method also constitutes a first step towards high-order methods (see Section 3.2.2).

We intend to pursue our contributions in the development of structure-preserving numerical methods, both based on simple TPFA finite volumes and on more advanced robust methods. We will keep working on always more complex porous media flows, more advanced semi-conductor devices, or on non-standard flow models.

3.2.2 High-order structure-preserving numerical methods

Taking advantage of our experience in the design of low-order structure-preserving numerical schemes, we intend to improve the accuracy of our numerical methods by going to high-order discretizations in the space and time variables.

There are important contributors in the community in these topics. For instance, the development of high-order in space methods allowing for general grids for diffusion problems was pushed forward in the last decade by several groups, for instance around Lourenço Beirão da Veiga and Franco Brezzi [84] for the Virtual Element Methods (VEM), around Daniele A. Di Pietro and Alexandre Ern [9, 120] for the Hybrid High-Order (HHO) methods, or around Bernardo Cockburn [117] for the Hybridizable Discontinuous Galerkin (HDG) methods.

Our team aims at designing high-order in space and entropy stable schemes based on the HHO technology. We also aim at developing high-order methods on general meshes for electromagnetism in the context of a collaboration with EDF (French electricity supply company), with application to the non-invasive control of nuclear plants (see Section 4.4).

Concerning the time discretization strategies, we take inspiration in the works by Giovanni Samaey [135] for projective integration schemes, and in those by Christophe Besse [86] and Jie Shen [94] for relaxation methods. It appears that (explicit) Strong Stability Preserving high-order time discretizations [129], which are very popular in the community working on hyperbolic systems, are not suitable for solving dissipation driven (and typically parabolic) systems for which implicit methods are commonly used.

At the moment, most of our energy stable methods rely on merely first-order time discretizations, typically Backward Euler or minimizing movement schemes [133]. The extension to higher order time discretizations is already the purpose of ongoing studies in our team. Two tracks have been identified so far and are already studied: (i) the variational BDF2 scheme [139] which generalizes to second order in time the minimizing movement scheme, and (ii) Runge-Kutta type schemes obtained after having

changed of main variables. Both approaches have their pros and their cons: (i) is difficult to implement, whereas (ii) might lead to non-conservative methods. Our goal for the next years on this topic is to be able to overpass the difficulties of (at least one of) these methods and to get efficient implementation strategies as well as theoretical foundations.

3.2.3 Asymptotic-preserving and multiscale numerical methods

It has been understood around year 2000 that the fine quantification of the entropy dissipation allows one to deduce fine properties on the asymptotic behavior of the solutions to dissipative PDEs [74, 108]. The extension to the discrete setting of this type of tools is more recent, see for instance [110, 87, 111]. Our team is involved in the study of the long-time behavior of numerical schemes for drift-diffusion models [88, 99, 6, 112] and kinetic equations [2, 77]. A future challenge is the study of the long time behavior properties for numerical schemes which can handle general meshes and high order accuracy (see Section 3.2.1 and Section 3.2.2).

We also contribute actively to the design and analysis of multiscale methods for highly heterogeneous (or highly oscillatory) diffusion problems. We have extended in [116] within the HHO framework the nonconforming multiscale method of [136] to arbitrary approximation orders (and its analysis also to the case of general meshes). We have also established in [114] an equivalence result between our multiscale HHO method and the MHM method of [73], improving in passing on both methods.

In the future we will continue our effort in the design of numerical schemes which enjoy accurate asymptotic properties in large time, extreme regimes of parameters and multiscale settings. This effort, which aims at increasing the robustness of our numerical methods, is strongly correlated with the preservation of energy or entropy dissipation structures at the discrete level (cf. Section 3.2.1), as explained above. A particular effort has begun in the investigation of asymptotic preserving schemes to pass from kinetic models to van Roosbroeck type models for semiconductor devices.

3.2.4 Numerical methods for optimal transport

In the last years, optimal transport and its generalisations have proven to be a powerful tool to analyse a large class of models, exposing useful mathematical structures which are responsible of their properties [72], and guiding the conception of novel numerical schemes. Due to its geometrical and physical meanings, optimal transport has also emerged as a useful modelling tool in different contexts including economics, biology or social sciences [155].

Transportation problems can often be cast as global space-time optimisation problems such as in variational mean field games or optimal planning problems [85]. Part of the activity of our team in this area is concerned with the analysis of such models in the discrete setting, which poses significant difficulties both in terms of the conception of schemes (which often passes through the definition of discrete variational problems) [146][145], and of the devising of efficient optimization algorithms to compute their solutions [26].

As currently many of these problems are still intractable at the numerical level (due to their high dimensionality and lack of smoothness), our aim is to further improve the current approaches, for example by using unstructured meshes in space-time, which would pave the way for the development of adaptive refinement techniques. Importantly, such new schemes could be used as a building block to construct new discretisations for PDEs with a variational structure related to optimal transport (such as Wasserstein gradient flows [147][27]). In particular, this could represent an additional research path to reach our objectives mentioned in Section 3.2.1.

3.3 Axis 3: Computational optimization of the numerical methods

Good numerical methods shall enjoy strong theoretical foundations allowing to guarantee their behavior in very general situations. They shall also be highly efficient from a computational point of view, so that they can be used in practice for solving real-world problems.

To increase the efficiency and applicability of our methods, we work on three tracks. First, we aim at building a unified and optimized software platform to implement, test and diffuse our numerical methods. Second, since our methods often yield nonlinear systems, the improvement of the nonlinear

solvers is also key to increase the efficiency of our methods. Finally, for high-dimensional models such as kinetic and particle systems, the curse of dimensionality makes numerical computations realistically feasible only if specific computationally efficient numerical strategies are deployed.

3.3.1 Development of the platform `ParaSkel++`

`ParaSkel++` [83] is a C++ platform, conceived by S. Lemaire and mainly developed since December 2022 by T. Zoto (succeeding L. Beaude), which is freely distributed under LGPL v3.0. The `ParaSkel++` platform aims at the high-performance, arbitrary-order, 2/3D numerical approximation of PDEs on general polytopal meshes using skeletal Galerkin methods (see [138]).

A first version (v1, August 2021) of the platform is operational, featuring a sequential implementation of all the main skeletal methods (Lagrange FE, VEM and HHO). The next, already ongoing, crucial development steps are the parallelization on shared and distributed memory, and the implementation of efficient quadrature formulas on polytopal cells. Eventually, the `ParaSkel++` platform is expected to possess five main assets with respect to other codes of the same nature from the community: (i) a unified 2/3D implementation, (ii) the native support of any type of DOF (vertex-, edge-, face-, and cell-based), (iii) an ultra-factorized architecture (with common-to-all-methods local elimination and global assembly steps), (iv) the use of efficient quadrature formulas on general polytopal cells (without the need for subtessellation), and (v) the embedding of parallel computation capabilities.

3.3.2 Design of robust nonlinear solvers

The entropy stable methods we build often yield nonlinear systems to be solved at each time step. It is therefore of paramount importance to have fast and robust nonlinear solvers at hand to address them, hence the increasing interest for so-called nonlinear preconditioning techniques. In [3], we proposed a strategy which consists in expressing the problem in terms of a new primary variable which, if well chosen, allows to remove the degeneracies of the system under consideration. This strategy has then been extended to the case of more complex systems arising in the context of porous media flows [80, 79]. In the framework of a collaboration with IFPEN, we develop new solvers for the computation of chemical equilibria (see [33]), with application to reactive transport. The methodology being developed in this framework will then be transposed to other contexts in an as generic as possible way.

3.3.3 Efficient numerical methods for high-dimensional systems

Physically-relevant problems usually involve regimes of validity. These regimes are characterized by the relative size of some dimensionless numbers. Developing numerical methods that are able to accurately reproduce the behaviors for such various regimes is then crucial when dealing with applications, whether theoretical or with an engineering goal. Nevertheless, because of the high dimensionality of the phase space in kinetic theory (up to 7 dimensions), this can become a real challenge to develop implicit methods able to deal with the different time scales of the problems.

A robust and fully explicit method that was developed and allows for time integration of (two-scale) stiff systems with arbitrary order of accuracy in time is called projective integration (PInt). It was proposed in [128] for stiff systems of ordinary differential equations with a clear gap in their eigenvalue spectrum. In [135], PInt was introduced and analyzed for linear kinetic equations with a diffusive scaling. It was then extended to the nonlinear Boltzmann equation in [140] and to gas mixtures in [78].

However, having robust numerical methods is not enough: one also needs these methods to be extremely accurate and implemented efficiently, in order to obtain relevant numerical results in reasonable time. Spectral methods based on the fast Fourier transform have been developed in this sense in the last two decades, and reached enough maturity to be incorporated in high performance computing codes [10]. Equilibrium preserving extensions were also introduced and analyzed in the series of papers [150, 149]. Finally, an extension to the more mathematically intricated quantum Boltzmann operator has been achieved in the code `KINEBEC` [142], which has been used to show Bose–Einstein condensation and Fermi–Dirac relaxation in [143].

4 Application domains

4.1 Subsurface CO2 storage

The capture and storage in the subsurface of carbon dioxide is commonly acknowledged as a promising solution to mitigate the emission of greenhouse gas from localized production sites, as for instance cement plants. The safety assessment of the subsurface sequestration sites requires advanced numerical tools building on theoretically certified numerical models and algorithms which remain valid in the long time limit. Among the numerous difficulties encountered in such a setting, let us mention the high level of coupling between the mechanics of the (solid) porous matrix [118], the multiphase and multicomponent character of the fluid which flows therein [82], and chemical reactions with a wide range of characteristic times [137]. Despite important differences (at the level of chemistry especially), similar problems occur in the emerging topic of dihydrogen subsurface storage, or native dihydrogen (generated by the corrosion of iron in an aqueous environment) migration in the context of nuclear waste repository management.

Together with colleagues from applied research institutes and academics, the RAPSODI project-team contributes to the derivation of so-called *thermodynamically consistent models*, the stability of which in the long-time limit being guaranteed by the second principle. The team also contributes to the design and the analysis of numerical schemes for multiphase and multicomponent flows in complex geometries (possibly allowing for general meshes), and to the design of fast and robust solvers for chemical equilibria.

4.2 Material sciences

The team is interested in the theoretical and numerical analysis of mathematical models describing the degradation of materials, as concrete carbonation and corrosion. The study of such models is an important environmental and industrial issue. Atmospheric carbonation degrades reinforced concretes and limits the lifetime of civil engineering structures. Corrosion phenomena issues occur for instance in the reliability of nuclear power plants and the nuclear waste repository. The study of the long time evolution of these phenomena is of course fundamental in order to predict the lifetime of the structures.

4.3 Complex fluid flows

The team is interested in numerical methods for the simulation of systems of PDEs describing complex flows, like for instance mixture flows, granular gases, rarefied gases, or quantum fluids.

Variable-density, low-Mach flows have been widely studied in the recent literature because of their applicability in various phenomena such as flows in high-temperature gas reactors, meteorological flows, flows with convective and/or conductive heat transfer or combustion processes. In such cases, the resolution of the full compressible Navier–Stokes system is not adapted, because of the sound waves' speed. The Boussinesq incompressible model is not a better alternative for such low-speed phenomena, because the compressibility effects cannot be totally cancelled due to large variations of temperature and density. Consequently, some models have been formally derived, leading to the filtering of the acoustic waves by the use of some formal asymptotic expansions and two families of methods have been developed in the literature in order to compute these flows. We are interested in particular in the so-called pressure-based methods, which are more robust than density-based solvers, although their range of validity is in general more limited.

The kinetic theory of molecular gases models a gas as a system of elastically colliding spheres, conserving mechanical energy during impact. Once initialized, it takes to a molecular gas no more than a few collisions per particle to relax to its equilibrium state, characterized by a Maxwellian velocity distribution and a certain homogeneous density (in the absence of external forces). A granular gas is a system of dissipatively colliding, macroscopic particles (grains). This slight change in the microscopic dynamics (converting energy into heat) causes drastic changes in the behavior of the gas: granular gases are open systems, which exhibit self-organized spatio-temporal cluster formations, and have no equilibrium distribution. They can be used to model silos, avalanches, pollen or planetary rings.

Quantum models can be used to describe superfluids, quantum semiconductors, weakly interacting Bose gases, or quantum trajectories of Bohmian mechanics. They have attracted considerable attention in the last decades, due in particular to the development of nanotechnology applications. To describe

quantum phenomena, there exists a large variety of models. In particular, there exist three different levels of description: microscopic, mesoscopic, and macroscopic. The quantum Navier–Stokes equations deal with a macroscopic description in which the quantum effects are taken into account through a third-order term called the quantum Bohm potential. This Bohm potential arises from the fluid dynamical formulation of the single-state Schrödinger equation. The nonlocality of quantum mechanics is approximated by the fact that the equations of state do not only depend on the particle density but also on its gradient. These equations were employed to model field emissions from metals and steady-state tunneling in metal-insulator-metal structures, and to simulate ultra-small semiconductor devices.

4.4 Electromagnetism for non-invasive control

The RAPSODI project-team works on the development of high-order polyhedral methods for electromagnetism. A well-known specificity in electromagnetism is that topology plays a crucial role in the well-posedness of the models. Dedicated analysis tools must then be deployed for their study [75]. We are interested in the devising of HHO methods in the curl/curl setting [115]. The mathematical analysis of HHO methods in this setting is particularly involved, as most of the needed discrete functional analysis tools are currently lacking. The design of (efficient and robust) multilevel linear solvers for statically condensed HHO approximations of electromagnetic models, as well as of computable (reliable and locally efficient) a posteriori error estimators on polyhedral cells are two other, still largely unexplored, aspects we are interested in. Our main target application, in the framework of a recently initiated collaboration with EDF, is the simulation of eddy current testing (ECT). ECT is used by EDF as a non-invasive control technique to assess the integrity of heat exchanger tubes in nuclear plants. The forward problem consists in solving the time-harmonic 3D Maxwell's equations in domains featuring more or less complex flaws. The use of high-order polyhedral methods is expected to yield improvements on two aspects. First, the support of polyhedral cells is expected to ease the full meshing process, and in particular enable to account for defects with complex geometries/topologies. Second, the increase in the approximation order is expected to yield a reduction of the noise on the computed control signal based on which the presence of a defect is inferred.

4.5 Large population models in epidemiology

Developing mathematical models to describe how infectious pathogens spread in animal populations is an essential step to identify the main biological mechanisms or environmental factors which contribute to the emergence of epidemics. When describing a pathogen spread at large scales, it is often relevant to model the distributions of hosts (which may represent individuals, animals or herds, for example) as spatially varying densities, and to model the pathogen dynamics via PDEs which describe the combined effect of neighbourhood interactions, large scale population dynamics, and environmental factors.

The team initiated a collaboration with INRAE (National Research Institute on Agriculture and Environment) on the modeling of different types of pathogen spread mechanisms in such continous models. A first focus of this collaboration is on neighbourhood interactions, which are a dominant factor in the infection dynamics of many pathogens (a specific example is the Bovine Viral Diarrhea Virus, an endemic disease present worldwide among industrial cattle herds, and causing annually large economic losses), and which at large scales may be described via non-local (convolution) terms. The analysis of the resulting model requires the development of dedicated mathematical tools, and will lead to a better understanding of the influence of neighborhood interactions on the spatial features of the epidemic dynamics. A second focus is on arboviruses, which are pathogens transmitted to mammals by the bite of arthropod vectors, mainly mosquitoes, and causing diseases such as the Zika virus, the Rift Valley fever and the West Nile virus. In this case, the aim is to produce a comprehensive description of the viral dynamics both in the vectors and in the hosts as well as to model their interaction in space (via diffusion processes and nonlocal interactions), which will then be used to identify the main mechanisms driving the virus spread.

4.6 Particle accelerators

Relativistic electron bunches are used in storage rings to produce intense radiation in various ranges of frequencies. The dynamics of these bunches is nonlinear because of interactions between electrons in the bunch. Moreover, these interactions occur in an asymmetric fashion because of the relativistic nature of the dynamics. The stability properties of the bunch (and thus the long-time properties of the dynamics) have been shown, both theoretically and experimentally, to be crucial in the understanding of the intensity of the emitted radiation [95, 123].

From a mathematical point of view, the dynamics of the electron density in the phase space can be described by a Vlasov–Fokker–Planck type equation [95] with a well suited mean-field self-interaction term [144]. The mathematical understanding of the long time behavior of solutions to this equation and the design of adapted numerical schemes constitutes a challenging and physically important problem.

5 New software, platforms, open data

5.1 New software

5.1.1 ParaSkel++

Keywords: PDEs, Polytopal meshes, High-order methods, HPC, C++

Functional Description: ParaSkel++ is a C++ platform, conceived by S. Lemaire and essentially developed by L. Beaude (02/2020–08/2021) and T. Zoto (12/2022–06/2024), which is freely distributed under GNU LGPL v3.0. The ParaSkel++ platform aims at the arbitrary-order, 2D/3D numerical approximation of PDEs on general polytopal meshes using skeletal Galerkin methods. Skeletal methods form a vast family of numerical approaches for the approximation of PDE-based models, which satisfy the following two building principles:

(1) the degrees of freedom (DoFs) of the method split into (i) skeleton DoFs, attached to the geometric entities (vertices, edges, faces) composing the mesh skeleton and common to all cells sharing the geometric entity in question, which prescribe the conformity properties of the underlying discrete functional space, and (ii) bulk DoFs (if any), attached to the interior of the cells, which play no role in the prescription of the conformity properties,

(2) the global discrete bilinear form of the problem (potentially after linearization, if the problem is nonlinear) writes as the sum over the mesh cells of cell-wise (referred to as local) bilinear contributions.

The very structure underpinning skeletal methods grants them the property of being amenable to static condensation, i.e. locally to each mesh cell, bulk DoFs can be eliminated in terms of the local skeleton DoFs by means of a local Schur complement. The final global system to solve thus writes in terms of the skeleton DoFs only. The skeletal family encompasses, in particular, standard FE methods as well as virtual-like Galerkin methods (VEM, HDG, HHO...). It does not contain (plain vanilla) IP-DG methods.

ParaSkel++ provides a high-performance, factorized C++ architecture for the implementation of arbitrary-order skeletal methods on general 2D/3D polytopal meshes. A first version (v1, August 2021) of the platform has been released, which features a sequential implementation of all the main skeletal methods on toy PDE problems. Ongoing developments still concern the parallelization of the code on shared and distributed memory, as well as the implementation of efficient quadrature formulas on polytopal cells.

Eventually, the ParaSkel++ platform is expected to possess five main assets setting it apart from other codes of the same nature from the community: (i) a unified 2D/3D implementation, (ii) the native support of any type of DoF (vertex-, edge-, face-, and cell-based), (iii) an ultra-factorized architecture (with common-to-all-methods local elimination and global assembly steps), (iv) the use of efficient quadrature formulas on polytopal cells (without the need for subtessellation), and (v) the embedding of advanced parallel computation capabilities.

URL: https://gitlab.inria.fr/simlemai/paraskel

Publication: hal-03517921

Contact: Simon Lemaire

Participants: Laurence Beaude, Thoma Zoto, Silvano Pitassi, Jeremy Dalphin

5.1.2 JuXim

Keywords: Chemical equilibrium, Complementarity problem, Nonlinear solver

Functional Description: Package for solving single- and multiphase chemical equilibria using the Julia language.

URL: https://gitlab.com/maxime.jonval/juxim

Contact: Maxime Jonval

6 New results

6.1 Modeling, analysis and numerical simulation of multi-component systems

Chemical equilibria computations, especially those with vanishing species in the aqueous phase, lead to nonlinear systems that are difficult to solve due to gradient blow up. Instead of the commonly used ad hoc treatments, M. Jonval, C. Cancès *et al.* propose in [33] two reformulations of the single-phase chemical equilibrium problem which are in line with the spirit of preconditioning but whose actual aims are to guarantee a better stability of Newton's method. The first reformulation is a parametrization of the graph linking species mole fractions to their chemical potentials. The second is based on an augmented system where this relationship is relaxed for the iterates by means of a Cartesian representation. We theoretically prove the local quadratic convergence of Newton's method for both reformulations. From a numerical point of view, we demonstrate that the two techniques are accurate, allowing to compute equilibria with chemical species having very low concentrations. Moreover, the robustness of our methods combined with a globalization strategy is superior to that of the literature.

In [13], C. Chainais-Hillairet, M. Herda *et al.* consider a drift-diffusion charge transport model for perovskite solar cells, where electrons and holes may diffuse linearly (Boltzmann approximation) or nonlinearly (e.g. due to Fermi-Dirac statistics). To incorporate volume exclusion effects, they rely on the Fermi-Dirac integral of order -1 when modeling moving anionic vacancies within the perovskite layer which is sandwiched between electron and hole transport layers. After non-dimensionalization, they first prove a continuous entropy-dissipation inequality for the model. Then, they formulate a corresponding two-point flux finite volume scheme on Voronoi meshes and show an analogous discrete entropy-dissipation inequality. This inequality helps them to show the existence of a discrete solution to the nonlinear discrete system with the help of a corollary of Brouwer's fixed point theorem and the minimization of a convex functional. Finally, they verify the theoretically proven properties numerically, simulating a realistic device setup and showing exponential decay in time with respect to the L^2-error as well as a physically and analytically meaningful relative entropy.

In [38], C. Chainais-Hillairet, M. Herda *et al.* present the numerical analysis and simulations of a multi-dimensional memristive device model. Memristive devices and memtransistors based on two-dimensional (2D) materials have demonstrated promising potential as components for next-generation artificial intelligence (AI) hardware and information technology. The charge transport model describes the drift-diffusion of electrons, holes, and ionic defects self-consistently in an electric field. They incorporate two types of boundary models: ohmic and Schottky contacts. The coupled drift-diffusion partial differential equations are discretized using a physics-preserving Voronoi finite volume method. It relies on an implicit time-stepping scheme and the excess chemical potential flux approximation. They demonstrate that the fully discrete nonlinear scheme is unconditionally stable, preserving the free-energy structure of the continuous system and ensuring the non-negativity of carrier densities. Novel discrete entropy-dissipation inequalities for both boundary condition types in multiple dimensions allow them to prove the existence of discrete solutions. They perform multi-dimensional simulations to understand the impact of electrode configurations and device geometries, focusing on the hysteresis behavior in lateral

2D memristive devices. Three electrode configurations – side, top, and mixed contacts – are compared numerically for different geometries and boundary conditions. These simulations reveal the conditions under which a simplified one-dimensional electrode geometry can well represent the three electrode configurations. This work lays the foundations for developing accurate, efficient simulation tools for 2D memristive devices and memtransistors, offering tools and guidelines for their design and optimization in future applications.

In [62], M. Herda *et al.* analyse an instationary drift–diffusion system for the electron, hole, and oxygen vacancy densities, coupled to the Poisson equation for the electric potential, in a bounded domain with mixed Dirichlet–Neumann boundary conditions. The electron and hole densities are governed by Fermi–Dirac statistics, while the oxygen vacancy density is governed by Blakemore statistics. The equations model the charge carrier dynamics in memristive devices used in semiconductor technology. The global existence of weak solutions is proved in up to three space dimensions. The proof is based on the free energy inequality, an iteration argument to improve the integrability of the densities, and estimations of the Fermi–Dirac integral. Under a physically realistic elliptic regularity condition, it is proved that the densities are bounded.

In [17], C. Cancès, C. Chainais-Hillairet *et al.* propose and study a one-dimensional model which consists of two cross-diffusion systems coupled via a moving interface. The motivation stems from the modelling of complex diffusion processes in the context of the vapor deposition of thin films. In the model, cross-diffusion of the various chemical species can be respectively modelled by a size-exclusion system for the solid phase and the Stefan-Maxwell system for the gaseous phase. The coupling between the two phases is modelled by linear phase transition laws of Butler-Volmer type, resulting in an interface evolution. The continuous properties of the model are investigated, in particular its entropy variational structure and stationary states. They introduce a two-point flux approximation finite volume scheme. The moving interface is addressed with a moving-mesh approach, where the mesh is locally deformed around the interface. The resulting discrete nonlinear system is shown to admit a solution that preserves the main properties of the continuous system, namely: mass conservation, nonnegativity, volume-filling constraints, decay of the free energy and asymptotics. In particular, the moving-mesh approach is compatible with the entropy structure of the continuous model. Numerical results illustrate these properties and the dynamics of the model.

In [42], C. Cancès, M. Herda *et al.* present a finite volume scheme for modeling the diffusion of charged particles, specifically ions, in constrained geometries using a degenerate Poisson-Nernst-Planck system with size exclusion yielding cross-diffusion. The method utilizes a two-point flux approximation and is part of the exponentially fitted schemes framework. The scheme is shown to be thermodynamically consistent, as it ensures the decay of some discrete version of the free energy. Classical numerical analysis results –existence of discrete solution, convergence of the scheme as the grid size and the time step go to 0– follow. They also investigate the long-time behavior of the scheme, both from a theoretical and numerical point of view. Numerical simulations confirm the findings, but also point out some possibly very slow convergence towards equilibrium of the system under consideration.

In [43], C. Cancès *et al.* study a system of drift-diffusion PDEs for a potentially infinite number of incompressible phases, subject to a joint pointwise volume constraint. The analysis is based on the interpretation as a collection of coupled Wasserstein gradient flows or, equivalently, as a gradient flow in the space of couplings under a 'fibered' Wasserstein distance. They prove existence of weak solutions, long-time asymptotics, and stability with respect to the mass distribution of the phases, including the discrete to continuous limit. A key step is to establish convergence of the product of pressure gradient and density, jointly over the infinite number of phases. The underlying energy functional is the objective of entropy regularized optimal transport, which allows us to interpret the model as the relaxation of the classical Angenent-Haker-Tannenbaum (AHT) scheme to the entropic setting. However, in contrast to the AHT scheme's lack of convergence guarantees, the relaxed scheme is unconditionally convergent. They conclude with numerical illustrations of the main results.

Multiphase poromechanics describes the evolution of multiphase flows in deformable porous media. Mathematical models for such multiphysics systems are inherently nonlinear, potentially degenerate and fully coupled systems of partial differential equations. In [40], C. Cancès *et al.* present a thermodynamically consistent multiphase poromechanics model falling into the category of Biot equations and obeying to a generalized gradient flow structure. It involves capillarity effects, degenerate relative permeabilities, and gravity effects. Contrary to established models it introduces a Lagrange multiplier associated to a

bound constraint on the effective porosity in particular ensuring its positivity. They establish existence of global weak solutions under the assumption of a weak coupling strength, implicitly utilizing the gradient flow structure, as well as regularization, a Faedo-Galerkin approach, and compactness arguments. This comprises the first global existence result for multiphase poromechanics accounting for degeneracies that are consistent with the multiphase nature of the flow.

The presence of moving interfaces is a characteristic feature of corrosion phenomena. The evolution of these interfaces is governed by nonlinear laws and poses significant difficulties in the theoretical and numerical treatment of the models. B. Merlet, J. Venel *et al.* attack these difficulties in [64], namely, they show the existence of solutions to a 1D reduced corrosion model with a moving interface. Their method is based on a minimizing movement scheme for some modified Wasserstein metric.

The efficiency of (In,Ga)N-based light emitting diodes (LEDs) is limited by the failure of holes to evenly distribute across the (In,Ga)N/GaN multi-quantum well stack which forms the active region. To tackle this problem, it is important to understand carrier transport in these alloys. In [37], J. Moatti *et al.* study the impact that random alloy fluctuations have on the distribution of electrons and holes in such devices. To do so, an atomistic tight-binding model is employed to account for alloy fluctuations on a microscopic level and the resulting tight-binding energy landscape forms input to a quantum corrected drift-diffusion model. Here, quantum corrections are introduced via localization landscape theory. Similar to experimental studies in the literature, they have focused on a multi-quantum well system where two of the three wells have the same In content while the third well differs in In content. By changing the order of wells in this 'multi-color' quantum well structure and looking at the relative radiative recombination rates of the different emitted wavelengths, they (i) gain insight into the distribution of carriers in such a system and (ii) can compare their findings to trends observed in experiment. They focus on three factors and evaluate the impact that each have on carrier distribution: an electron blocking layer, quantum corrections and random alloy fluctuations. They find that the electron blocking layer is of secondary importance. However, in order to recover experimentally observed features – namely that the p-side quantum well dominates the light emission – both quantum corrections and random alloy fluctuations should be considered. The widely assumed homogeneous virtual crystal approximation fails to capture the characteristic light emission distribution across a multi-quantum well stack.

6.2 Analysis and numerical simulation in electromagnetism and related fields

In [36], S. Lemaire and S. Pitassi prove discrete versions of the first and second Weber inequalities on $\boldsymbol{H}(\mathbf{curl}) \cap \boldsymbol{H}(\mathrm{div})$-like hybrid spaces spanned by polynomials attached to the faces and to the cells of a polyhedral mesh. The proven hybrid Weber inequalities are optimal in the sense that (i) they are formulated in terms of $\boldsymbol{H}(\mathbf{curl})$- and $\boldsymbol{H}(\mathrm{div})$-like hybrid semi-norms designed so as to embed optimally (polynomially) consistent face penalty terms, and (ii) they are valid for face polynomials in the smallest possible stability-compatible spaces. The results are valid on domains with general, possibly non-trivial topology. In a second part are also proved, within a general topological setting, related discrete Maxwell compactness properties.

In [56], S. Lemaire, S. Pitassi *et al.* devise and analyze hybrid polyhedral methods of arbitrary order for the approximation of div-curl systems on three-dimensional domains featuring non-trivial topology. The systems they focus on stem from magnetostatics, and can either be first-order (field formulation) or second-order (vector potential formulation). The well-posedness of the methods essentially relies on topologically generic hybrid versions of the first and second Weber inequalities. The error analysis is performed for regular solutions. Finally, leveraging (co)homology computation techniques from the literature, a comprehensive numerical validation of the methodology is provided.

In [50], T. Chaumont-Frelet *et al.* analyze the conforming approximation of the time-harmonic Maxwell's equations using Nédélec (edge) finite elements. They prove that the approximation is asymptotically optimal, i.e., the approximation error in the energy norm is bounded by the best-approximation error times a constant that tends to one as the mesh is refined and/or the polynomial degree is increased. Moreover, under the same conditions on the mesh and/or the polynomial degree, they establish discrete inf-sup stability with a constant that corresponds to the continuous constant up to a factor of two at most. Their proofs apply under minimal regularity assumptions on the exact solution, so that general domains, material coefficients, and right-hand sides are allowed.

In [47], T. Chaumont-Frelet proposes a novel a posteriori error estimator for the Nédélec finite

element discretization of time-harmonic Maxwell's equations. After the approximation of the electric field is computed, he proposes a fully localized algorithm to reconstruct approximations to the electric displacement and the magnetic field, with such approximations respectively fulfilling suitable divergence and curl constraints. These reconstructed fields are in turn used to construct an a posteriori error estimator which is shown to be reliable and efficient. Specifically, the estimator controls the error from above up to a constant that tends to one as the mesh is refined and/or the polynomial degree is increased, and from below up to constant independent of p. Both bounds are also fully-robust in the low-frequency regime. The properties of the proposed estimator are illustrated on a set of numerical examples.

In [48], T. Chaumont-Frelet considers interior penalty discontinuous Galerkin discretizations of time-harmonic wave propagation problems modeled by the Helmholtz equation, and derives novel a priori and a posteriori estimates. His analysis classically relies on duality arguments of Aubin–Nitsche type, and its originality is that it applies under minimal regularity assumptions. The estimates he obtains directly generalize known results for conforming discretizations, namely that the discrete solution is optimal in a suitable energy norm and that the error can be explicitly controlled by a posteriori estimators, provided the mesh is sufficiently fine.

In [49], T. Chaumont-Frelet *et al.* derive a priori and a posteriori error estimates for the discontinuous Galerkin (dG) approximation of the time-harmonic Maxwell's equations. Specifically, they consider an interior penalty dG method, and establish error estimates that are valid under minimal regularity assumptions and involving constants that do not depend on the frequency for sufficiently fine meshes. The key result of the a priori error analysis is that the dG solution is asymptotically optimal in an augmented energy norm that contains the dG stabilization. Specifically, up to a constant that tends to one as the mesh is refined, the dG solution is as accurate as the best approximation in the same norm. The main insight is that the quantities controlling the smallness of the mesh size are essentially those already appearing in the conforming setting. They also show that for fine meshes, the inf-sup stability constant is as good as the continuous one up to a factor two. Concerning the a posteriori analysis, they consider a residual-based error estimator under the assumption of piecewise constant material properties. They derive a global upper bound and local lower bounds on the error with constants that (i) only depend on the shape-regularity of the mesh if it is sufficiently refined and (ii) are independent of the stabilization bilinear form.

In [55], T. Chaumont-Frelet *et al.* consider the h-version of the finite element method, where accuracy is increased by decreasing the meshwidth h while keeping the polynomial degree p constant, applied to the Helmholtz equation. Although the question "how quickly must h decrease as the wavenumber k increases to maintain accuracy?" has been studied intensively since the 1990s, none of the existing rigorous wavenumber-explicit analyses take into account the approximation of the geometry. In this paper they prove that for nontrapping problems solved using straight elements the geometric error is of order kh, which is then less than the pollution error $k(kh)^2p$ when k is large; this fact is then illustrated in numerical experiments. More generally, they prove that, even for problems with strong trapping, using degree four (in 2-d) or degree five (in 3-d) polynomials and isoparametric elements ensures that the geometric error is smaller than the pollution error for most large wavenumbers.

In [51], T. Chaumont-Frelet *et al.* derive a posteriori error estimates for the the scalar wave equation discretized in space by continuous finite elements and in time by the explicit leapfrog scheme. The analysis combines the idea of invoking extra time-regularity for the right-hand side, as previously introduced in the space semi-discrete setting, with a novel, piecewise quartic, globally twice-differentiable time-reconstruction of the fully discrete solution. The main results show that the proposed estimator is reliable and efficient in a damped energy norm. These properties are illustrated in a series of numerical examples.

In [52], T. Chaumont-Frelet *et al.* prove sharp wavenumber-explicit error bounds for first- or second-type-Nédélec-element (a.k.a. edge-element) conforming discretisations, of arbitrary (fixed) order, of the variable-coefficient time-harmonic Maxwell equations posed in a bounded domain with perfect electric conductor (PEC) boundary conditions. The PDE coefficients are allowed to be piecewise regular and complex-valued; this set-up therefore includes scattering from a PEC obstacle and/or variable real-valued coefficients, with the radiation condition approximated by a perfectly matched layer (PML). In the analysis of the h-version of the finite element method, with fixed polynomial degree p, applied to the time-harmonic Maxwell equations, the asymptotic regime is when the meshwidth, h, is small enough (in a wavenumber-dependent way) that the Galerkin solution is quasioptimal independently of the

wavenumber, while the preasymptotic regime is the complement of the asymptotic regime. The results of this paper are the first preasymptotic error bounds for the time-harmonic Maxwell equations using first-type Nédélec elements or higher-than-lowest-order second-type Nédélec elements. Furthermore, they are the first wavenumber-explicit results, even in the asymptotic regime, for Maxwell scattering problems with a non-empty scatterer.

In [66], T. Chaumont-Frelet *et al.* consider the finite element solution of time-harmonic wave propagation problems in heterogeneous media with hybridizable discontinuous Galerkin (HDG) methods. In the case of homogeneous media, it has been observed that the iterative solution of the linear system can be accelerated by hybridizing with transmission variables instead of numerical traces, as performed in standard approaches. In this work, they extend the HDG method with transmission variables, which is called the CHDG method, to the heterogeneous case with piecewise constant physical coefficients. In particular, they consider formulations with standard upwind and general symmetric fluxes. The CHDG hybridized system can be written as a fixed-point problem, which can be solved with stationary iterative schemes for a class of symmetric fluxes. The standard HDG and CHDG methods are systematically studied with the different numerical fluxes by considering a series of 2D numerical benchmarks. The convergence of standard iterative schemes is always faster with the extended CHDG method than with the standard HDG methods, with upwind and scalar symmetric fluxes.

In [25], E. Creusé *et al.* propose an a posteriori goal-oriented error estimator for the harmonic ($\boldsymbol{A}$–Φ) formulation arising in the modeling of eddy current problems, approximated by nonconforming finite element methods. It is based on the resolution of a dual problem associated with the initial one. For each of these two problems, a guaranteed equilibrated estimator is developed using some flux reconstructions. These fluxes also allow to obtain a goal-oriented error estimator that is fully computable and can be split in a principal part and a remainder one. Their theoretical results are illustrated by numerical experiments.

In [54], T. Chaumont-Frelet *et al.* consider time-harmonic elastodynamic problems in heterogeneous media. They focus on scattering problems in the high-frequency regime and in nearly incompressible media, where the angular frequency ω and ratio of the Lamé parameters λ/μ may both be large. They derive stability estimates controlling the norm of the solution by the norm of the right-hand side up to a fully-explicit constant. Crucially, under natural assumptions on the domain and coefficients, this constant increases linearly with ω and is uniform in the ratio λ/μ.

6.3 Analysis of dissipative models and their discretization

In [63], M. Herda *et al.* design, analyze and simulate a finite volume scheme for a cross-diffusion system which models chemotaxis with local sensing. This system has the same gradient flow structure as the celebrated minimal Keller–Segel system, but unlike the latter, its solutions are known to exist globally in 2D. The long-time behavior of solutions is only partially understood which motivates numerical exploration with a reliable numerical method. They propose a linearly implicit, two-point flux finite volume approximation of the system. They show that the scheme preserves, at the discrete level, the main features of the continuous system, namely mass, non-negativity of solutions, entropy, and duality estimates. These properties allow them to prove the well-posedness, unconditional stability and convergence of the scheme. They also show rigorously that the scheme possesses an asymptotic preserving (AP) property in the quasi-stationary limit. They complement their analysis with thorough numerical experiments investigating convergence and AP properties of the scheme as well as its reliability with respect to stability properties of steady solutions.

In [45], C. Cancès, A. Natale *et al.* propose a fully discrete finite volume scheme for the standard Fokker–Planck equation. The space discretization relies on the well-known square-root approximation, which falls into the framework of two-point flux approximations. The time discretization is novel and relies on a tailored nonlinear mid-point rule, designed to accurately capture the dissipative structure of the model. They establish well-posedness for the scheme, positivity of the solutions, as well as a fully discrete energy-dissipation inequality mimicking the continuous one. They then prove the convergence of the scheme under mildly restrictive conditions on the unstructured grids, which can be easily satisfied in practice. Numerical simulations show that the scheme is second order accurate both in time and space, and that one can solve the discrete nonlinear systems arising at each time step using Newton's method with low computational cost.

In [39], P. Gervais *et al.* prove a criterion justifying propagation and appearance of L^p–norms for

solutions to the spatially homogeneous Boltzmann equation with very soft potentials without cutoff. Such a criterion also provides a new conditional stability and uniqueness result for classical solutions to the equation. They first derive an energy estimate, which they close thanks to a new "ϵ-Poincaré inequality", allowing then for an estimate on the appearance rate of L^p–norms. The strategy is then refined to handle weights and stability estimates.

In [59], P. Gervais and M. Herda prove sufficient conditions for uniqueness and stability of stationary solutions to Vlasov–Fokker–Planck equation with self consistent interactions and a confining force. They first prove existence under general assumptions, and then uniqueness for interaction kernels with small negative Fourier modes. They then prove stability under the extra assumption of small imaginary Fourier modes through hypocoercive and hypoelliptic methods.

In [58], P. Gervais proves hypoelliptic estimates and averaging lemmas for kinetic equations in presence of a confining potential. This work adapts results from the work of F. Bouchut [90] and P.-E. Jabin [131] to the standard weighted framework of stability theory in confined kinetic equations.

In [15], T. Laidin *et al.* consider an implicit finite volume discretization of a non-linear kinetic reaction model describing the interactions of two species. They show that the discrete solutions converge exponentially fast towards the steady state. The proof relies on a small perturbation argument and the proof of a maximum principle on the non-linear system.

In [34], T. Laidin *et al.* construct spectral methods that allow to exactly preserve the moments of the unknown at the discrete level. The method is general and relies on a constrained minimization problem that can be solved explicitly. The robustness of the method is illustrated through various numerical experiments ranging from bounded and unbounded domains to applications to Fokker–Planck type equations.

In [41], C. Calgaro, R. Colombier and E. Creusé propose a Finite-Volume scheme on cartesian grids for the numerical approximation of some solutions to the Quantum Navier–Stokes (QNS) equations. The QNS system corresponds to a generalization of the usual Navier–Stokes system when quantum effects need to be taken into account, as in certain physical phenomena such as superfluids evolution or electron flow in semiconductors. The main difficulty lies in the presence of the Bohm potential in the momentum equation, which corresponds to a third-order term, increasing the complexity of the numerical scheme used to obtain approximate solutions. The idea is then to introduce a new variable $\nabla f(\rho)/\rho$ where the function f must be specified and to add to the original third-order system an additional equation, allowing it to be reduced to a second-order one. The originality of this contribution is to propose a scheme allowing to provide some discrete BD-entropy inequalities (Bresch–Desjardins), similarly to the continuous case (see [92]). The numerical scheme is based on a time splitting, where the hyperbolic step is discretized with a classical Finite-Volume scheme, whereas the parabolic step remains linear. Discrete BD-entropy inequalities are established, and numerical tests in 1D and 2D illustrate the efficiency of the scheme in several configurations.

In [21], C. Chainais-Hillairet *et al.* propose a new numerical two-point flux for a quasilinear convection-diffusion equation. This numerical flux is shown to be an approximation of the numerical flux derived from the solution of a two-point Dirichlet boundary value problem for the projection of the continuous flux onto the line connecting neighboring collocation points. The latter approach generalizes an idea first proposed by Scharfetter and Gummel for linear drift-diffusion equations. Convergence of the scheme is established, as well as relative entropy decay properties.

In [14], S. Lemaire *et al.* study the numerical approximation of sign-shifting problems of elliptic type. They fully analyze and assess the method briefly introduced in [67]. The method, which is based on domain decomposition and optimization, is proved to be convergent as soon as, for a given loading, the continuous problem admits a unique solution of finite energy. Departing from the T-coercivity approach, which relies on the use of geometrically fitted mesh families, the method works for arbitrary (interface-compliant) meshes. Moreover, it is shown convergent for a class of problems for which T-coercivity is not applicable. A comprehensive set of test-cases complements the analysis.

In [35], S. Lemaire and J. Moatti are interested in the high-order approximation of anisotropic, potential-driven advection-diffusion models on general polytopal partitions. They study two hybrid schemes, both built upon the Hybrid High-Order technology. The first one hinges on exponential fitting and is linear, whereas the second is nonlinear. The existence of solutions is established for both schemes. Both schemes are also shown to possess a discrete entropy structure, ensuring that the long-time behaviour of discrete solutions mimics the PDE one. For the nonlinear scheme, the positivity of discrete

solutions is a built-in feature. In contrast, numerical evidence is displayed indicating that the linear scheme violates positivity, whatever the order. Finally, they verify numerically that the nonlinear scheme has optimal order of convergence, expected long-time behaviour, and that raising the polynomial degree results, also in the nonlinear case, in an efficiency gain.

In [20], M. Herda *et al.* study a self-consistent Vlasov–Fokker–Planck equation which describes the longitudinal dynamics of an electron bunch in the storage ring of a synchrotron particle accelerator. They show existence and uniqueness of global classical solutions under physical hypotheses on the initial data. The proof relies on a mild formulation of the equation and hypoelliptic regularization estimates. They also address the problem of the long-time behavior of solutions. They prove the existence of steady states, called Haissinski solutions, given implicitly by a nonlinear integral equation. When the beam current (*i.e.* the nonlinearity) is small enough, they show uniqueness of steady state and local asymptotic nonlinear stability of solutions in appropriate weighted Lebesgue spaces. The proof is based on hypocoercivity estimates. Finally, they discuss the physical derivation of the equation and its particular asymmetric interaction potential.

Neuron models have attracted a lot of attention recently, both in mathematics and neurosciences. In [32], M. Herda *et al.* are interested in studying long-time and large-population emerging properties in a simplified toy model. From a mathematical perspective, this amounts to study the long-time behaviour of a degenerate reflected diffusion process. Using coupling arguments, the flow is proven to be a contraction of the Wasserstein distance for long times, which implies the exponential relaxation toward a (non-explicit) unique globally attractive equilibrium distribution. The result is extended to a McKean–Vlasov type non-linear variation of the model, when the mean-field interaction is sufficiently small. The ergodicity of the process results from a combination of deterministic contraction properties and local diffusion, the noise being sufficient to drive the system away from non-contractive domains.

In [16], C. Calgaro, C. Cancès and E. Creusé perform the convergence analysis of a finite volume scheme for a convection-diffusion equation involving a Joule effect term which was introduced in the former contribution [96] emanating from the team. The proof proposed in [16] relies on compactness arguments. In order to treat the Joule effect term, a second order discrete Gagliardo–Nirenberg inequality is established by the authors. By going beyond the (nowadays usual) framework of discrete functional inequalities involving first order discrete differential operators, this contribution seems to be a genuine novelty in the field of discrete functional analysis.

6.4 Complementary topics in numerical analysis

In [53], T. Chaumont-Frelet *et al.* rewrite the standard nodal virtual element method as a generalised gradient method. This re-formulation allows for computing a reliable and efficient error estimator by locally reconstructing broken fluxes and potentials. They prove the usual upper and lower bounds with constants independent of the stabilisation of the method and, under technical assumptions on the mesh, the degree of accuracy.

In [23], T. Chaumont-Frelet *et al.* analyze constrained and unconstrained minimization problems on patches of tetrahedra sharing a common vertex with discontinuous piecewise polynomial data of degree p. They show that the discrete minimizers in the spaces of piecewise polynomials of degree p conforming in the H^1, $\boldsymbol{H}(\mathbf{curl})$, or $\boldsymbol{H}(\mathrm{div})$ spaces are as good as the minimizers in these entire (infinite-dimensional) Sobolev spaces, up to a constant that is independent of p. These results are useful in the analysis and design of finite element methods, namely for devising stable local commuting projectors and establishing local-best/global-best equivalences in a priori analysis and in the context of a posteriori error estimation. Unconstrained minimization in H^1 and constrained minimization in $\boldsymbol{H}(\mathrm{div})$ have been previously treated in the literature. Along with improvement of the results in the H^1 and $\boldsymbol{H}(\mathrm{div})$ cases, our key contribution is the treatment of the $\boldsymbol{H}(\mathbf{curl})$ framework. This enables us to cover the whole de Rham diagram in three space dimensions in a single setting.

In [22], T. Chaumont-Frelet *et al.* design an operator from the infinite-dimensional Sobolev space $\boldsymbol{H}(\mathbf{curl})$ to its finite-dimensional subspace formed by the Nédélec piecewise polynomials on a tetrahedral mesh that has the following properties: 1) it is defined over the entire $\boldsymbol{H}(\mathbf{curl})$, including boundary conditions imposed on a part of the boundary; 2) it is defined locally in a neighborhood of each mesh element; 3) it is based on simple piecewise polynomial projections; 4) it is stable in the $\boldsymbol{L}^2$-norm, up to data oscillation; 5) it has optimal (local-best) approximation properties; 6) it satisfies the commuting property with its

sibling operator on $\boldsymbol{H}(\mathbf{curl})$; 7) it is a projector, i.e., it leaves intact objects that are already in the Nédélec piecewise polynomial space. This operator can be used in various parts of numerical analysis related to the $\boldsymbol{H}(\mathbf{curl})$ space. The authors employ it here to establish the two following results: i) equivalence of global-best, tangential-trace-and curl-constrained, and local-best, unconstrained approximations in $\boldsymbol{H}(\mathbf{curl})$ including data oscillation terms; and ii) fully h- and p- (meshsize- and polynomial-degree-) optimal approximation bounds valid under the minimal Sobolev regularity only requested elementwise. As a result of independent interest, they also prove a p-robust equivalence of curl-constrained and unconstrained best-approximations on a single tetrahedron in the $\boldsymbol{H}(\mathbf{curl})$ setting, including hp data oscillation terms.

6.5 Analysis and numerical simulation of variational models

Derived from the concentration-compactness principle, the concept of generalized minimizer can be used to define generalized solutions of variational problems which may have components "infinitely" distant from each other. In [46], and under mild assumptions, J. Candau-Tilh establishes existence and density estimates of generalized minimizers of perturbed isoperimetric problems. His hypotheses encapsulate a wide class of functionals including the classical, anisotropic and fractional perimeter. The perturbation term may for instance take the form of a potential, a translation invariant kernel or a nonlocal term involving the Wasserstein distance.

In [57], A. Natale *et al.* study a variational problem providing a way to extend for all times minimizing geodesics connecting two given probability measures, in the Wasserstein space. This is simply obtained by allowing for negative coefficients in the classical variational characterization of Wasserstein barycenters. They show that this problem admits two equivalent convex formulations: the first can be seen as a particular instance of Toland duality and the second is a barycentric optimal transport problem. They also propose an efficient numerical scheme to solve this latter formulation based on entropic regularization and a variant of Sinkhorn algorithm.

In [30], B. Merlet, M. Pegon *et al.* establish a $C^{1,\alpha}$-regularity theorem for almost-minimizers of the functional $\mathscr{F}_{\varepsilon,\gamma} = P - \gamma P_\varepsilon$, where $\gamma \in (0,1)$, P is the classical perimeter, and P_ε is a nonlocal energy converging to the perimeter as ε vanishes. The theorem provides a criterion for $C^{1,\alpha}$-regularity at a point of the boundary which is uniform as the parameter ε goes to 0. As a consequence they obtain that volume-constrained minimizers of $\mathscr{F}_{\varepsilon,\gamma}$ are balls for any ε small enough. For small ε, this minimization problem corresponds to the large mass regime for a Gamow-type problem where the nonlocal repulsive term is given by an integrable kernel G with sufficiently fast decay at infinity.

In [44], C. Cancès *et al.* consider the convergence of a finite element discretization of a degenerate parabolic equation of q-Laplace type with an additional external potential. The main novelty of the approach presented therein is that the authors use the underlying gradient flow structure in the L^p-Wasserstein metric: from the abstract machinery of metric gradient flows, the convergence of the scheme is obtained solely on the basis of estimates that result naturally from the equation's variational structure. In particular, the limit is identified as the unique gradient flow solution without reference to monotonicity methods.

In [29], B. Merlet (former member of the team) *et al.* introduce and study the notion of *tensor rectifiable chains* which form a two-dimensional chain complex of normed groups. They complete the theory of tensor flat chains in [60] by establishing a deformation theorem in this setting and by identifying isometrically some subgroups of tensor flat chains with corresponding subgroups of classical chains.

In [28], the same authors define and prove the existence of the decomposition in "connected components" for some objects which are very weak generalizations of surfaces (called flat chains). This result is used in the higher dimensional case of the previous paper to reduce the study of the jump set to the study of its "connected components" and then to understand their fine geometrical structure.

In [61], B. Merlet *et al.* study a variant of the Eikonal equation in 2D. The classical model arises in various physical models from the study of micromagnetism or liquid crystals and consists in the differential inclusion $\nabla u \in \mathbb{S}^1$ for functions $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$. The regularity and even the dimension of the singular set of ∇u assuming that its entropy production is a finite measure is still an important unsolved problem. Here, the authors consider instead the differential inclusion $\nabla u \in [-1,1] \times \{0\} \cup \{0\} \times [-1,1]$ or equivalently $\partial_1 u \, \partial_2 u = 0$ (the circle is replaced by the cross formed by a vertical and a horizontal line). This model comes from anisotropic Ising models. In this variant, the regularity problem is easier and the

authors show that the singular set is made of lines. They also establish similar results in higher dimension. This work introduces new lines of research for the study of the standard Eikonal equation.

In [31], motivated by some models of pattern formation involving an unoriented director field in the plane, B. Merlet, M. Pegon *et al.* study a family of unoriented counterparts to the Aviles–Giga functional. They introduce a nonlinear curl operator for such unoriented vector fields as well as a family of even entropies which they call "trigonometric entropies". Using these tools they show two main theorems which parallel some results in the literature on the classical Aviles–Giga energy. The first is a compactness result for sequences of configurations with uniformly bounded energies. The second is a complete characterization of zero-states, that is, the limit configurations when the energies go to 0. Their methods provide alternative proofs in the classical Aviles–Giga context.

In [19], J. Candau-Tilh, B. Merlet *et al.* consider a variant of the optimal transport problem and investigate the existence and characterization of its maximizers. In particular, they show that among sets of any fixed volume, the ball is the unique solution up to translation of this problem.

In [65], A. Natale studies a class of discrete models in which a collection of particles evolves in time following the gradient flow of an energy depending on the cell areas of an associated Laguerre (i.e. a weighted Voronoi) tessellation. Using a modulated energy argument, it is proven that in the limit of a high number of particles, the discrete solutions converge towards smooth solutions of nonlinear diffusion PDEs of porous medium type.

6.6 PhD theses

In his thesis entitled "Hybrid kinetic/fluid and structure preserving numerical methods for collisional kinetic equations", and defended on September 27 2024, T. Laidin focused on the development and analysis of efficient numerical methods for approximating solutions of potentially nonlinear kinetic collisional equations. These equations arise in various fields such as physics, notably in the study of semiconductors and gas dynamics. They also appear in biology in modelling the movement of cells within tissue. These models exhibit a multiscale aspect where there is, on one hand, a mesoscopic (or kinetic) description that gives the evolution of the distribution function of particles, molecules, or cells. On the other hand, through a process of averaging, one obtains the so-called macroscopic (or fluid) scale which allows to track the evolution of observable physical quantities: the moments of the distribution function. These moments correspond to the density, average velocity, and temperature of the considered particles. Throughout his manuscript, T. Laidin presents various ways to take advantage of fluid dynamics to construct and study efficient numerical methods for the kinetic scale. In the first part, he explores discretization methods aiming to preserve the structure of continuous equations. He begins by introducing an implicit finite volume scheme for a nonlinear reaction kinetic model. He studies the long-time behaviour of the discrete solution using hypocoercivity methods. Then, he examines a spectral method, based on general orthogonal polynomials, capable of preserving the moments of the solution while ensuring good convergence properties. The second part is dedicated to the design of numerical methods aiming to reduce the cost of kinetic simulations. To do this, he studies two approaches exploiting the evolution of the unknown's moments. The first, a hybrid kinetic/fluid method, involves adopting dynamically and locally in position a less costly fluid description of the system instead of the more expensive kinetic one. The second approach also relies on the use of a fluid model, but this time to accelerate the temporal iterations of the method. Here, he proposes a prototype of a multiscale parareal method, using a fluid model as a coarse solver and a kinetic model as a fine solver.

In his thesis entitled "Theoretical and numerical analysis of perturbed isoperimetric problems", and defended on October 11 2024, J. Candau-Tilh focused on perturbed isoperimetric problems. These problems involve the minimisation of an energy composed of a perimeter term that promotes mass aggregation, countered by a perturbation term favouring disaggregation. In his manuscript, J. Candau-Tilh begins by presenting the concepts used as well as past and current research conducted on the isoperimetric problem and its variants. In Chapter 1, he studies a problem where the perimeter interacts with a non-local term called an exterior transport term, defined using optimal transport theory. He demonstrates the existence of solutions to this problem and, in regimes where the perimeter dominates, he proves that the minimisers are balls. Chapter 2 is dedicated to the exterior transport term. In a general framework, he shows that the variational problem defining it has solutions and a dual formulation. Using stronger assumptions, he finally shows that this term is maximised only by balls. In Chapter 3, he presents

a numerical study in dimension 2 of the problem from Chapter 1. He approximates the minimisers of the energy considered via a gradient descent algorithm. The numerical results lead to conjecture the existence of a critical mass above which the minimisers are no longer balls, but elongated shapes with two axes of symmetry. Chapter 4 focuses on a perturbed isoperimetric problem where the perimeter and perturbation terms are not explicit. He exhibits a general set of assumptions under which a relaxed version of the problem admits minimisers. Under stronger hypotheses, he then investigates whether these minimisers have density estimates.

In his thesis entitled "Advanced numerical methods for high stiffness problems in reactive transport", realized in collaboration with IFPEN, and defended on November 18 2024, M. Jonval tackled the simulation of reactive transport problems in porous media, which is a major challenge for numerous IFPEN projects. Unfortunately, the performance of the reactive transport codes is nowadays strongly limited by numerical issues related to chemical modeling. These difficulties take various forms, all of which stemming from the stiffness of the equations to be solved. The goal of M. Jonval's thesis was to design new approaches for a more efficient resolution of the equations governing chemistry, first at equilibrium and then including kinetics. To this end, he made use of nonlinear preconditioning techniques. Besides, advanced time integration techniques adapted to stiffness have been investigated in order to by-pass difficulties coming from the intrinsic multi-scale aspect of chemical kinetics. Finally, the aforementioned contributions have been coupled with transport in porous media, with the ultimate goal of obtaining a numerical strategy which is robust with respect to large time steps.

7 Bilateral contracts and grants with industry

7.1 Bilateral contracts with industry

C. Cancès heads the MATHSOUT project (1M euros, 2024–2029) together with I. Faille (IFPEN). This project involves academic partners (INRIA, UniCA, CNRS) as well as IFPEN and the French Geological survey (BRGM). N.D.Q. Dang started her PhD at IFPEN in November 2024 in the framework of the MATHSOUT project. The contract follows the lines of the bilateral agreement between INRIA and IFPEN.

The PhD thesis of M. Jonval (supervised by C. Cancès), that started in October 2021, was co-funded by INRIA (salaries) and IFPEN (overhead costs). The contract also followed the lines of the bilateral agreement between INRIA and IFPEN.

A 2-year research collaboration contract was signed in 2022 between INRIA and EDF R&D in the framework of the France Relance recovery plan. The contract followed the lines of the bilateral agreement between INRIA and EDF. The research project was coordinated by S. Lemaire and involved S. Pitassi, whose post-doc position (from 10/2022 to 07/2024) was funded in this framework ("Dispositif 4 de l'action de Préservation de l'Emploi de R&D"). The project concerned the development of high-order polyhedral methods for the numerical simulation of eddy current testing.

7.2 Bilateral grants with industry

In 2023, the PRCE project HIPOTHEC (HIgh-order POlyhedral meTHods for Eddy Current testing simulations) has been funded in the generic ANR call. This 6-year project, which started in January 2024, is coordinated by S. Lemaire, and is a collaboration between INRIA, EDF, and 3 additional academic partners. The aim of the project is to pursue, within an enlarged academic consortium, the research efforts initiated in the framework of the France Relance collaboration between the team and EDF R&D. More details about the HIPOTHEC project can be found in Section 8.2.2.

CEA (C. Bataillon) and ANDRA (L. Trenty) have been involved in the EURAD project on corrosion modeling together with the RAPSODI project-team (C. Cancès, C. Chainais-Hillairet, and B. Merlet). The final report is available [24].

8 Partnerships and cooperations

8.1 International research visitors

8.1.1 Visits of international scientists

N. J. Walkington

Status: Professor

Institution of origin: Carnegie Mellon University

Country: USA

Dates: 31/05/2024 to 30/06/2024

Context of the visit: Collaboration with C. Cancès on mathematical and numerical models for multiphase porous media flows

Mobility program/type of mobility: Invited professor position, funded by the LabEx CEMPI

F. Raimondi

Status: Post-doctoral researcher

Institution of origin: University of Salerno

Country: Italy

Dates: 12/02/2024 to 23/02/2024

Context of the visit: Collaboration with C. Cancès and C. Chainais-Hillairet on the mathematical analysis of corrosion models

Mobility program/type of mobility: Funded by the H2020 European Joint Program EURAD

Paolo Bignardi

Status: PhD student

Institution of origin: Università di Pavia

Country: Italy

Dates: 01/02/2024 to 30/04/2024

Context of the visit: Hosted by T. Chaumont-Frelet in the context of his PhD thesis

Euan Spence

Status: Professor

Institution of origin: University of Bath

Country: UK

Dates: 08/01/2024 to 12/01/2024

Context of the visit: Collaboration with T. Chaumont-Frelet

Mobility program/type of mobility: Funded by the AEx POPEG

Lorenzo Mascotto

Status: Associate professor

Institution of origin: University of Milano Bicocca

Country: Italy

Dates: 13/05/2024 to 17/05/2024

Context of the visit: Collaboration with T. Chaumont-Frelet

Mobility program/type of mobility: Funded by the University of Milano Bicocca

Gregor Gantner

Status: Professor

Institution of origin: University of Bonn

Country: Germany

Dates: 21/10/2024 to 25/10/2024

Context of the visit: Collaboration with T. Chaumont-Frelet

Mobility program/type of mobility: Funded by the University of Bonn

Heiko Gimperlein

Status: Professor

Institution of origin: University of Innsbruck

Country: Austria

Dates: 25/12/2024 to 29/12/2024

Context of the visit: Collaboration with T. Chaumont-Frelet

Mobility program/type of mobility: Funded by the ANR JCJC `APOWA`

8.1.2 Visits of scientists from French institutions

The RAPSODI team has hosted a number of one/two-day visits from French colleagues. Below are only listed the longer visits.

Maxime Laborde

Status: Researcher

Institution of origin: University Paris Cité

Country: France

Dates: 01/07/2024 to 05/07/2024

Context of the visit: Collaboration with M. Pegon

Mobility program/type of mobility: Funded by PEPS-JCJC

K. Fourteau and K. Jondeau

Status: Researchers

Institution of origin: Météo France

Country: France

Dates: 09/04/2024 to 11/04/2024 and 01/07/2024 to 05/07/2024

Context of the visit: Collaboration with C. Cancès on snow models

Mobility program/type of mobility: Supported by the IMPT grant S-NOW

8.2 National initiatives

8.2.1 France 2030 program

C. Cancès is the co-PI, together with I. Faille (IFPEN), of the MATHSOUT project of the PEPR Mathematics in Interaction (Maths-VivES) funded by the ANR in the framework of the France 2030 program. The project essentially aims at lifting, thanks to mathematical studies, scientific locks identified by practitioners in Numerical Geosciences. The project involves 4 institutional partners (INRIA Univ. Lille, IFPEN, UniCA, and BRGM) as well as colleagues from CNRS—UGA and from Sorbonne Université.

- Title: MATHématiques SOUTerraines
- Type: PEPR
- ANR reference: ANR-23-EXMA-0010
- Duration: 2024–2029 (5 years)
- Budget: ~1 000 000 euros
- Coordinators: C. Cancès and I. Faille (IFPEN)

8.2.2 ANR projects

C. Cancès and M. Herda are members of the ANR JCJC project MICMOV. This project aims at gathering PDE analysts, probability theorists, and theoretical physicists to work on the derivation of macroscopic properties of physical systems from their microscopic description. The rigorous microscopic description of moving interfaces, the understanding of macroscopic nonlocal effects, and the mathematical apprehension of the underlying atomic mechanisms, are particularly important matters of this project.

- Title: MICroscopic description of MOVing interfaces
- Type: JCJC
- ANR committee: Mathématiques (CE40) - 2019
- ANR reference: ANR-19-CE40-0012
- Duration: 2020–2024 (48 months)
- Budget: 132 256 euros
- Coordinator: M. Simon (Université Lyon 1)

M. Alfaro is a member of the ANR PRC project DEEV, whose goal is to analyze multi-scale integro-differential equations, with possible stochastic components, modeling the evolutionary dynamics of structured populations.

- Title: Integro-Differential Equations from EVolutionary biology

- Type: PRC
- ANR committee: Mathématiques (CE40) - 2020
- ANR reference: ANR-20-CE40-0011
- Duration: 2020–2024 (48 months)
- Budget: 159 320 euros
- Coordinator: S. Mirrahimi (Institut de Mathématiques de Toulouse)

T. Chaumont-Frelet is the PI of the ANR JCJC project APOWA, funded in the 2023 generic call. The APOWA project aims at the development, analysis and implementation of a posteriori error estimators and adaptive finite element schemes for time-dependent wave propagation problems.

- Title: A POsteriori error estimates for WAve equations
- Type: JCJC
- ANR committee: Mathématiques (CE40) - 2023
- ANR reference: ANR-23-CE40-0019
- Duration: 2024–2027 (48 months)
- Budget: 266 725 euros
- Coordinator: T. Chaumont-Frelet

S. Lemaire is the PI of the ANR PRCE project HIPOTHEC, funded in the 2023 generic call. This project aims at developing accurate and flexible numerical solvers for eddy current testing simulations, based on high-order polyhedral methods. The target application, of industrial interest, is the non-invasive detection of flaws within steam generators in nuclear plants.

- Title: HIgh-order POlyhedral meTHods for Eddy Current testing simulations
- Type: PRCE, in partnership with EDF
- ANR committee: Modèles numériques, simulation, applications (CE46) - 2023
- ANR reference: ANR-23-CE46-0013
- Duration: 2024–2028 (60 months)
- Budget: 604 193 euros (in total), with 143 464 euros for INRIA Lille
- Coordinator: S. Lemaire
- Consortium: INRIA (Lille), UPHF (Valenciennes) - EDF (Palaiseau) - Université de Montpellier, Université Côte d'Azur (Nice)

In the framework of the HIPOTHEC project, it has been agreed that all the software developments will be implemented within the prototyping platform ParaSkel++ developed by RAPSODI.

8.2.3 LabEx CEMPI

Through their affiliation to the Laboratoire Paul Painlevé of University of Lille, RAPSODI team members benefit from the support of the LabEx CEMPI.

- Title: Centre Européen pour les Mathématiques, la Physique et leurs Interactions
- Partners: Laboratoire Paul Painlevé (LPP) and Laser Physics department (PhLAM), Université de Lille
- ANR reference: 11-LABX-0007
- Duration: February 2012 - December 2024 (the project has been renewed in 2019)
- Budget: 6 960 395 euros
- Coordinator: E. Fricain (LPP, Université de Lille)

The "Laboratoire d'Excellence" CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions), a project of the Laboratoire de mathématiques Paul Painlevé (LPP) and the laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), was created in the context of the "Programme d'Investissements d'Avenir" in February 2012. The association Painlevé-PhLAM creates in Lille a research unit for fundamental and applied research and for training and technological development that covers a wide spectrum of knowledge stretching from pure and applied mathematics to experimental and applied physics. The CEMPI research is at the interface between mathematics and physics. It is concerned with key problems coming from the study of complex behaviors in cold atoms physics and nonlinear optics, in particular fiber optics. It deals with fields of mathematics such as algebraic geometry, modular forms, operator algebras, harmonic analysis, and quantum groups, that have promising interactions with several branches of theoretical physics.

The PhD thesis of A.-A. Diallo, which started in November 2024 in collaboration with the PhLAM laboratory, and which is co-supervised by M. Herda, is funded by the LabEx CEMPI.

8.2.4 HQI: France Hybrid HPC Quantum Initiative

C. Guichard is a member of the WP4 of the HQI initiative. The HQI initiative aims at serving academic and industrial research scientists, who want to evaluate the potential of quantum and/or hybrid computing for their applications.

- Title: HQI: France Hybrid HPC Quantum Initiative
- Type: Programme d'Investissements d'Avenir (PIA4)
- Duration: January 2022 - December 2026
- Budget: 72 300 000 euros
- Coordinator of WP4: P. Tremblin (Maison de la Simulation & CEA)

8.2.5 Mathematical Institute for Planet Earth (IMPT)

C. Cancès is the co-PI, together with K. Fourteau (Météo France Grenoble), of the S-NOW project (2023-2024) funded (15k€) by the Mathematical Institute for Planet Earth (IMPT). The goal of the S-NOW project is to assess the compatibility of the models used to describe snow with thermodynamics, and introduce as minor as possible corrections if needed.

A. Natale is leading with G. Beaunée (INRAE) the project "Calibration of epidemic models on graphs with Optimal Transport and derivative-free optimization" (2023-2024) financed (55k€) by the Mathematical Institute for Planet Earth (IMPT). The project deals with the design of inference methods for epidemiological models on graphs. State-of-the-art inference methods to determine unknown parameters in this context often rely on extensive manipulations of the model outputs to match simulated results

with measurements, which limits their robustness and reliability. This project aims at developing optimal transport metrics to compare epidemic scenarios, and use these to construct more robust calibration techniques via minimum discrepancy estimators. The post-doc position of C. Sarrazin was funded in the framework of this project.

8.2.6 Exploratory Actions (AEx)

T. Chaumont-Frelet is the PI of the "Action exploratoire" AEx POPEG funded by INRIA. The aim of the POPEG project is to develop innovative Galerkin methods for high-frequency wave propagation problems. Specifically, the objective is to use Gaussian coherent state basis functions in order to drastically reduce the number of degrees of freedom compared to finite element basis functions for the same accuracy when the frequency is high. The PhD position of F. Proust (UniCA) is supported by this project.

8.2.7 SMAI BOUM

M. Pegon is the recipient of a SMAI BOUM 2023 grant aiming at funding (~ 1k€) the participation of young researchers to the conference "Calculus of Variations in Lille - 4th edition" which took place in Lille in June 2024.

8.2.8 PEPS-JCJC

M. Pegon is the recipient of a PEPS-JCJC grant (~ 3.5k€) of the INSMI section of the CNRS. C. Sarrazin is also a member of this project. It is dedicated to the numerical resolution of isoperimetric problems involving non-local energies. The non-local energies considered can be either of Gamow-type (such as Riesz potentials or non-local perimeters) or related to optimal transport.

8.3 Regional initiatives

8.3.1 Technological Development Actions (ADT)

S. Lemaire is the coordinator of the ADT project ParaSkel++, funded by INRIA and the Hauts-de-France region, which started in February 2020 and was renewed for two more years in 2022. The aim of the project is to develop an optimized parallel C++ platform for the arbitrary-order numerical approximation of PDEs on general polytopal meshes. T. Zoto was hired in December 2022 for 2 years as the new lead developer of the platform. He left the team in June 2024.

8.3.2 CPER WaveTech

The regional initiative CPER WaveTech "Ondes et Matière pour la Deep Tech" aims at investigating, in relation with the regional industrial and socio-economical spheres, advanced subjects in photonics, TeraHertz, and quantum mechanics. The post-doc of P. Gervais, supervised by M. Herda in the framework of a collaboration with the PhLAM laboratory, is funded by the CPER WaveTech.

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

C. Cancès was a co-organizer of the Workshop on the mathematical and numerical modeling of CO_2 storage held on January 31–February 2 at IFPEN, Rueil-Malmaison. He also co-organized the kick-off meeting of the MATHSOUT project at IFPEN, Rueil-Malmaison, on December 2-3.

C. Calgaro co-organized the event "Applied Analysis and Modeling: a conference in honor of Olivier Goubet", which took place on November 4-6. The objective of this conference was to celebrate the illustrious career of O. Goubet, and his contributions in Applied Analysis and Modeling. The program consisted of plenary talks, short communications and a poster session.

J. Venel was part of the organizing committee of the Journée Analyse Appliquée Hauts-de-France held on October 17 at the Université Polytechnique Hauts-de-France.

C. Guichard co-organises the working group NumerIQ. This working group meets bimonthly with the aim of demystifying quantum computing and highlighting its potential benefits in the numerical resolution of PDEs.

B. Merlet, A. Natale, M. Pegon, and J. Venel organized the "Conference on Calculus of Variations in Lille - 4th edition" from June 24 to June 28 2024, at Polytech Lille. The aim of this 5-day workshop was to bring together experts and young researchers in Calculus of Variations with applications in different areas of physics, mechanics, and image processing. This conference featured 16 invited plenary lectures, 11 contributing talks, and a poster session.

A. Natale co-organized the workshop "Finite Volumes and Optimal Transport: past, present and perspectives" from November 19 to November 21 2024, at the Institut de Mathématiques d'Orsay. This workshop brought together experts in Finite Volumes and Optimal Transport (and related disciplines) with the main aim of exploring the connections between the two fields and discuss open problems. This workshop featured 19 invited plenary lectures.

T. Chaumont-Frelet organized the APOWA kick-off meeting at INRIA Lille. The workshop had 12 speakers and its goal was to bring together different experts working on a posteriori error estimation for time-dependent wave propagation problems. He also co-organized the Semiclapp Summer School dedicated to "Semiclassical analysis and applications" and held in May in the University of Nice. He finally co-organized the minisymposium "Advances in p- and hp-, and problem oriented Galerkin methods" at the CMAM conference held in Bonn in June.

M. Alfaro was one of the organizers of the international workshop "Mathematical modelling of epidemiological dynamics" in Le Havre, June 17-21, and of the "Normand Meeting on theoretical and numerical aspects of PDEs" in Rouen, November 4-8. The three first days were dedicated to an autumn school and the last two days to a conference, covering a large spectrum of PDE issues, such as their applications in biology, numerical methods for PDEs or mean-field games.

S. Lemaire organized the kick-off workshop of the ANR project HIPOTHEC on March 7-8 in Wissant (Hauts-de-France region). For this occasion, the members of the consortium, as well as a few external invited researchers, gathered for two days. T. Zoto also attended this event.

M. Herda and S. Lemaire organized the mini-symposium "Advanced numerical methods for dissipative systems" in the framework of the ALGORITMY 2024 international conference, that was held on March 15-20 in Podbanské (Slovakia).

Together with A. Zurek (UTC), C. Cancès, C. Chainais-Hillairet, M. Herda, and S. Lemaire organized the international workshop "New Trends in the Numerical Analysis of PDEs" which was held on June 10-13 within the INRIA Lille research center. The scientific programme consisted of 20 invited talks from renowned experts, plus a poster session for young researchers. This event gathered around 50 participants from Europe, North Africa, and North America (mainly).

9.1.2 Scientific events: selection

C. Cancès was program chair of the 2024 French Congress on Numerical Analysis (CANUM 2024). He was also a member of the scientific committee of the first annual meeting of the French Network on Mathematics for Planet Earth and Energy (RTTE).

9.1.3 Journal - Member of the editorial boards

C. Chainais-Hillairet is editor-in-chief of the book series Mathématiques et Applications and member of the editorial boards of ESAIM: Mathematical Modelling and Numerical Analysis, IMA Journal of Numerical Analysis, and North-Western European Journal of Mathematics.

9.1.4 Reviewer - reviewing activities

RAPSODI permanent team members are regular reviewers for all the main international journals in PDEs, calculus of variations, numerical analysis, and scientific computing.

9.1.5 Scientific talks

M. Alfaro gave a talk on his joint work with C. Chainais-Hillairet [71] in the Séminaire d'Analyse Appliquée d'Aix-Marseille in February.

C. Cancès was invited in Oberwolfach (Germany) on February 5–9 to attend the MFO Workshop on Applications of Optimal Transportation, and he attended the first annual meeting of the French Network on Mathematics for Planet Earth and Energy (RTTE). He was an invited speaker in the ALGORITMY 2024 conference held in Podbanské (Slovakia) on March 15–20, in the fourth Gradient Flows face-to-face workshop held on September 9–12 in Raitenhaslach (Germany), in the workshop Finite Volumes and Optimal Transportation: past, present and perspectives held in Orsay on November 19–21, and during the annual IFPEN—INRIA joint workshop held in Paris on December 9.

P. Gervais gave talks at the conferences on Kinetic equation, Mathematical Physics and Probability on June 20, and on Modeling, theory and numerics for PDEs (kinetic and hyperbolic systems) on October 10. He also gave talks in several seminars at Université de Rennes and Université Libre de Bruxelles, as well as in the online French-Korean webinar.

Jules Candau-Tilh gave a talk at the bi-montly seminar of the GT CalVa "Calculus of Variations" (CNRS), co-hosted by the Paris-Cité, Paris-Dauphine and Paris-Saclay Universities on September 23. He also gave a talk on the theory of optimal transport at the PhD students' seminar of Paris-Saclay University on March 5.

T. Laidin gave talks in international conferences, including the NumAspYoung 2024 conference held in Ferrara on December 17–19, the CJC-MA 2024 held at ENS Lyon on October 28–30, the EWM-EMS Summer School: Kinetic Theory Arising from Mathematical Biology held at the Mittag–Leffler Institute (Stockholm) on July 1–5, and the conference Theoretical and Analytical Aspects of Kinetic equations in Plasmas held at CIRM (Marseille) on March 25–29. T. Laidin also gave several seminars at Laboratoire de Mathématiques Jean Leray (Nantes), Laboratoire JAD (Nice), and Laboratoire de Mathématiques Bretagne Atlantique (Brest).

J.Venel gave a seminar in Université de Versailles Saint-Quentin in April.

A. Natale gave a talk at the Oberwolfach workshop "Applications of Optimal Transportation" (MFO, Oberwolfach), at the "Journées SMAI MODE 2024" (Lyon), at the "Congrès national d'Analyse NUMérique" (CANUM 2024, Île de Ré), at the 77th Course of the International School of Mathematics Guido Stampacchia: "Variational analysis and applications 2024" (Erice, Italy), and at the 6th "Dolomites Workshop on Constructive Approximation and Applications" (Canazei, Italy).

M. Pegon gave a talk in the Oberwolfach workshop Calculus of Variations in August. He also gave a talk in the Analysis and PDE seminar at Université Libre de Bruxelles.

T. Chaumont-Frelet gave two talks at the WONAPDE 2024 conference in January. He was invited to give a seminar at the Herriot–Watt University of Edinburgh in February, and at the Universities of Sussex and Nothingam in March. He also gave a talk at the kick-off workshops of the ANR projects HIPOTHEC and APOWA in March.

S. Lemaire gave a talk at the ALGORITMY 2024 international conference held in Podbanské (Slovakia) on March 15–20. He also gave invited talks during the kick-off workshop of the ERC SyG project "NEw-generation MEthods for numerical SImulationS" (NEMESIS), which took place in Montpellier on June 19–21, as well as for the conference on "POlytopal Element Methods in Mathematics and Engineering" (POEMs V) held in Paris on December 3-6. Finally, S. Lemaire attended the kick-off workshops of the ANR project APOWA held in Lille in March, and of the MATHSOUT project (PEPR Maths-VivES) held at IFPEN (Rueil-Malmaison) in December.

M. Herda was invited to give talks in the "Modeling, theory and numerics for PDEs (kinetic and hyperbolic systems)" workshop (October 8–11, Centre Paul Langevin, Aussois), the workshop "The many facets of Kinetic Theory" (September 23–27, ICMS, Edinburgh, UK), the conference "Applied Mathematics and Simulation for Semiconductor Devices" (AMaSiS 2024) (September 10–13, WIAS, Berlin, Germany), and the workshop "Theoretical and Analytical Aspects of Kinetic equations in Plasmas" (March 25–29, CIRM, Marseille). He also gave a seminar talk at the Laboratoire JAD (Nice).

C. Chainais-Hillairet gave talks at the AMaSiS 2024 conference that was held in Berlin on September 10–13, at the workshop "Modeling, theory and numerics for PDEs (kinetic and hyperbolic systems)" (ANR MUFFIN) that was held in Aussois on October 8–11, and at the workshop "Finite Volumes and Optimal Transport: past, present and perspectives" that was held in Orsay on November 19–21. She also gave

several seminars (Toulouse, Versailles, Compiègne, CEA-DAM) and a colloquium in Nantes.

9.1.6 Leadership within the scientific community

C. Chainais-Hillairet is a member of the scientific committee of the Institut Henri Poincaré. She was also member of the jury for the SMAI/GAMNI Blaise Pascal prize delivered by the Académie des Sciences.

9.1.7 Scientific expertise

In 2024, S. Lemaire was a member of the hiring committees (i) for an associate professor position (MCF 26) within the AN-EDP team of the Laboratoire Paul Painlevé (Univ. Lille), as well as (ii) for young researcher positions (CRCN and ISFP) within the INRIA Lille research center.

C. Chainais-Hillairet was part of the selection committees for full professor (PR) positions at Aix-Marseille Université, Sorbonne Université, and Paris-Saclay Université.

9.1.8 Research administration

M. Alfaro is deputy director of the Doctoral School "Mathématiques, Information, Ingénierie des Systèmes" (MIIS), handling about 200 students in Normandy.

C. Cancès is a member of the Bureau du Comité des Équipes-Projets (BCEP) of the INRIA Lille research center. He also heads the Research Jobs Committee (Commission des Emplois de Recherche, CER for short), and represents INRIA in the council of the MADIS graduate school. He also acts as a member of the Mathematical Domain Board (Bureau de Domaine) of the MADIS graduate school. Besides, he is a member of the Administration Council of the French Society for Applied and Industrial Mathematics (SMAI).

T. Laidin was a member of the Commission Mixte of the Laboratoire Paul Painlevé, representing PhD students and post-doctoral researchers.

C. Calgaro is a member of the management team of the Faculté des Sciences et Technologies at Université de Lille, and she is a member of the Commission Mixte of the Laboratoire Paul Painlevé.

J. Venel is a member of the Conseil de la Fédération Mathématique des Hauts-de-France.

S. Lemaire has been responsible since 2022, for the INRIA Lille research center (15 research teams), of the coordination of the yearly activity reports campaign. Since September 2024, he is also a substitute member of the INRIA Lille Center Committee, as well as a member of the Catering Commission (in charge of the attribution of the catering market within the center). Finally, he is the webmaster of the RAPSODI website.

C. Chainais-Hillairet is vice-director of the Laboratoire Paul Painlevé, in charge of human resources for researchers, professors, and assistant professors.

M. Herda is an elected member of the Conseil de Laboratoire and of the Commission Mixte related to the math laboratory and the math department, respectively. M. Herda is also substitute member of the INRIA Lille Center Committe, and nominated member of the Commission des Utilisateurs des Moyens Informatiques (CUMI) at INRIA Lille. He is coordinating and writing the annual activity report for the RAPSODI team since 2022.

A. Natale co-organizes the Numerical Analysis and PDEs (AN-EDP) seminar of the Laboratoire Paul Painlevé.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

RAPSODI team members are strongly involved in teaching at Université de Lille and Université Polytechnique des Hauts-de-France (UPHF, Valenciennes), as well as in the engineering schools Centrale Lille and Polytech Lille, and in SKEMA Business School.

Faculty members of the project-team ensure their teaching duties (~192h yearly), as well as important administrative tasks in the math departments. E. Creusé is the head of the mathematics department of the CERAMATHS laboratory at UPHF. C. Calgaro is a member of the Conseil de Département de Mathématiques at Université de Lille. M. Pegon is in charge of the students' recruitment for a department

of the engineering school Polytech Lille. C. Guichard is a member of the Master's Council of the UFR of Mathematics at Sorbonne University. C. Guichard is also responsible for the "IMPE" training of the Master 2 "Mathematical Engineering" at Sorbonne University.

INRIA members of the project-team also take an important part in teaching activities. C. Cancès was in charge of the course "Mathematical Tools for Simulation - Hyperbolic PDEs" (27h) of the M2 Scientific Computing at Université de Lille. A. Natale taught the course "Refresher in Mathematics" (20h) in the framework of the M2 Data Science of Université de Lille and Centrale Lille. He also taught the course "Numerical solution of nonlinear problems" (49h) in the framework of the M1 Scientific Computing at Université de Lille. S. Lemaire taught the course "Mathematical Tools for Simulation - Elliptic & Parabolic PDEs" (44h) in the framework of the M2 Scientific Computing at Université de Lille. M. Herda was in charge of the course "Scientific computing" (28h) for 1st year (~L3) students in Centrale Lille.

Finally, PhD students and post-docs also contribute in the teaching activities (up to 64h yearly), either at Université de Lille (J. Candau-Tilh, P. Gervais, T. Laidin) or in SKEMA Business School and Centrale Lille (M. Jonval).

9.2.2 Supervision

Post-docs

- **In progress -** P. Gervais (CNRS): *Self-consistent Vlasov–Fokker–Planck equations, and application to the modeling of electron beams*, supervised by M. Herda, since September 2023, funded by the CPER WaveTech.
- C. Sarrazin (INRAE/INRIA): *Calibration of epidemic models on graphs with Optimal Transport and derivative-free optimization*, co-supervised by A. Natale and G. Beaunée (INRAE), from November 2023 to August 2024, funded by the Mathematical Institute for Planet Earth (IMPT).
- S. Pitassi (EDF/INRIA): *High-order polyhedral methods for eddy current testing simulation*, co-supervised by S. Lemaire, J. Dalphin (EDF), and J.-P. Ducreux (EDF), from October 2022 to July 2024, funded via the research collaboration contract between INRIA and EDF (France Relance recovery plan).

PhD students

- **In progress -** A.-A. Diallo (Université de Lille): *Numerical simulation of relativistic beams of charged particles in particle accelerators*, co-supervised by M. Herda, S. Bielawski (PhLAM, Univ. Lille), and C. Évain (PhLAM, Univ. Lille), since November 2024, funded by the LabEx `CEMPI`.
- **In progress -** N. D. Q. Dang (IFPEN/INRIA): *Acceleration of Newton-type methods for nonlinear systems by pre-flattening techniques*, co-supervised by Q.-H. Tran (IFPEN), C. Cancès, and I. Ben Gharbia (IFPEN), since November 2024, funded by the PEPR Maths-VivES, project `MATHSOUT`.
- **In progress -** A. Dupouy (INRIA): *Mathematical and numerical analysis of dissipative problems with free boundaries*, supervised by C. Cancès and C. Chainais-Hillairet, since October 2023, co-funded by INRIA and the Hauts-de-France region.
- **In progress -** R. Colombier (UPHF, Valenciennes): *Numerical schemes for solving the macroscopic quantum hydrodynamics equations*, co-supervised by E. Creusé (UPHF) and C. Calgaro, since November 2022, co-funded by UPHF and the Hauts-de-France region.
- M. Jonval (IFPEN/INRIA): *Advanced numerical methods for stiff problems in the context of reactive transport*, co-supervised by C. Cancès, I. Ben Gharbia, T. Faney, and Q.-H. Tran (IFPEN), from October 2021 to November 2024, co-funded by INRIA and IFPEN in the framework of the bilateral contract.
- J. Candau-Tilh (Université de Lille): *Isoperimetric problems with Wasserstein interactions*, co-supervised by B. Merlet and M. Goldman (CMAP, École Polytechnique), from September 2021 to October 2024, funded by an ENS fellowship.

- T. Laidin (Université de Lille): *Hybrid kinetic/fluid numerical methods and discrete hypocoercivity for the Boltzmann equation for semiconductors*, co-supervised by T. Rey and M. Bessemoulin-Chatard (CNRS & Université de Nantes), from October 2021 to September 2024, co-funded by the LabEx CEMPI and the Hauts-de-France region.

Engineers

- T. Saouzanet (CNRS, then INRIA): Development of a Python code for the simulation of a thermodynamically consistent corrosion model, supervised by C. Cancès, C. Chainais-Hillairet, and J. Venel (UPHF), from February to July 2024. The position was partially funded by the European Joint Program EURAD on Nuclear Waste Management.
- T. Zoto (INRIA): Development of the ParaSkel++ platform, supervised by S. Lemaire, from December 2022 to June 2024, funded by INRIA and the Hauts-de-France region (ADT ParaSkel++).

Interns

- **In progress -** A. Leloir (Univ. Lille and Centrale Lille), M2 internship: *Evaluation of the entropy production rate in a corrosion model*, supervised by C. Cancès.
- N. Delattre (Univ. Lille), M2 internship: *A posteriori analysis for hybrid high-order methods*, supervised by S. Lemaire, from April to September 2024, funded by EDF (research collaboration).
- K. Jondeau (ISAE & EPFL), M2 internship: *Use of the second principle of thermodynamics as a numerical stability criterion in snow models*, supervised by K. Fourteau (Météo France) and C. Cancès, from April to August 2024, funded by the S-NOW project, supported by the Mathematical Institute for Planet Earth (IMPT).
- A. Salvador Carrasco Urbina (Universidad Técnica Federico Santa María, Chile), Master internship: *Development of numerical algorithms for the Wasserstein extrapolation problem*, supervised by A. Natale, from January to March 2024, funded by INRIA Chile.
- J.-P. Valois (Univ. Lille), M1 internship: *Implementation of a 3D population dynamics model*, August 2024.
- C. Magnier (UPHF), L3 internship: *Mathematical modeling of chemical equilibria*, from April to May 2024.

9.2.3 Juries

Habilitation à Diriger des Recherches (HDR)

- C. Chainais-Hillairet was a referee and a member of the Habilitation defense committee of Khaled Saleh (Université Lyon 1) on March 7 2024. Title: *Contributions à l'analyse mathématique et numérique pour les écoulements mono et multiphasiques compressibles et incompressibles.*

PhD defenses

- M. Alfaro was a referee and a member of the PhD defense committee of Maxime Estavoyer (Université de Lyon and INRIA) on November 18 2024. Title: *Propagation et émergence de motifs en biologie.*
- C. Cancès was a referee and a member of the PhD defense committee of Stefan Portisch (TU Vienna) on October 22 2024. Title: *Analysis of nonlocal cross-diffusion and nonlinear drift-diffusion systems using Entropy Methods.*
- C. Cancès was a referee and a member of the PhD defense committee of Thomas Crozon (École Centrale de Nantes) on December 12 2024. Title: *Finite Volumes for compressible/incompressible two-phase flows in porous media with discontinuous capillary pressure.*

- C. Cancès was a member of the PhD defense committee of Ari Rappaport (Sorbonne Université, INRIA Paris and ANDRA) on March 22 2024. Title: *A posteriori error estimates and adaptivity in numerical approximation of PDEs: regularization, linearization, discretization, and floating point precision.*
- J. Venel was a member of the PhD defense committee of Jules Candau-Tilh (Université de Lille) on October 11 2024. Title: *Theoretical and numerical analysis of perturbed isoperimetric problems.*
- J. Venel was a member of the PhD defense committee of Oscar Dufour (Université de Lyon) on December 6 2024. Title: *Enhanced agent-based models for pedestrian crowds: insights from empirical data at the Festival of Lights and refinements of mechanical interactions, pedestrian shapes and decisional aspects.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Arthur Tételin (Université Toulouse III, ISAE-SUPAERO) on June 14 2024. Title: *Reconstruction des variables vectorielles dans le cadre des méthodes volumes finis sur maillages non-structurés généraux.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Wassim Aboussi (Université Paris XIII-Sorbonne Paris Nord and Université Sidi Mohamed Ben Abdallah) on June 26 2024. Title: *Étude théorique et numérique des écoulements de Bingham.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Lucas Coeuret (Université Toulouse III) on July 12 2024. Title: *Stability of discrete shock profiles for systems of conservation laws.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Joyce Ghantous (Université de Pau et des Pays de l'Adour) on September 23 2024. Title: *Prise en compte de conditions aux bords d'ordre élevé et analyse numérique de problèmes de diffusion sur maillages courbes à l'aide d'éléments finis d'ordre élevé.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Tino Laidin (Université de Lille) on September 27 2024. Title: *Méthodes numériques hybrides cinétique/fluide et préservant la structure pour des équations cinétiques collisionnelles.*
- C. Chainais-Hillairet was a member of the PhD defense committee of Théo Belin (Université Paris-Saclay) on December 10 2024. Title: *Autour de la frontière libre d'une équation parabolique avance-rétrograde.*

Other Juries

- M. Alfaro was a member of the committee for the *Agrégation externe de mathématiques* in 2024.

9.3 Popularization

M. Alfaro has facilitated a workshop "Modèles d'invasions: des lapins de Fibonacci aux crapauds buffles" at the "Journées Nationales de l'APMEP (Association des Professeurs de Mathématiques de l'Enseignement Public)", in Le Havre, on October 21.

S. Lemaire is since September 2024 (co-) Scientific Officer in charge of Mediation for the INRIA Lille research center. He is responsible of both internal (organization of the monthly scientific event "30 MIN. de sciences") and external (through different actions, intended for high school students, in particular) scientific outreach. He co-organized on October 21-22 the "Rendez-vous des Jeunes Mathématiciennes et Informaticiennes" (RJMI), which is specifically geared towards female high school students, in order to promote scientific careers amongst them. In May, S. Lemaire also realized an intervention in the framework of the national scientific outreach program "1 scientifique, 1 classe / Chiche !" in a 2nde class of the Lycée Raymond Queneau in Villeneuve d'Ascq.

P. Gervais took part in the "Rendez-vous des Jeunes Mathématiciennes et Informaticiennes" (RJMI), which consisted on the first day, in a 3-hour research workshop on a simple geometric problem, and on the second day, in a 10-minute presentation.

J. Venel co-organized the internship Maths C pour L at Université Polytechnique Hauts-de-France. This event is open to around twenty female undergraduate mathematics students for one week. The students work in small groups on research topics and, thanks to various presentations by female researchers, doctoral students, and engineers, they can discover the various possible careers in mathematics. This week was co-funded by INRIA.

C. Chainais-Hillairet gave a talk at Lycée Faidherbe in Lille in order to promote the women's careers in mathematics. She was also in the organizing committee of the week-long event « Les Fourmis », proposed to secondary school girls experiencing gender non-mixing.

10 Scientific production

10.1 Major publications

[1] M. Bessemoulin-Chatard and C. Chainais-Hillairet. 'Exponential decay of a finite volume scheme to the thermal equilibrium for drift–diffusion systems'. In: *Journal of Numerical Mathematics* 25.3 (2017), pp. 147–168. DOI: 10.1515/jnma-2016-0007. URL: https://hal.archives-ouvertes.fr/hal-01250709.

[2] M. Bessemoulin-Chatard, M. Herda and T. Rey. 'Hypocoercivity and diffusion limit of a finite volume scheme for linear kinetic equations'. In: *Mathematics of Computation* 89 (Jan. 2020), pp. 1093–1133. DOI: 10.1090/mcom/3490. URL: https://hal.archives-ouvertes.fr/hal-01957832 (cit. on p. 7).

[3] K. Brenner and C. Cancès. 'Improving Newton's method performance by parametrization: the case of Richards equation'. In: *SIAM Journal on Numerical Analysis* 55.4 (2017), pp. 1760–1785. URL: https://hal.archives-ouvertes.fr/hal-01342386 (cit. on p. 8).

[4] C. Cancès, T. Gallouët and L. Monsaingeon. 'Incompressible immiscible multiphase flows in porous media: a variational approach'. In: *Analysis & PDE* 10.8 (2017), pp. 1845–1876. DOI: 10.2140/apde.2017.10.1845. URL: https://hal.archives-ouvertes.fr/hal-01345438 (cit. on p. 5).

[5] C. Cancès and C. Guichard. 'Numerical analysis of a robust free energy diminishing Finite Volume scheme for parabolic equations with gradient structure'. In: *Foundations of Computational Mathematics* 17.6 (2017), pp. 1525–1584. URL: https://hal.archives-ouvertes.fr/hal-01119735 (cit. on p. 6).

[6] C. Chainais-Hillairet and M. Herda. 'Large-time behaviour of a family of finite volume schemes for boundary-driven convection-diffusion equations'. In: *IMA Journal of Numerical Analysis* 40.4 (1st Oct. 2020), pp. 2473–2505. DOI: 10.1093/imanum/drz037. URL: https://hal.archives-ouvertes.fr/hal-01885015 (cit. on p. 7).

[7] T. Chaumont-Frelet and M. Vohralík. 'p-robust equilibrated flux reconstruction in H(curl) based on local minimizations. Application to a posteriori analysis of the curl-curl problem'. In: *SIAM Journal on Numerical Analysis* 61.4 (2023), pp. 1783–1818. DOI: 10.1137/21M141909X. URL: https://inria.hal.science/hal-03227570.

[8] F. Chave, D. A. Di Pietro and S. Lemaire. 'A discrete Weber inequality on three-dimensional hybrid spaces with application to the HHO approximation of magnetostatics'. In: *Mathematical Models and Methods in Applied Sciences* 32.1 (2022), pp. 175–207. DOI: 10.1142/S0218202522500051. URL: https://hal.archives-ouvertes.fr/hal-02892526.

[9] D. A. Di Pietro, A. Ern and S. Lemaire. 'An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators'. In: *Computational Methods in Applied Mathematics* 14.4 (June 2014), pp. 461–472. DOI: 10.1515/cmam-2014-0018. URL: https://hal.archives-ouvertes.fr/hal-00978198 (cit. on p. 6).

[10] G. Dimarco, R. Loubère, J. Narski and T. Rey. 'An efficient numerical method for solving the Boltzmann equation in multidimensions'. In: *Journal of Computational Physics* 353 (2018), pp. 46–81. DOI: 10.1016/j.jcp.2017.10.010. URL: https://hal.archives-ouvertes.fr/hal-01357112 (cit. on p. 8).

[11] T. Gallouët, A. Natale and F.-X. Vialard. 'Generalized compressible flows and solutions of the H(div) geodesic problem'. In: *Archive for Rational Mechanics and Analysis* (2020). DOI: 10.1007/s00205-019-01453-x. URL: https://hal.archives-ouvertes.fr/hal-01815531.

[12] B. Merlet. 'A highly anisotropic nonlinear elasticity model for vesicles I. Eulerian formulation, rigidity estimates and vanishing energy limit'. In: *Arch. Ration. Mech. Anal.* 217.2 (2015), pp. 651–680. DOI: 10.1007/s00205-014-0839-5. URL: https://hal.archives-ouvertes.fr/hal-00848547.

10.2 Publications of the year

International journals

[13] D. Abdel, C. Chainais-Hillairet, P. Farrell and M. Herda. 'Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells'. In: *IMA Journal of Numerical Analysis* 44.2 (Mar. 2024), pp. 1090–1129. DOI: 10.1093/imanum/drad034. URL: https://hal.science/hal-03779230 (cit. on p. 12).

[14] A. Abdulle and S. Lemaire. 'An optimization-based method for sign-changing elliptic PDEs'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 58.6 (2024), pp. 2187–2223. DOI: 10.1051/m2an/2024013. URL: https://hal.science/hal-04140542 (cit. on p. 17).

[15] M. Bessemoulin-Chatard, T. Laidin and T. Rey. 'Discrete hypocoercivity for a nonlinear kinetic reaction model'. In: *IMA Journal of Numerical Analysis* (2025). DOI: 10.1093/imanum/drae058. URL: https://hal.science/hal-04494454. In press (cit. on p. 17).

[16] C. Calgaro, C. Cancès and E. Creusé. 'Discrete Gagliardo-Nirenberg inequality and application to the finite volume approximation of a convection-diffusion equation with a Joule effect term'. In: *IMA Journal of Numerical Analysis* 44.4 (2024), pp. 2394–2436. DOI: 10.1093/imanum/drad063. URL: https://hal.science/hal-03881410 (cit. on p. 18).

[17] C. Cancès, J. Cauvin-Vila, C. Chainais-Hillairet and V. Ehrlacher. 'Cross-diffusion systems coupled via a moving interface'. In: *Interfaces and Free Boundaries : Mathematical Analysis, Computation and Applications* (2025). URL: https://hal.science/hal-04654232. In press (cit. on p. 13).

[18] C. Cancès, V. Ehrlacher and L. Monasse. 'Finite Volumes for the Stefan-Maxwell Cross-Diffusion System'. In: *IMA Journal of Numerical Analysis* 44.2 (2024), pp. 1029–1060. DOI: 10.1093/imanum/drad032. URL: https://hal.science/hal-02902672 (cit. on p. 6).

[19] J. Candau-Tilh, M. Goldman and B. Merlet. 'An exterior optimal transport problem'. In: *Calculus of Variations and Partial Differential Equations* 64.2 (6th Jan. 2025), p. 45. DOI: 10.1007/s00526-024-02900-8. URL: https://hal.science/hal-04196005 (cit. on p. 20).

[20] L. Cesbron and M. Herda. 'On a Vlasov-Fokker-Planck equation for stored electron beams'. In: *Journal of Differential Equations* 404 (25th Sept. 2024), pp. 316–353. DOI: 10.1016/j.jde.2024.05.056. URL: https://hal.science/hal-04173543 (cit. on p. 18).

[21] C. Chainais-Hillairet, R. Eymard and J. Fuhrmann. 'A monotone numerical flux for quasilinear convection diffusion equation'. In: *Mathematics of Computation* 93.345 (Jan. 2024), pp. 203–231. DOI: 10.1090/mcom/3870. URL: https://hal.science/hal-03791166 (cit. on p. 17).

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