2021
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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Project-Team RAPSODI

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2   Overall objectives

2.1   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 solutions of 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), the decay of physically motivated entropies, 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 of physical parameters.

We aim to develop methods fulfilling the above quality criteria for physical models which all display a dissipative behavior, and that are motivated by industrial collaborations or multidisciplinary projects. In particular, we have identified a couple of specific situations we plan to investigate: models from corrosion science (in the framework of nuclear waste repository) [65], low-frequency electromagnetism [84], and mechanics of complex inhomogeneous fluids arising in avalanches [75] or in porous media [66].

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 compose with existing codes. The numerical algorithms have thus to be optimized under this constraint.

2.2   Scientific context

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.

Let us mention for example the review paper by Jérôme Droniou [89], where it is highlighted that all the linear methods for solving diffusion equations on general meshes suffer from the same lack of monotonicity and preserve neither the positivity of the solutions nor the decay of the entropy. Moreover, there is no complete convergence proof for the nonlinear methods exposed in [89]. The first convergence proof for a positivity preserving and entropy diminishing method designed to approximate transient dissipative equations on general meshes was proposed recently in [78]. The idea and the techniques introduced in [78] should be extended to practical applications.

In systems of PDEs, the values of the physical parameters often change the qualitative behavior of the solutions. Then, one challenge in the numerical approximation of such systems is the design of methods which can be applied for a large range of parameters, as in particular in the regime of singular perturbations. Such schemes, called *asymptotic-preserving* (AP) schemes [96], are powerful tools as they allow the use of the same scheme for a given problem and for its limit with fixed discretization parameters. In many cases, the AP property of numerical schemes is just empirically established, without any rigorous proof. We aim to extend the techniques recently introduced in [72] for the drift-diffusion system, and based on the control of the numerical dissipation of entropy, to other dissipative systems in order to prove the AP property of numerical schemes.

The question of the robustness of the numerical methods with respect to the physical parameters is also fundamental for fluid mixture models. The team already developed such schemes for the variable density Navier–Stokes system [74, 75]. We aim to propose new ones for more complex models with the same philosophy in mind. On the one hand, we will be interested in high-order schemes, which must be as simple as possible in view of 3D practical implementations. Let us stress that combining high order accuracy and stability is very challenging. On the other hand, the optimization of the computations will have to be considered, in particular with the development of some a posteriori error estimators. Impressive progresses have been achieved in this field [87], allowing important computational savings without compromising the accuracy of the results. Recently, we successfully applied this strategy to the Reissner–Mindlin model arising in solid mechanics [86], the dead-oil model for porous media flows [77], or the Maxwell equations in their quasi-static approximation for some eddy current problems [84, 85]. We aim to develop new a posteriori estimators for other dissipative systems, like fluid mixture models.

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 shall focus on the following objectives, which are necessary for the applications we have in mind:

1. Design and analysis of structure-preserving numerical methods.

2. Computational optimization.

3   Research program

3.1   Design and analysis of structure-preserving schemes

3.1.1   Numerical analysis of nonlinear numerical methods

Up to now, almost all numerical methods dedicated to degenerate parabolic problems that the mathe-maticians are able to analyze rely on the use of mathematical transformations (like, e.g., the Kirchhoff's transform). It forbids the extension of the analysis to complex realistic models. The methods used in the industrial codes for solving such complex problems rely on the use of what we call NNM, i.e., on methods that preserve all the nonlinearities of the problem without reducing them thanks to artificial mathematical transforms. Our aim is to take advantage of the recent breakthrough proposed by C. Cancès and Cindy Guichard in [4] and [78] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness with respect to physical parameters, etc).

3.1.2   Design and analysis of asymptotic-preserving schemes

There has been an extensive effort in the recent years to develop numerical methods for diffusion equations that are robust with respect to heterogeneities, anisotropy, and the mesh (see for instance [89] for a comprehensive discussion on such methods). On the other hand, the understanding of the role of nonlinear stability properties in the asymptotic behaviors of dissipative systems increased significantly in the last decades (see for instance [79, 99]).

Recently, C. Chainais-Hillairet and co-authors [72, 80, 81] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization character-istic parameters, or in the long-time asymptotics. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes, etc) are required in [72, 80, 81]. The schemes proposed in [4] and [78] allow to handle nonlinear test functions in the analysis without restrictions on the mesh and on the anisotropy of the problem. Combining the nonlinear schemes *à la* [78] with the methodology of [72, 80, 81] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would also be robust under adaptive mesh refinement.

3.1.3   Design and stability analysis of numerical methods for low-Mach models

We aim at extending the range of the NS2DDV software [98] by introducing new physical models, like for instance the low-Mach model, which gives intermediate solutions between the compressible Navier–Stokes model and the incompressible Navier–Stokes one. This model was introduced in [97] as a limit system which describes combustion processes at low Mach number in a confined region. Within this scope, we will propose a theoretical study for proving the existence of weak solutions for a particular class of models for which the dynamic viscosity of the fluid is a specific function of the density. We will also propose the extension of a combined Finite Volume-Finite Element method, initially developed for the simulation of incompressible and variable density flows, to this class of models.

3.2   Optimizing the computational efficiency

3.2.1   High-order nonlinear numerical methods

The numerical experiments carried out in [78] show that in case of very strong anisotropy, the convergence of the proposed NNM becomes too slow (less than first order). Indeed, the method appears to strongly overestimate the dissipation. In order to make the method more competitive, it is necessary to estimate

the dissipation in a more accurate way. Preliminary numerical results show that second-order accuracy in space can be achieved in this way. One also aims to obtain (at least) second-order accuracy in time without jeopardizing the stability. For many problems, this can be done by using so-called two-step backward differentiation formulas (BDF2) [92].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the solution of the mass equation. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider Residual Distribution schemes, that appear as an alternative to Finite Volume methods. Residual Distribution schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D entails reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [95, 100], with high-order accuracy [58, 59], or for parabolic problems [56, 57] make them very competitive. Relying on these breakthroughs, we aim at designing new Residual Distribution schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2   A posteriori error control

The question of the a posteriori error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuška and Rheinboldt more than thirty years ago [64], a posteriori error estimators have been widely studied. We will take advantage of the huge corresponding bibliographical database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g., [84, 85]) to the temporal magnetodynamic one, for which space-time a posteriori error estimators have to be developed. A space-time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop a posteriori estimators for the variable density Navier–Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [74, 75] we developed combines features from Finite Elements and Finite Volumes. Fortunately, there exists a significant literature on the subject. Some recent references are devoted to the unsteady Navier–Stokes model in the Finite Element context [69, 93]. In the Finite Volume context, recent references deal with unsteady convection-diffusion equations [62, 77, 88, 101]. We want to adapt some of these results to the variable density Navier–Stokes system, and to be able to design an efficient space-time remeshing algorithm.

3.2.3   Efficient computation of pairwise interactions in large systems of particles

Many systems are modeled as a large number (N) of pointwise individuals with pairwise interaction, i.e., with $N(N-1)/2$ interactions. Such systems are ubiquitous, they are found in chemistry (Van der Waals interaction between atoms), in astrophysics (gravitational interactions between stars, galaxies or galaxy clusters), in biology (flocking behavior of birds, schooling of fish) or in the description of crowd motions. Building on the special structure of convolution type of the interactions, the team develops computational methods based on the nonuniform Fast Fourier Transform [94]. This reduces the $O(N^2)$ naive computational cost of the interactions to $O(N\log N)$, allowing numerical simulations involving millions of individuals.

4   Application domains

4.1   Porous media flows

Porous media flows are of great interest in many contexts, like, e.g., oil engineering, water resources management, nuclear waste repository management, or carbon dioxide sequestration. We refer to [66, 67] for an extensive discussion on porous media flow models.

From a mathematical point of view, the transport of complex fluids in porous media often leads to possibly degenerate parabolic conservation laws. The porous rocks can be highly heterogeneous and anisotropic. Moreover, the grids on which one intends to solve numerically the problems are prescribed

by the geological data, and might be nonconformal with cells of various shapes. Therefore, the schemes used for simulating such complex flows must be particularly robust.

4.2 Corrosion and concrete carbonation

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.

From a mathematical point of view, the modeling of concrete carbonation (see [61]) as the modeling of corrosion in an underground repository (DPCM model developed by Bataillon et al. [65]) lead to systems of PDEs posed on moving domains. The coupling between convection-diffusion-reaction equations and moving boundary equations leads to challenging mathematical questions.

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 Stratigraphy

The knowledge of the geology is a prerequisite before simulating flows within the subsoil. Numerical simulations of the geological history thanks to stratigraphy numerical codes allow to complete the knowl-

edge of the geology where experimental data are lacking. Stratigraphic models consist in a description of the erosion and sedimentation phenomena at geological scales.

The characteristic time scales for the sediments are much larger than the characteristic time scales for the water in the river. However, the (time-averaged) water flux plays a crucial role in the evolution of the stratigraphy. Therefore, defining appropriate models that take the coupling between the rivers and the sediments into account is fundamental and challenging. Once the models are at hand, efficient numerical methods must be developed.

4.5 Low-frequency electromagnetism

Numerical simulation is nowadays an essential tool in order to design electromagnetic systems, by estimating the electromagnetic fields generated in a wide variety of devices. An important challenge for many applications is to quantify the intensity of the electric field induced in a conductor by a current generated in its neighborhood. In the low-frequency regime, we can for example cite the study of the impact on the human body of a high-tension line or, for higher frequencies, the one of a smartphone. But the ability to simulate accurately some electromagnetic fields is also very useful for nondestructive control, in the context of the maintenance of nuclear power stations for example. The development of efficient numerical tools, among which a posteriori error estimators, is consequently necessary to reach a high precision of calculation in order to provide estimations that are as reliable as possible.

5 Highlights of the year

5.1 Promotions

C. Cancès was promoted senior Inria researcher (DR2) as of October 2021.

I. Lacroix-Violet was promoted from associate professor at Université de Lille to full professor at Université de Lorraine (Nancy, France). She left the project-team at the end of August 2021.

5.2 Award

On November 23, 2021 C. Cancès was awarded the Blaise Pascal Prize from the Académie des Sciences: see here. The Blaise Pascal Prize is awarded every year by the Académie des Sciences after consultation of the SMAI-GAMNI group. It aims at rewarding outstanding achievements on the devising and mathematical analysis of numerical methods for the solution of PDEs realized by an under-40 researcher in France.

5.3 ABPDE IV conference

From November 16 to November 19, 2021 was held in Lille (at Polytech Lille engineering school) the 4th edition of the conference "Asymptotic Behaviors of systems of PDEs arising in Physics and Biology" (ABPDE IV), organized by C. Cancès, C. Chainais-Hillairet, M. Herda, I. Lacroix-Violet, Alexandre Mouton (Université de Lille), and T. Rey. This event gathered around 70 participants. The ABPDE conference has now become a well-established recurrent event (every 3 years); see also Section 10.1.1.

6 New software and platforms

For the self-assessment of our platforms and codes, we adopt the framework defined by Inria Evaluation Committee (Software family, Audience, Evolution and maintenance, Duration of the development, Contribution of the team, Web page, Description).

6.1 Platform ParaSkel++

Family={research, vehicle}; Audience={partners}; Evolution={lts}; Duration={2}; Contribution={leader}; URL={Software Heritage deposit}

`ParaSkel++` [54] is a C++ platform (freely distributed under LGPL), developed by L. Beaude and S. Lemaire, for the high-performance, arbitrary-order, 2/3D numerical approximation of PDEs on general polytopal meshes using skeletal Galerkin methods. Skeletal Galerkin methods are a vast family of numerical methods for the approximation of PDE-based models that satisfy the following two building principles (see [27]):

- the degrees of freedom (DOF) of the method split into (i) skeleton DOF, 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 DOF (if need be), attached to the interior of the cells, which play no role in the prescription of the conformity properties of the underlying discrete functional space;

- 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 cell, bulk DOF can be eliminated in terms of the local skeleton DOF by means of a Schur complement. The final global system to solve thus writes in terms of the skeleton DOF only. The skeletal family encompasses in particular standard FE methods and virtual-like Galerkin methods (VEM, HHO, HDG...). It does not contain (plain vanilla) DG methods. `ParaSkel++` offers a high-performance factorized C++ architecture for the implementation of arbitrary-order skeletal methods on general 2/3D polytopal meshes. A first version (v1, August 2021) of the platform is operational, featuring a sequential implementation of all the main skeletal methods. The next crucial development steps will be the parallelization on shared memory (before considering 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 facilities.

6.2   Code `KINEBEC`

Family={vehicle}; Audience={partners}; Evolution={lts}; Duration={2}; Contribution={leader};
URL={Software Heritage deposit}

`KINEBEC` (Kinetic Bose–Einstein Condensates) [55] is a C code (freely distributed under GPL), developed by Alexandre Mouton (CNRS permanent engineer at Université de Lille) and T. Rey, devoted to the simulation of collisional kinetic equations of Boltzmann type using a deterministic, spectral Galerkin approach. While mainly devoted to the numerical simulation of the Boltzmann–Nordheim equation (BNE) for fermions and bosons, this code can also be used to solve the classical Boltzmann equation (BE). It relies on state-of-the-art fast spectral approaches to solve with high accuracy and efficiency both the BNE and BE. It has been parallelized on shared memory (OpenMP), but also has a native MPI support for heterogeneous architectures, as well as CUDA capabilities.

6.3   Other codes

6.3.1   Code `FPfrac`

Family={vehicle}; Audience={team}; Evolution={nofuture}; Duration={1}; Contribution={leader};
URL={gitlab.inria.fr/herda/fpfrac}

The Matlab code `FPfrac`, developed by M. Herda, was used to produce the numerical simulations of the article "On a structure-preserving numerical method for fractional Fokker–Planck equations" [38].

6.3.2   Code `FV4SM`

Family={vehicle}; Audience={team}; Evolution={nofuture}; Duration={0.5}; Contribution={instigator}; URL={10.5281/zenodo.3934285}

     The Julia code `FV4SM` [91], developed by C. Cancès, Virginie Ehrlacher (ENPC & Inria Paris), and Laurent Monasse (Inria Nice), was used to produce the numerical simulations of the article "Finite Volumes for the Stefan–Maxwell cross-diffusion system" [43]. It simulates the Stefan–Maxwell equations on Cartesian grids thanks to an entropy-diminishing TPFA Finite Volume scheme.

6.3.3   Code `DPCM-proof`

Family={vehicle}; Audience={partners}; Evolution={basic}; Duration={1}; Contribution={instigator}; URL={github.com/MaximeBreden/DPCM}

     The Matlab code `DPCM-proof`, developed by Maxime Breden (École Polytechnique), C. Chainais-Hillairet, and Antoine Zurek (Université de Technologie de Compiègne), was used to perform the computer-assisted proofs of the article "Existence of traveling wave solutions for the Diffusion Poisson Coupled Model: a computer-assisted proof" [15].

7   New results

7.1   Modeling and numerical simulation of complex fluids

In [34], C. Cancès et al. establish an error estimate, within the generic framework for the spatial discretisation of partial differential equations of the Gradient Discretisation Method (GDM), for a class of degenerate parabolic problems. This result is obtained under very mild regularity assumptions on the exact solution. Their study covers well-known models like the porous medium equation and the fast diffusion equations, as well as the strongly degenerate Stefan problem. Several schemes are then compared in a last section devoted to numerical results.

     In [44], C. Cancès and his co-author prove the existence of weak solutions to a system of two diffusion equations that are coupled by a pointwise volume constraint. The time evolution is given by gradient dynamics for a free energy functional. Their primary example is a model for the demixing of polymers, the corresponding energy is the one of Flory, Huggins and de Gennes. Due to the nonlocality in the equations, the dynamics considered here is qualitatively different from the one found in the formally related Cahn–Hilliard equations. Their angle of attack stems from the theory of optimal mass transport, that is, they consider the evolution equations for the two components as two gradient flows in the Wasserstein distance with one joint energy functional that has the volume constraint built in. The main difference with their previous work [76] is the nonlinearity of the energy density in the gradient part, which becomes singular at the interface between pure and mixed phases.

     In [12], S. Bassetto, C. Cancès et al. are concerned with the numerical approximation of the Richards equation in a heterogeneous domain, each subdomain of which is homogeneous and represents a rocktype. Their first contribution is to rigorously prove convergence toward a weak solution of cell-centered finite volume schemes with upstream mobility and without Kirchhoff's transform. Their second contribution is to numerically demonstrate the relevance of locally refining the grid at the interface between subregions, where discontinuities occur, in order to preserve an acceptable accuracy for the results computed with the schemes under consideration.

     In [42], S. Bassetto, C. Cancès et al. further benchmark several numerical approaches building on upstream mobility two-point flux approximation finite volumes to solve Richards' equation in domains made of several rocktypes. Their study encompasses four different schemes corresponding to different ways to approximate the nonlinear transmission condition systems arising at the interface between different rocks, as well as different resolution strategies based on Newton's method with variable switch. The different methods are compared on filling and drainage test-cases with standard nonlinearities of Brooks–Corey and van Genuchten type, as well as with challenging steep nonlinearities.

     In [15], C. Chainais-Hillairet et al. present and apply a computer-assisted method in order to prove the existence of traveling wave solutions to the Diffusion Poisson Coupled Model arising in corrosion modeling. They also establish a precise and certified description of the solutions.

In [25], A. Natale et al. develop a novel particle discretization for compressible isentropic fluids and porous media flow. The main idea of the method is to replace the internal energy of the fluid by its Moreau–Yosida regularization in the L^2 sense, which can be efficiently computed as a semi-discrete optimal transport problem. Using a modulated energy argument which exploits the convexity of the energy in Eulerian variables, they prove quantitative convergence estimates towards smooth solutions.

In [35], T. Rey et al. review recent mathematical results in kinetic granular materials, especially for those which arose since the last review by Villani on the same subject. This model describes the nonequilibrium behavior of materials composed of a large number of interacting, nonnecessarily microscopic particles, such as grains or planetary rings. This theoretical knowledge is then used to validate a new high-order numerical method for this equation, highlighting through numerics some theoretical open problems.

7.2   Numerical simulation in low-frequency electromagnetism

In [24], E. Creusé et al. study the $\mathbf{A} - \varphi - \mathbf{B}$ magnetodynamic Maxwell system, given in its potential and space-time formulation. First, the existence of strong solutions with the help of the theory of Showalter on degenerate parabolic problems is established. Second, using energy estimates, the existence and the uniqueness of the weak solution to the $\mathbf{A} - \varphi - \mathbf{B}$ system is inferred.

In [23], S. Lemaire et al. prove a discrete version of the first Weber inequality on three-dimensional hybrid spaces spanned by vectors of polynomials attached to the elements and faces of a polyhedral mesh. They then introduce two Hybrid High-Order methods for the approximation of the magnetostatics model, in both its (first-order) field and (second-order) vector potential formulations. These methods are applicable on general polyhedral meshes, and allow for arbitrary orders of approximation. Leveraging the previously established discrete Weber inequality, they perform a comprehensive analysis of the two methods, that they finally validate on a set of test-cases.

7.3   Structure-preserving numerical methods

In [14], C. Chainais-Hillairet et al. develop their work [71]. They establish a priori estimates which lead to the existence of a solution to the scheme, and they prove the exponential decay of the discrete relative entropy towards the thermal equilibrium. Moreover, numerical results assess the good behavior of the numerical schemes.

In [46], C. Chainais-Hillairet, M. Herda, S. Lemaire and J. Moatti devise and study three Hybrid Finite Volume methods for an heterogeneous and anisotropic linear advection-diffusion equation on general meshes. They consider two linear methods, as well as a new, nonlinear scheme. They prove the existence of a solution to each scheme, and positivity of the discrete solutions to the nonlinear scheme. For the three schemes, they show that the discrete solutions converge exponentially fast in time towards their associated discrete steady-states. Their theoretical results are illustrated by numerical simulations.

In [17], C. Cancès, C. Chainais-Hillairet, B. Gaudeul et al. consider an unipolar degenerate drift-diffusion system arising in the modeling of organic semiconductors. They design four different Finite Volume schemes based on four different formulations of the fluxes. They provide a stability analysis and existence results for the four schemes; the convergence is established for two of them.

In [49], B. Gaudeul and his co-author consider a nonlinear cross-diffusion system arising from the consideration of nonzero various ions sizes in a Nernst–Planck–Poisson model. For two different Finite Volume schemes based on two different formulations of the fluxes of the problem, they discuss stability and existence results. For both of them, they report a convergence proof under a non-degeneracy assumption. Numerical experiments illustrate the behavior of the schemes.

In [20], C. Cancès et al. propose a Finite Element scheme for the numerical approximation of degenerate parabolic problems in the form of a nonlinear anisotropic Fokker–Planck equation. The scheme is energy-stable, only involves physically motivated quantities in its definition, and is able to handle general unstructured grids. Its convergence is rigorously proven thanks to compactness arguments, under very general assumptions. Although the scheme is based on Lagrange Finite Elements of degree 1, it is locally conservative after a local post-processing giving rise to an equilibrated flux. This also allows to derive a guaranteed a posteriori error estimate for the approximate solution. Numerical experiments are

presented in order to give evidence of a very good behavior of the proposed scheme in various situations involving strong anisotropy and drift terms.

In [19], C. Cancès and his co-author study a time-implicit Finite Volume scheme for the degenerate Cahn–Hilliard model proposed in [90] and studied mathematically in [76]. The scheme is shown to preserve the key properties of the continuous model, namely mass conservation, positivity of the concentrations, the decay of the energy, and the control of the entropy dissipation rate. This allows to establish the existence of a solution to the nonlinear algebraic system corresponding to the scheme. Furthermore, thanks to compactness arguments, the approximate solution is shown to converge towards a weak solution to the continuous problem as the discretization parameters tend to 0. Numerical results illustrate the behavior of the numerical scheme.

In [43], C. Cancès et al. propose a provably convergent Finite Volume scheme for the so-called Stefan–Maxwell model, which describes the evolution of the composition of a multi-component mixture and reads as a cross-diffusion system. The proposed scheme relies on a Two-Point Flux Approximation, and preserves at the discrete level some fundamental theoretical properties of the continuous model, namely the non-negativity of the solutions, the conservation of mass, and the preservation of the volume-filling constraints. In addition, the scheme satisfies a discrete entropy-entropy dissipation relation, very close to the relation which holds at the continuous level. In this article, C. Cancès et al. present the scheme together with its numerical analysis, and finally illustrate its behavior with some numerical results.

In [45], C. Cancès and his co-auhor propose and study an implicit finite volume scheme for a general model which describes the evolution of the composition of a multi-component mixture in a bounded domain. They assume that the whole domain is occupied by the different phases of the mixture, which leads to a volume filling constraint. In the continuous model, this constraint yields the introduction of a pressure, which should be thought as a Lagrange multiplier for the volume filling constraint. The pressure solves an elliptic equation, to be coupled with parabolic equations, possibly including cross-diffusion terms, which govern the evolution of the mixture composition. The system admits an entropy structure, which is the cornerstone of the analysis. The main objective of their work is the design of a two-point flux approximation finite volume scheme which preserves the key properties of the continuous model, namely the volume filling constraint and the control of the entropy production. Thanks to these properties, and in particular to the discrete entropy-entropy dissipation relation, the authors are able to prove the existence of solutions to the scheme and its convergence. Finally, they illustrate the behavior of their scheme through different applications.

In [29], A. Natale and his co-author construct and analyze Two-Point Flux Approximation Finite Volume discretizations of the quadratic optimal transport problem in its dynamic form. They show numerically that these types of discretizations are prone to form instabilities in their more natural implementation, and propose a variation based on nested meshes in order to overcome these issues. Moreover, they introduce a strategy based on the barrier method to solve the discrete optimization problem.

In [48], E. Facca et al. give a new characterization of the cut locus of a point on a compact Riemannian manifold as the zero set of the optimal transport density solution of the Monge–Kantorovich equations, a PDE formulation of the optimal transport problem with cost equal to the geodesic distance. Combining this result with an optimal transport numerical solver based on the so-called dynamical Monge–Kantorovich approach, they propose a novel framework for the numerical approximation of the cut locus of a point in a manifold. They show the applicability of the proposed method on a few examples settled on 2d-surfaces embedded in $\mathbb{R}^3$ and discuss advantages and limitations.

In [30], T. Rey and his co-author focus on the stability properties of some recently introduced spectral methods that preserve equilibrium. Thanks to the high accuracy and the possibility to use fast algorithms, spectral methods represent an effective way to approximate the Boltzmann collision operator. On the other hand, the loss of some local invariants leads to the wrong long time behavior. A way to overcome this drawback, without sacrificing spectral accuracy, has been proposed recently with the construction of equilibrium-preserving spectral methods. Despite the ability to capture the steady-state with arbitrary accuracy, the theoretical properties of the method have never been studied in details. In this paper, using the perturbation argument developed by Filbet and Mouhot for the homogeneous Boltzmann equation, the authors prove stability, convergence, and spectrally accurate long-time behavior of the equilibrium-preserving approach.

In [52], T. Rey and his co-author introduce a novel Fourier-Galerkin spectral method that improves the

classical spectral method by making it conservative on the moments of the approximated distribution, without sacrificing its spectral accuracy or the possibility of using fast algorithms. The method is derived directly using a constrained best approximation in the space of trigonometric polynomials and can be applied to a wide class of problems where preservation of moments is essential. The authors then apply the new spectral method to the evaluation of the Boltzmann collision term, and prove spectral consistency and stability of the resulting Fourier-Galerkin approximation scheme. They illustrate their theoretical findings by various numerical experiments.

In [41], R. Bailo and T. Rey propose fully explicit projective integration and telescopic projective integration schemes for the multispecies Boltzmann and BGK equations. Projective integration has been recently proposed as a viable alternative to fully implicit and micro-macro methods for providing light, nonintrusive and almost AP integrators for collisional kinetic equations. The methods employ a sequence of small forward-Euler steps, intercalated with large extrapolation steps. The telescopic approach repeats said extrapolations as the basis for an even larger step. This hierarchy renders the computational complexity of the method essentially independent of the stiffness of the problem, which permits the efficient solution of equations in the hyperbolic scaling with very small Knudsen numbers. The schemes are validated on a range of scenarios, demonstrating their prowess in dealing with extreme mass ratios, fluid instabilities, and other complex phenomena.

In [40], R. Bailo et al. develop finite volume schemes for the Cahn–Hilliard equation that unconditionally and discretely satisfy the boundedness of the phase field and the free-energy dissipation. Their numerical framework is applicable to a variety of free-energy potentials including the Ginzburg–Landau and Flory–Huggins, general wetting boundary conditions and degenerate mobilities. Its central thrust is the finite volume upwind methodology, which we combine with a semi-implicit formulation based on the classical convex-splitting approach for the free-energy terms. Extension to an arbitrary number of dimensions is straightforward thanks to their cost-saving dimensional-splitting nature, which allows to efficiently solve higher-dimensional simulations with a simple parallelization. The numerical schemes are validated and tested in a variety of prototypical configurations with different numbers of dimensions and a rich variety of contact angles between droplets and substrates.

In [39], R. Bailo et al. propose finite volume schemes for general continuity equations which preserve positivity and global bounds that arise from saturation effects in the mobility function. In the particular case of gradient flows, the schemes dissipate the free energy at the fully discrete level. Moreover, these schemes are generalised to coupled systems of non-linear continuity equations, such as multispecies models in mathematical physics or biology, preserving the bounds and the dissipation of the energy whenever applicable. These results are illustrated through extensive numerical simulations which explore known behaviours in biology and showcase new phenomena not yet described by the literature.

In [38], M. Herda et al. introduce and analyze numerical schemes for the homogeneous and the kinetic Lévy–Fokker–Planck equation. The discretizations are designed to preserve the main features of the continuous model such as conservation of mass, heavy-tailed equilibrium and (hypo)coercivity properties. They perform a thorough analysis of the numerical schemes and show exponential stability. Along the way, they introduce new tools of discrete functional analysis, such as discrete nonlocal Poincaré and interpolation inequalities adapted to fractional diffusion. Their theoretical findings are illustrated and complemented with numerical simulations.

In [13], I. Lacroix-Violet et al. focus on the numerical integration in time of nonlinear Schrödinger equations using different methods preserving the energy or a discrete analog of it. In particular, they give a rigorous proof of the order of the relaxation method (presented in [70] for cubic nonlinearities) and they propose a generalized version that allows to deal with general power law nonlinearities. Numerical simulations for different physical models show the efficiency of these methods.

7.4 Cost reduction for numerical methods

In [27], S. Lemaire presents a unifying viewpoint on Hybrid High-Order (HHO) [6] and Virtual Element (VE) [68] methods on general polytopal meshes in dimension 2 or 3, in terms of both formulation and analysis. The focus is on a model Poisson problem. To bridge the two paradigms, (i) he transcribes the (conforming) VE method into the HHO framework and (ii) proves H^m approximation properties for the local polynomial projector in terms of which the local VE discrete bilinear form is defined. This allows him to perform a unified analysis of VE/HHO methods, that differs from standard VE analyses by the fact that

the approximation properties of the underlying virtual space are not explicitly used. As a complement to this unified analysis, he also studies interpolation in local virtual spaces, shedding light on the differences between the conforming and nonconforming cases.

In [22], S. Lemaire et al. establish the equivalence between the Multiscale Hybrid-Mixed (MHM) [63] and the Multiscale Hybrid High-Order (MsHHO) [83] methods for a variable diffusion problem with piecewise polynomial source term. Under the idealized assumption that the local problems defining the multiscale basis functions are exactly solved, they prove that the equivalence holds for general polytopal (coarse) meshes and arbitrary approximation orders. They finally leverage the interchange of properties to perform a unified convergence analysis, as well as to improve on both methods.

In [47], I. Lacroix-Violet and her co-author introduce a new class of numerical methods for the time integration of evolution equations set as Cauchy problems of ODEs or PDEs. The systematic design of these methods mixes the Runge–Kutta collocation formalism with collocation techniques, in such a way that the methods are linearly implicit and have high order. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods are expected to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so.

In [51], T. Rey and his co-author present an efficient implementation of a spectral Fourier-Galerkin algorithm for the quantum Boltzmann–Nordheim equation (BNE) for fermions and bosons. The BNE was first formulated by Uehling and Uhlenbeck starting from a classical Boltzmann equation with heuristic arguments. Using novel parallelization techniques, they investigate some of the conjectured properties of the large time behavior of the solutions to this equation. In particular, they are able to observe numerically both Bose–Einstein condensation and Fermi–Dirac relaxation, and to make some conjectures on their stability.

In [18], C. Cancès and his co-author propose a reduced model for the migration of hydrocarbons in heterogeneous porous media. Their model keeps track of the time variable. This allows to compute steady-states that cannot be reached by the commonly used ray-tracing and invasion-percolation algorithms. An efficient Finite Volume scheme allowing for very large time steps is then proposed.

7.5 Asymptotic analysis

In [16], I. Lacroix-Violet et al. consider global weak solutions to compressible Navier–Stokes–Korteweg equations with density dependent viscosities, in a periodic domain $\Omega = \mathbb{T}^3$, with a linear drag term with respect to the velocity. The main result concerns the exponential decay to equilibrium of such solutions using log-Sobolev type inequalities. In order to show such a result, the starting point is a global weak-entropy solutions definition, introduced in [73]. Assuming extra assumptions on the shear viscosity when the density is close to vacuum and when the density tends to infinity, I. Lacroix-Violet et al. conclude the exponential decay to equilibrium. The result also covers the quantum Navier–Stokes system with a drag term.

In [11], following the ideas of V. V. Zhikov and A. L. Pyatnitskii, and more precisely the stochastic two-scale convergence, B. Merlet et al. establish a homogenization theorem in a stochastic setting for two nonlinear equations: the equation of harmonic maps into the sphere, and the Landau–Lifshitz equation. Homogenization results for nonlinear problems are known to be difficult. In this particular case, the equations have strong nonlinear features; in particular, in general, their solutions are not unique. Here, the authors take advantage of the different equivalent definitions of weak solutions to the nonlinear problem to apply typical linear homogenization recipes.

In [53], F. Raimondi tackles the homogenization of a quasilinear elliptic problem having a singular lower-order term and posed in a two-component domain with an ϵ-periodic imperfect interface. A Dirichlet condition is prescribed on the exterior boundary, while the continuous heat flux is assumed to be proportional to the jump of the solution on the interface via a function of order ϵ^γ. An homogenization result for $-1 < \gamma < 1$ is proved by means of the periodic unfolding method, adapted to two-component domains by P. Donato, K. H. Le Nguyen and R. Tardieu. One of the main tools in the homogenization process is the study of a suitable auxiliary linear problem and a related convergence result. It shows that the gradient of u^ϵ behaves like that of the solution of the auxiliary one, associated with a weak cluster

point of the sequence $\{u^\epsilon\}$, as $\epsilon \to 0$. This allows not only to pass to the limit in the quasilinear term, but also to study the singular term near its singularity, via an accurate a priori estimate.

7.6 Applied calculus of variations

In [21], B. Merlet et al. establish new results on the approximation of k-dimensional surfaces (k-rectifiable currents) by polyhedral surfaces with convergence in h-mass and with preservation of the boundary (the approximating polyhedral surface has the same boundary as the limit). This approximation result is required in the convergence study of [82].

In [26], B. Merlet and his co-author study a family of functionals penalizing oblique oscillations. These functionals naturally appear in some variational problems related to pattern formation and are somewhat reminiscent of those introduced by Bourgain, Brezis and Mironescu to characterize Sobolev functions. More precisely, for a function u defined on a tensor product $\Omega_1 \times \Omega_2$, the family of functionals $\{E_\varepsilon(u)\}_{\varepsilon > 0}$ that they consider vanishes if u is of the form $u(x_1)$ or $u(x_2)$. They prove the converse property and related quantitative results. In particular, they describe the fine properties of functions with $\sup_\varepsilon E_\varepsilon(u) < \infty$ by showing that, roughly, such u is piecewise of the form $u(x_1)$ or $u(x_2)$ on domains separated by lines where the energy concentrates. It turns out that this problem naturally leads to the study of various differential inclusions, and has connections with branched transportation models.

In [31], M. Pegon studies large volume minimizers of isoperimetric problems derived from Gamow's liquid drop model for the atomic nucleus, involving the competition of a perimeter term and repulsive nonlocal potentials. Considering a large class of potentials, given by general radial nonnegative kernels which are integrable on $\mathbb{R}^n$, such as Bessel potentials, M. Pegon proves the existence of minimizers of arbitrarily large mass, provided that the first moment of the kernels is below an explicit threshold. This contrasts with the case of Riesz potentials, where minimizers do not exist above a critical mass. In addition, renormalizing to a fixed volume, any sequence of minimizers converges to the ball as the mass goes to infinity. Finally, M. Pegon shows that the threshold on the first moment of the kernels is sharp, in the sense that large balls go from stable to unstable. A direct consequence of the instability of large balls above this threshold is that there exist nontrivial compactly supported kernels for which the problems admit minimizers which are not balls, that is, symmetry breaking occurs.

In [28], B. Merlet and M. Pegon consider an isoperimetric problem in which the standard perimeter $P(E)$ is replaced by $P(E) - \gamma P_\varepsilon(E)$, with $0 < \gamma < 1$ and P_ε a nonlocal energy such that $P_\varepsilon(E) \to P(E)$ as ε vanishes. They prove that unit area minimizers are disks for $\varepsilon > 0$ small enough. This isoperimetric problem is equivalent to a generalization of the liquid drop model for the atomic nucleus introduced by Gamow, where the nonlocal repulsive potential is given by a radial, sufficiently integrable kernel. In that formulation, their result states that if the first moment of the kernel is smaller than an explicit threshold, there exists a critical mass m_0 such that for any $m > m_0$, the disk is the unique minimizer of area m up to translations.

In [50], 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.

8 Bilateral contracts and grants with industry

8.1 Bilateral contracts with industry

The PhD thesis of S. Bassetto was funded by IFPEn. The contract followed the lines of the bilateral contract between Inria and IFPEn. S. Bassetto defended on December 16, 2021.

The PhD thesis of M. Jonval, that started in October 2021, is co-funded by Inria (salaries) and IFPEn (overhead costs). The contract follows the lines of the bilateral contract between Inria and IFPEn.

8.2 Bilateral grants with industry

CEA (Christian Bataillon) and ANDRA (Laurent Trenty) are involved in the EURAD project on corrosion modeling together with the RAPSODI project-team (C. Cancès, C. Chainais-Hillairet, B. Merlet, and F. Raimondi). More details on the project can be found in Section 9.2.1.

9 Partnerships and cooperations

9.1 International research visitors

Between October 19 and November 19, C. Chainais-Hillairet and M. Herda invited Patricio Farrell, research group leader at WIAS (Berlin, Germany), and Dilara Abdel, PhD student within P. Farrell's group, to work on the numerical simulation of perovskite semiconductors. P. Farrell was invited as a visiting professor funded by the LabEx CEMPI (see Section 9.3.2), whereas D. Abdel received funding from the French Embassy in Berlin.

The team was also visited by national researchers.

S. Lemaire invited Théophile Chaumont-Frelet (Inria Nice) to visit him in Lille on November 8-10.

C. Cancès invited Flore Nabet (École Polytechnique) to visit him in Lille on June 15-17, as well as on December 5-6.

9.2 European initiatives

9.2.1 FP7 & H2020 projects

C. Cancès, C. Chainais-Hillairet and B. Merlet are involved in the H2020 project EURAD (EUropean Joint Programme on RADioactive Waste Management). Inside EURAD, the DONUT work-package is concerned with the development and improvement of numerical methods and tools for modelling coupled processes. The task of the RAPSODI project-team inside EURAD/DONUT is to establish an energetic formulation of the Diffusion Poisson Coupled Model leading to new long-time robust numerical methods for the simulation of the corrosion processes in an underground repository. The project started in 2019, and the RAPSODI project-team received a grant of 138 750 euros. The first technical report (2020) is available [60]. The post-doc position of F. Raimondi is funded by EURAD.

9.2.2 Other european programs/initiatives

M. Herda is the French P. I. of a bilateral French-Austrian PHC AMADEUS 2021 program. The two-year project is entitled "Design and analysis of structure-preserving numerical schemes for cross-diffusion systems" and has been submitted in collaboration with an Austrian research team at the Institute for Analysis and Scientific Computing, T. U. Vienna. The project involves other members of the RAPSODI project-team (C. Cancès, C. Chainais-Hillairet, B. Gaudeul, and T. Rey). The grant of 4 400 euros is dedicated to cover travel expenses.

9.3 National initiatives

9.3.1 ANR

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: Mathématiques (CE40) - 2019

- ANR reference: ANR-19-CE40-0012

- Duration: March 2020 - October 2024

- Budget: 132 256 euros

- Coordinator: Marielle Simon (Inria Lille, PARADYSE project-team)

C. Cancès is a member of the ANR JCJC project COMODO. This project focuses on the mathematical and numerical study of cross-diffusion systems in moving domains. The targeted application is the simulation of the production of photovoltaic devices by a vapor deposition process.

- Title: CrOss-diffusion equations in MOving DOmains

- Type: Modèles numériques, simulation, applications (CE46) - 2019

- ANR reference: ANR-19-CE46-0002

- Duration: January 2020 - December 2023

- Budget: 213 810 euros

- Coordinator: Virginie Ehrlacher (ENPC & Inria Paris)

C. Chainais-Hillairet and T. Rey are members of the ANR JCJC project MOHYCON. This project is related to the analysis and simulation of multiscale models of semiconductors. As almost all current electronic technology involves the use of semiconductors, there is a strong interest for modeling and simulating the behavior of such devices, which was recently reinforced by the development of organic semiconductors used for example in solar panels or in mobile phones and television screens (among others).

- Title: Multiscale MOdels and HYbrid numerical methods for semiCONductors

- Type: Mathématiques (CE40) - 2017

- ANR reference: ANR-17-CE40-0027

- Duration: January 2018 - March 2022

- Budget: 113 940 euros

- Coordinator: Marianne Bessemoulin-Chatard (CNRS & Université de Nantes)

9.3.2 LabEx CEMPI

Through their affiliation to the Laboratoire Paul Painlevé of Université de 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: Emmanuel 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 post-doc position of M. Pegon is funded by the LabEx CEMPI. The research stay in Lille of Patricio Farrell (WIAS, Berlin, Germany) between October and November 2021 was also supported by the LabEx CEMPI.

9.3.3 CNRS NEEDS

C. Chainais-Hillairet has been a member of the CNRS NEEDS (Nuclear power, Energy, Environment, Waste, Society) project POCO (Preuves assistées par Ordinateur pour un modèle de COrrosion) from 2020 to 2021. The project was coordinated by Maxime Breden (École Polytechnique). It focused on computer-assisted proofs for a corrosion model (see [15]).

9.3.4 BOUM

J. Candau-Tilh and M. Pegon received funding (~1000 euros) through the 2021 BOUM (BOUge tes Mathématiques) call for projects of the Société de Mathématiques Appliquées et Industrielles (SMAI). The aim of their project is to invite and fund 5 young researchers to present their work at the 3rd edition of the Conference on Calculus of Variations to be held in Lille on July 4-6, 2022, and co-organized by J. Candau-Tilh, B. Merlet, A. Natale and M. Pegon.

9.4   Regional initiatives

9.4.1 ERC Generator

The MANAKINEQO (MAthematical and Numerical Advances in KINetic EQuatiOns) project (referenced as R-ERCGEN-19-007-REY) is a proposal funded (116 545 euros) within the ERC Generator program from I-SITE ULNE. Between February 2020 and January 2022, T. Rey, P. I. of the project, aims at investigating mathematical properties, as well as developing efficient numerical schemes, for multiscale collisional kinetic equations of the Boltzmann type. The 18-month post-doc of R. Bailo has been funded by this grant, as well as most of the ABPDE IV conference (see Section 10.1.1).

9.4.2 Technological Development Action (ADT)

S. Lemaire is the P. I. of the ADT project ParaSkel++ (funded by Inria Lille), that started in February 2020. The aim of the project is to develop an optimized parallel C++ platform for the arbitrary-order numerical approximation of PDEs by skeletal methods on general 2/3D polytopal meshes (more details in Section 6.1). L. Beaude was hired as a temporary engineer for this project. She left the team at the end of August 2021 for a permanent engineer position at BRGM (Orléans, France).

9.4.3 STIMulE

C. Calgaro, E. Creusé and T. Rey are members of the SQUAW (Super QUantum fluids and shAllow Water equations) project, headed by Olivier Goubet (Université de Lille) and funded by the 2021 STIMulE regional call. The SQUAW project brings together the skills of applied mathematicians from four research units of the FMHF (Fédération de recherche Mathématique des Hauts-de-France). One scientific direction of the projet is the coupling of quantum models with classical fluid models (Navier–Stokes type). The challenge

is to successfully concatenate two completely different types of models, the numerical simulation of which currently requires completely different approaches. The fields of application of these models range from superfluids to semiconductors. Two Master 2 internships (one in Lille and one in Valenciennes) will be funded by the SQUAW project.

10   Dissemination

10.1   Promoting scientific activities

10.1.1   Scientific events: organisation

Conferences and workshops

C. Cancès, C. Chainais-Hillairet, M. Herda, I. Lacroix-Violet, and T. Rey co-organized the 4th edition of the conference "Asymptotic Behaviors of systems of PDEs arising in Physics and Biology" (ABPDE IV), that was held in Lille (at Polytech Lille engineering school) from November 16 to November 19, 2021. The event gathered around 70 participants and featured 10 plenary talks, 19 contributed talks, and 12 posters.

E. Creusé co-organized the event "PDE, Analysis and Applications - Conference in honor of the 60th birthday of Serge Nicaise", that was held in Valenciennes on November 2-5, 2021.

E. Creusé also co-organized the 3rd edition of the event "Analyse Appliquée en Hauts-de-France", that was held in Valenciennes on July 6, 2021.

C. Cancès co-organized the DONUT scientific days within the EURAD project (see Section 9.2.1), held online on January 27-28, 2021.

A. Natale co-organized the "Journée du Laboratoire Paul Painlevé 2021", that was held in La Piscine Museum (Roubaix) on November 25, 2021.

Mini-symposia

R. Bailo co-organized, together with Sergio Perez (Imperial College London, UK), a mini-symposium on the "Challenges in structure-preserving numerical methods for PDEs" at the British Applied Mathematics Colloquium, that was held remotely on April 6-9, 2021.

C. Cancès co-organized, together with Jakub W. Both (Bergen University, Norway), a mini-symposium on "Dissipation-driven nonlinear and coupled processes in porous media" at the SIAM Conference on Mathematical and Computational Issues in the Geosciences (SIAM GS21), that was held remotely on June 21-24, 2021.

S. Lemaire co-organized, together with Andrea Borio (Politecnico di Torino, Italy), Ilario Mazzieri (Politecnico di Milano, Italy), and Giuseppe Vacca (Università di Milano Bicocca, Italy), a mini-symposium on the "Advances in polygonal and polyhedral methods" at the WCCM XIV & ECCOMAS 2020 conference, that was held remotely on January 11-15, 2021.

S. Lemaire co-organized, together with Alexandre Ern (ENPC & Inria Paris) and Théophile Chaumont-Frelet (Inria Nice), a mini-symposium on "High-order face-based discretization methods" at the ICOSA-HOM 2020 conference, that was held remotely on July 12-16, 2021.

10.1.2   Scientific events: selection

C. Chainais-Hillairet was a member of the scientific committees of the tenth SMAI Congress held in June 2021 in La Grande-Motte, and of the CEA-SMAI/GAMNI Workshop to be held in Paris in January 2022.

10.1.3   Journal

Member of the editorial boards   C. Chainais-Hillairet is a member of the editorial board of the North-Western European Journal of Mathematics.

Reviewer - reviewing activities   RAPSODI permanent team members are regular reviewers for all the main international journals in PDEs, numerical analysis, and scientific computing.

10.1.4 Invited talks

R. Bailo gave an online talk at the kinetic mini-symposium (co-organized by himself) of the British Applied Mathematics Colloquium held remotely on April 6-9. He also gave an online talk in the ANEDP seminar of the Laboratoire Paul Painlevé.

C. Cancès was an invited speaker at the Jacques-Louis Lions Hispano-French School on Numerical Simulation in Physics and Engineering held in Madrid between August 30 and September 3. He also gave a contributed talk at the AMaSiS 2021 conference held online on September 6-9. C. Cancès was finally invited to take part in the Oberwolfach workshop "Applications of Optimal Transportation in the Natural Sciences" held online on February 22-26.

J. Candau-Tilh presented a poster at the event "Rencontre en Calcul des Variations" held on December 8-10 in Nancy.

C. Chainais-Hillairet was an invited keynote speaker at the AMaSiS 2021 conference held online on September 6-9. She also gave a seminar at the Université de Nantes.

B. Gaudeul gave online talks at the Numerische Mathematik Seminar in WIAS (Berlin, Germany), as well as at the PhD Students Seminar of the Laboratoire Jacques-Louis Lions (Sorbonne Université).

M. Herda gave a talk in the Summer School "Multi-scale modeling for pattern formation in biological systems", within the mini-symposium "Kinetic approaches in biological systems". The event was originally planned at the Mittag-Leffler Institute (Stockholm, Sweden) but was eventually held online on July 19-23. M. Herda also gave an online talk at the Workshop MOME (Mathematical MOdelling in Ecology) held remotely on April 2.

I. Lacroix-Violet gave an online seminar for the PDEs Webinar at Université de Lorraine.

S. Lemaire gave online talks at the WCCM XIV & ECCOMAS 2020 conference held remotely on January 11-15, as well as in the ICOSAHOM 2020 conference (in the mini-symposium co-organized by himself) held remotely on July 12-16, 2021.

B. Merlet gave talks at the workshop "Geometric Measure Theory and Applications" held between August 30 and September 3 in Cortona (Italy), and at the workshop "Variational methods and applications" held on September 6-10 at the Centro di Ricerca Matematica Ennio De Giorgi in Pisa (Italy). He also gave an online talk for the PDE team seminar at Université de Poitiers.

J. Moatti presented posters at the AMaSiS 2021 conference held online on September 6-9, at the "Congrès des Jeunes Chercheuses et Chercheurs en Mathématiques Appliquées" held in École Polytechnique (Palaiseau) on October 27-29, and for the ABPDE IV conference held in Lille on November 16-19.

A. Natale gave a talk at the Oberwolfach workshop "Applications of Optimal Transportation in the Natural Sciences" held online on February 22-26. He also gave a talk for the "Journée du Laboratoire Paul Painlevé 2020" held in the Laboratoire Paul Painlevé on July 1st, as well as for the ANEDP seminar of the Laboratoire Paul Painlevé.

M. Pegon gave talks for the "Journée d'équipe ANEDP 2020" held online on February 4, 2021, for the "Journées Jeunes EDPistes 2021" held online on March 24-26, at the tenth SMAI Congress held on June 21-25 in La Grande-Motte, at the workshop "Variational methods and applications" held on September 6-10 at the Centro di Ricerca Matematica Ennio De Giorgi in Pisa (Italy), at the "Journée du Laboratoire Paul Painlevé 2021" held on November 25 in La Piscine Museum (Roubaix), and at the event "Rencontre en Calcul des Variations" held on December 8-10 in Nancy. He also gave an online seminar at the Virginia Commonwealth University (see here).

F. Raimondi gave a talk for the "Journée d'équipe ANEDP 2020" held online on February 4, 2021. She also presented posters at the "Congrès des Jeunes Chercheuses et Chercheurs en Mathématiques Appliquées" held in École Polytechnique (Palaiseau) on October 27-29, as well as for the ABPDE IV conference held in Lille on November 16-19.

T. Rey gave online talks at the kinetic mini-symposium (co-organized by R. Bailo) of the British Applied Mathematics Colloquium held remotely on April 6-9, and at the conference "Recent Development in Numerical Kinetic Theory" held remotely on June 21-25. He also gave an online seminar for the KinetiCAM work group of Cambridge University, as well as a talk in the Applied Mathematics Seminar at Université de Strasbourg.

10.1.5 Leadership within the scientific community

C. Cancès is the leader of the task "Numerical methods for high-performance computing of coupled processes" in the `DONUT` work-package on the development and improvement of numerical methods and tools for modelling coupled processes within the H2020 project `EURAD` on the management of nuclear waste at the European level (see Section 9.2.1).

10.1.6 Scientific expertise

C. Calgaro was part of the selection committee for a tenured assistant professor (MCF) position at Université du Littoral Côte d'Opale (Calais), as well as of the selection committee for 4 tenured junior research scientist (CRCN and ISFP) positions at Inria Lille.

C. Chainais-Hillairet was part of the selection committee for a tenured assistant professor (MCF) position at Université de Lille, as well as of the selection committee for a full professor (PR) position at Université de Versailles Saint-Quentin-en-Yvelines.

E. Creusé was the president of the selection committee for a temporary assistant professor (MCF article 19) position at Université Polytechnique Hauts-de-France (Valenciennes).

E. Creusé was also an HCERES expert for the evaluation of the Laboratoire de Mathématiques Jean Leray in Nantes.

I. Lacroix-Violet was part of the selection committee for a tenured assistant professor (MCF) position at Université de Montpellier, as well as of the selection committee (together with C. Calgaro) for a tenured assistant professor (MCF) position at Université du Littoral Côte d'Opale (Calais).

10.1.7 Research administration

C. Cancès is a member of the scientific advisory board (BSC) of the Inria Lille research center.

C. Chainais-Hillairet is vice-director of the Laboratoire Paul Painlevé, in charge of human resources for researchers, professors and assistant professors. She was also an elected member of the Conseil de la Faculté des Sciences et Technologies at Université de Lille until the end of April 2021.

E. Creusé is the director of the Département de Mathématiques et Applications de Valenciennes (DEMAV), within the Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS) at Université Polytechnique Hauts-de-France (Valenciennes). He is also responsible for the MAS (Modélisation, Simulation, Aléa) team of the DEMAV.

Until the end of August 2021, B. Gaudeul was the delegate of the PhD students at the Commission Mixte, and was a member of the Commission Égalité, whose aim is to fight against gender-based discriminations.

Since 2019, M. Herda is the co-organizer of the weekly Numerical Analysis and PDEs (ANEDP) seminar of the Laboratoire Paul Painlevé. He is also an elected member of the Conseil de Laboratoire and of the Commission Mixte which, every few months, provide consultative advice and votes on matters (budget, promotions...) related to the math laboratory and the math department. M. Herda is also substitute member of the Inria Lille Comité de Centre.

Until the end of August 2021, I. Lacroix-Violet was a member of the Conseil de la Fédération de Recherche des Hauts-de-France, and of the Commission Emploi Recherche (CER) of the Inria Lille research center.

S. Lemaire is a member of the Commission de Développement Technologique (CDT) of the Inria Lille research center.

B. Merlet is in charge of the Numerical Analysis and PDEs (ANEDP) team of the Laboratoire Paul Painlevé. He is also a member of the Commission Mixte.

T. Rey is a member of the Opération Postes, the local correspondent of the biomath-oriented research group GdR `MathSAV`, a member of the council of the Graduate Programme "Information and Knowledge Society", and the point of contact concerning sustainable development at Laboratoire Paul Painlevé.

10.2   Teaching - Supervision - Juries

10.2.1   Teaching

RAPSODI team members are strongly involved in teaching at Université de Lille (and Université Polytechnique Hauts-de-France, Valenciennes).

Faculty members of the project-team ensure their teaching duties (~192h yearly), as well as important administrative tasks in the math departments. C. Calgaro is in charge of the Master "Mathematics and Applications", and is a member of the Conseil de Département de Mathématiques at Université de Lille. B. Merlet was in charge of the Master 2 "Scientific Computing" until August 2021. Since September 2021, T. Rey substituted him in this task. Until August 2021, I. Lacroix-Violet was responsible of the first year of the Production department at Polytech Lille engineering school.

Inria members of the project-team also take an important part in teaching activities. In 2021, C. Cancès taught the course "Fundamental notions in Mathematics" (32h) in the framework of the Master 1 "Data Science" of Université de Lille and École Centrale Lille, as well as a course on differential equations and their approximation (28h) for first-year students at École Centrale Lille. M. Herda gave tutorials (16h) in the introductory course to scientific computing for first-year students at École Centrale Lille. He also gave tutorials (36h) on multivariate calculus to second-year undergraduate students at Université de Lille. M. Jonval taugh a refresher course in maths (30h) at SKEMA Business School for first-year students. He also taught a course on Fourier and Laplace transforms (20h) at ISEN Lille for third-year students. S. Lemaire taught the course "Mathematical Tools for Simulation" (44h) in the framework of the Master 2 "Scientific Computing" at Université de Lille. J. Moatti gave tutorials on linear algebra (36h) for L1 MIASHS students at Université de Lille. He also gave tutorials (18h) for a refresher course in L2 LAS at Université de Lille. He finally gave tutorials (10h) in L1 SESI at Université de Lille. A. Natale taught the course "Refresher in Mathematics" (16h) in the framework of the Master 2 "Data Science" of Université de Lille and École Centrale Lille. He also taugh the course "Numerical approximation of nonlinear problems" (22h) in the framework of the Master 1 "Scientific Computing" at Université de Lille.

10.2.2   Supervision

In progress

Post-doc of E. Facca (Inria): "Locally conservative methods for the approximation of dynamical transport on unstructured meshes", advised by A. Natale, since October 2021, funded by Inria.

Post-doc of F. Raimondi (CNRS): "Variational modeling of corrosion", co-advised by C. Cancès, C. Chainais-Hillairet and B. Merlet, since October 2020, funded by the H2020 project `EURAD`.

Post-doc of M. Pegon (Université de Lille): "Theoretical shape optimization problems", advised by B. Merlet, since September 2020, funded by the LabEx `CEMPI`.

PhD of M. Jonval (Inria/IFPEn): "Advanced numerical methods for stiff problems in the context of reactive transport", co-supervised by Ibtihel Ben Gharbia (IFPEn), C. Cancès, Thibault Faney (IFPEn) and Quang-Huy Tran (IFPEn), since October 2021, co-funded by Inria and IFPEn in the framework of the bilateral contract. Prior to his recruitment as a PhD student, M. Jonval joined the team as a research assistant between May 1st and September 30.

PhD of T. Laidin (Université de Lille): "Hybrid kinetic/fluid numerical methods and discrete hypocoercivity for the Boltzmann equation for semi-conductors", co-supervised by Marianne Bessemoulin-Chatard (CNRS & Université de Nantes), C. Chainais-Hillairet and T. Rey, since October 2021, co-funded by the LabEx `CEMPI` and the Hauts-de-France region.

PhD of J. Candau-Tilh (Université de Lille): "Isoperimetric problems with Wasserstein interactions", co-supervised by Michael Goldman (Université Paris Diderot) and B. Merlet, since September 2021, funded by an ENS fellowship.

PhD of J. Moatti (Inria): "Design and analysis of high-order methods for convection-diffusion models, study of the long-time behavior", co-supervised by C. Chainais-Hillairet, M. Herda and S. Lemaire, since October 2020, funded by Inria.

Ended in 2021

Post-doc of R. Bailo (Université de Lille): "Projective integration of the multiple-species Boltzmann

equation", advised by T. Rey, from June 2020 until October 2021, funded by the ERC Generator project `MANAKINEQO`.

PhD of S. Bassetto (IFPEn): "Towards a more robust and accurate treatment of capillary effects in multiphase flow simulations in porous media", co-supervised by C. Cancès, Guillaume Enchéry (IFPEn) and Quang-Huy Tran (IFPEn), defended on December 16 [36], co-funded by IFPEn and Inria in the framework of the bilateral contract.

PhD of B. Gaudeul (Université de Lille): "Numerical approximation of cross-diffusion systems arising in physics and biology", co-supervised by C. Cancès and C. Chainais-Hillairet, defended on August 30 [37], funded by an ENS fellowship.

Engineer position of L. Beaude (Inria) on the development of the `ParaSkel++` platform, supervised by S. Lemaire, from February 2020 until August 2021, funded by Inria (ADT `ParaSkel++`).

Internships

M2 internship of T. Laidin (Université de Nantes): "Hybrid kinetic/fluid numerical methods for the linear BGK equation", co-supervised by Marianne Bessemoulin-Chatard (CNRS & Université de Nantes) and T. Rey, April-September 2021.

M2 internship of A. Salheddine (Université Polytechnique Hauts-de-France, Valenciennes): "Numerical simulation of incompressible fluid flows by a BGK method", supervised by E. Creusé, July-December 2021.

M2 internship of A. Spadotto (Politecnico di Milano, Italy): "Hybrid High-Order methods for magnetostatics", co-supervised by Daniele A. Di Pietro (Université de Montpellier) and S. Lemaire, April-September 2021.

M2 project of Fabian Polvin, Chaimae Elbaraka and Ismail Bouhmala (Université Polytechnique Hauts-de-France, Valenciennes): "Implementation of the 2D MAC-FD scheme for the numerical simulation of the boundary layer equations", supervised by E. Creusé, January-May 2021.

M1 internship of L. Cleenewerck (Université de Lille): "Implementation of numerical schemes for simulations in population dynamics", supervised by M. Herda, June-July 2021.

M1 internship of S. Despierres (Université de Lille): "Projective integration for kinetic chemotaxis", supervised by T. Rey, June-July 2021.

M1 internship of J. Drappier (Université de Lille): "Finite element approximation of mean field games", supervised by A. Natale, June-July 2021.

M1 internship of K.-H. N'Gakosso (Université de Lille): "Implementation of some numerical schemes for a corrosion model", supervised by C. Chainais-Hillairet, June-July 2021.

M1 internship of F. Pigot (Université de Lille): "Micro-macro correspondence of models for pedestrian dynamics", supervised by R. Bailo, June-July 2021.

M1 internship of J. Rouzé (Université de Lille): "Inverse models for sachet salads", supervised by C. Calgaro, in collaboration with Bonduelle, June-July 2021.

M1 project of S. Despierres and F. Pigot (Université de Lille): "Asymptotic-preserving schemes for linear kinetic equations", supervised by T Rey, February-May 2021.

M1 project of Charbel Ghosn (Université de Lille): "Projective integration for nonlinear ODEs", supervised by T. Rey, January-May 2021.

L3 internship of C. Delbergue (Université de Lille): "Integration schemes for mass action kinetics", supervised by M. Jonval, October-December 2021.

10.2.3   Juries

C. Cancès was a jury member for the PhD defense of Aya Oussaily (Université de Technologie de Compiègne) on October 11. He was also part of the jury, as co-superviser, for the PhD defenses of B. Gaudeul (Université de Lille) on August 30, of Gabriele Todeschi (Université Paris Dauphine) on December 13, and of S. Bassetto (Université de Lille) on December 16.

C. Chainais-Hillairet reported on 3 PhD theses, respectively written by Gopikrishnan Chirappurathu Remesan (IIT Bombay, India & Monash University, Australia), Guissel Dongmo (Université Paris-Saclay), and Virgile Dubos (Sorbonne Université). She was also a jury member for the PhD defenses of Guissel Dongmo on December 13 and Virgile Dubos on December 14, and a jury member as well as the president of the jury for the PhD defenses of Hélène Bloch (Université Paris-Saclay) on September 23 and S. Bassetto

(Université de Lille) on December 16. She was finally part of the jury, as co-superviser, for the PhD defense of B. Gaudeul (Université de Lille) on August 30.

E. Creusé reported on the PhD thesis of Jérémy Alloul (Université d'Orléans), defended on June 21. He was also a jury member for the PhD defense of Joanna Bisch (Université de Lille) on October 22.

M. Herda was a jury member for the PhD defense of Mohamad Rachid (Université de Nantes) on December 7.

B. Merlet reported on the PhD thesis of Chih-Kang Huang (Université Lyon 1), defended on October 15. He also reported on the Habilitation of Matthieu Bonnivard (Université Paris Diderot), to be defended on January 7, 2022.

10.3 Popularization

10.3.1 Internal or external Inria responsibilities

C. Calgaro is in charge of the communication of the Laboratoire Paul Painlevé. She regularly gives/organizes conferences in high schools in the framework of the "Mathématiques itinérantes".

10.3.2 Education

T. Laidin welcomed a schoolboy (3ème) for half a day to introduce him to the research world.

10.3.3 Interventions

In October 2021, C. Chainais-Hillairet took part in the "Rendez-vous des Jeunes Mathématiciennes et Informaticiennes" organized in Lille, where she gave a talk to an audience of high school female students. C. Chainais-Hillairet and F. Raimondi also participated to speed meeting exchanges with the schoolgirls.

In October 2021, J. Venel gave a popularization conference for an audience of high school female students during the event "Filles, maths et informatique : une équation lumineuse" organized in Arras.

11 Scientific production

11.1 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] C. Calgaro, E. Creusé, T. Goudon and S. Krell. 'Simulations of non homogeneous viscous flows with incompressibility constraints'. In: *Mathematics and Computers in Simulation* 137 (2017), pp. 201–225. URL: https://hal.archives-ouvertes.fr/hal-01246070.

[3] 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.

[4] 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.

[5] C. Chainais-Hillairet, B. Merlet and A. Vasseur. 'Positive Lower Bound for the Numerical Solution of a Convection-Diffusion Equation'. In: *FVCA8 2017 - International Conference on Finite Volumes for Complex Applications VIII*. Lille, France: Springer, June 2017, pp. 331–339. DOI: 10.1007/978-3-319-57397-7_26. URL: https://hal.archives-ouvertes.fr/hal-01596076.

[6] 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.

[7] 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.

[8] F. Filbet and M. Herda. 'A finite volume scheme for boundary-driven convection-diffusion equations with relative entropy structure'. In: *Numerische Mathematik* 137.3 (2017), pp. 535–577. URL: https://hal.archives-ouvertes.fr/hal-01326029.

[9] I. Lacroix-Violet and A. Vasseur. 'Global weak solutions to the compressible quantum Navier–Stokes equation and its semi-classical limit'. In: *Journal de Mathématiques Pures et Appliquées* 114 (2018), pp. 191–210. URL: https://hal.archives-ouvertes.fr/hal-01347943.

[10] 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.

11.2 Publications of the year

International journals

[11] F. Alouges, A. de Bouard, B. Merlet and L. Nicolas. 'Stochastic homogenization of the Landau-Lifshitz-Gilbert equation'. In: *Stochastics and Partial Differential Equations: Analysis and Computations*. Stochastic Partial Differential Equations. Analysis and Computations 9.4 (2nd Jan. 2021), pp. 789–818. DOI: 10.1007/s40072-020-00185-4. URL: https://hal.archives-ouvertes.fr/hal-02020241.

[12] S. Bassetto, C. Cancès, G. Enchéry and Q.-H. Tran. 'Upstream mobility finite volumes for the Richards equation in heterogenous domains'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.5 (Sept. 2021), pp. 2101–2139. DOI: 10.1051/m2an/2021047. URL: https://hal.archives-ouvertes.fr/hal-03377035.

[13] C. Besse, S. Descombes, G. Dujardin and I. Lacroix-Violet. 'Energy preserving methods for nonlinear Schrödinger equations'. In: *IMA Journal of Numerical Analysis* 41.1 (Jan. 2021), pp. 618–653. DOI: 10.1093/imanum/drz067. URL: https://hal.archives-ouvertes.fr/hal-01951527.

[14] M. Bessemoulin-Chatard, C. Chainais-Hillairet and H. Mathis. 'Analysis of numerical schemes for semiconductors energy-transport models'. In: *Applied Numerical Mathematics* 168 (Oct. 2021), pp. 143–169. DOI: 10.1016/j.apnum.2021.05.030. URL: https://hal.archives-ouvertes.fr/hal-02940224.

[15] M. Breden, C. Chainais-Hillairet and A. Zurek. 'Existence of traveling wave solutions for the Diffusion Poisson Coupled Model: a computer-assisted proof'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.4 (13th July 2021), pp. 1669–1697. DOI: 10.1051/m2an/2021037. URL: https://hal.archives-ouvertes.fr/hal-03082893.

[16] D. Bresch, M. Gisclon, I. Lacroix-Violet and A. F. Vasseur. 'On the Exponential decay for Compressible Navier-Stokes-Korteweg equations with a Drag Term'. In: *Journal of Mathematical Fluid Mechanics* (2021). URL: https://hal.archives-ouvertes.fr/hal-02542115.

[17] C. Cancès, C. Chainais-Hillairet, J. Fuhrmann and B. Gaudeul. 'A numerical analysis focused comparison of several Finite Volume schemes for an Unipolar Degenerated Drift-Diffusion Model'. In: *IMA Journal of Numerical Analysis* 41.1 (2021), pp. 271–314. DOI: 10.1093/imanum/draa002. URL: https://hal.archives-ouvertes.fr/hal-02194604.

[18] C. Cancès and D. Maltese. 'a gravity current model with capillary trapping for oil migration in multilayer geological basins'. In: *SIAM Journal on Applied Mathematics* 81.2 (2021), pp. 454–484. DOI: 10.1137/19M1284233. URL: https://hal.archives-ouvertes.fr/hal-02272965.

[19]   C. Cancès and F. Nabet. 'Finite Volume approximation of a two-phase two fluxes degenerate Cahn-Hilliard model'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.3 (2021), pp. 969–1003. DOI: 10.1051/m2an/2021002. URL: https://hal.archives-ouvertes.fr/hal-02561981.

[20]   C. Cancès, F. Nabet and M. Vohralík. 'Convergence and a posteriori error analysis for energy-stable finite element approximations of degenerate parabolic equations'. In: *Mathematics of Computation* 90.328 (2021), pp. 517–563. DOI: 10.1090/mcom/3577. URL: https://hal.archives-ouvertes.fr/hal-01894884.

[21]   A. Chambolle, L. A. D. Ferrari and B. Merlet. 'Strong approximation in h-mass of rectifiable currents under homological constraint'. In: *Advances in Calculus of Variation* 14.3 (1st July 2021), pp. 343–363. DOI: 10.1515/acv-2018-0079. URL: https://hal.archives-ouvertes.fr/hal-01813234.

[22]   T. Chaumont-Frelet, A. Ern, S. Lemaire and F. Valentin. 'Bridging the Multiscale Hybrid-Mixed and Multiscale Hybrid High-Order methods'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* (2021). DOI: 10.1051/m2an/2021082. URL: https://hal.archives-ouvertes.fr/hal-03235525.

[23]   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* (2021). DOI: 10.1142/S0218202522500051. URL: https://hal.archives-ouvertes.fr/hal-02892526.

[24]   E. Creusé, S. Nicaise and R. V. Sabariego. 'Existence results for the $\mathbf{A} - \varphi - \mathbf{B}$ magnetodynamic formulation of the Maxwell system with skin and proximity effects'. In: *Applicable Analysis* (2021). DOI: 10.1080/00036811.2020.1836351. URL: https://hal.archives-ouvertes.fr/hal-03122785.

[25]   T. Gallouët, Q. Merigot and A. Natale. 'Convergence of a Lagrangian discretization for barotropic fluids and porous media flow'. In: *SIAM Journal on Mathematical Analysis* (2021). URL: https://hal.archives-ouvertes.fr/hal-03234144.

[26]   M. Goldman and B. Merlet. 'Non-convex functionals penalizing simultaneous oscillations along independent directions: rigidity estimates'. In: *Annali della Scuola Normale Superiore di Pisa, Classe di Scienze*. Annali della Scuola Normale Superiore di Pisa. Classe di Scienze. Serie V 22.3 (2021), pp. 1473–1509. DOI: 10.2422/2036-2145.201906_006. URL: https://hal.archives-ouvertes.fr/hal-02132896.

[27]   S. Lemaire. 'Bridging the Hybrid High-Order and Virtual Element methods'. In: *IMA Journal of Numerical Analysis* 41.1 (2021), pp. 549–593. DOI: 10.1093/imanum/drz056. URL: https://hal.archives-ouvertes.fr/hal-01902962.

[28]   B. Merlet and M. Pegon. 'Large mass rigidity for a liquid drop model in 2D with kernels of finite moments'. In: *Journal de l'École polytechnique — Mathématiques* (12th Nov. 2021). URL: https://hal.archives-ouvertes.fr/hal-03181775.

[29]   A. Natale and G. Todeschi. 'Computation of optimal transport with finite volumes'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.5 (Sept. 2021), pp. 1847–1871. DOI: 10.1051/m2an/2021041. URL: https://hal.archives-ouvertes.fr/hal-03348217.

[30]   L. Pareschi and T. Rey. 'On the stability of equilibrium preserving spectral methods for the homogeneous Boltzmann equation'. In: *Applied Mathematics Letters* 120 (Nov. 2021), p. 107187. URL: https://hal.archives-ouvertes.fr/hal-03000138.

[31]   M. Pegon. 'Large mass minimizers for isoperimetric problems with integrable nonlocal potentials'. In: *Nonlinear Analysis: Theory, Methods and Applications* 211 (31st Oct. 2021). URL: https://hal.archives-ouvertes.fr/hal-02496313.

Conferences without proceedings

[32] T. Chaumont-Frelet, A. Ern, S. Lemaire and F. Valentin. 'Bridging the multiscale hybrid-mixed and multiscale hybrid high-order methods'. In: GS21 - SIAM Conference on Mathematical and Computational Issues in the Geosciences. Milan / Virtual, Italy, 21st June 2021. URL: https://hal.inria.fr/hal-03403903.

[33] T. Chaumont-Frelet, A. Ern, S. Lemaire and F. Valentin. 'Bridging the multiscale hybrid-mixed and multiscale hybrid high-order methods'. In: ICOSAHOM 2020 - International Conference on Spectral and High-Order Methods. Vienna / Virtual, Austria, 12th July 2021. URL: https://hal.inria.fr/hal-03403920.

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