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Université de Lille

Activity Report 2019

Project-Team RAPSODI

Reliable numerical approximations of dissipative systems.

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

RESEARCH CENTER
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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:

1. 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.);
2. provide accurate numerical approximations at a reasonable computational cost (and ultimately maximize the accuracy at a fixed computational effort);
3. robustness with respect to physical conditions: the computational cost for a given accuracy should be essentially insensitive to 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) [71], low-frequency electromagnetism [88], and mechanics of complex inhomogeneous fluids arising in avalanches [82] or in porous media [73].

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 apart, but combining them still leads to unsolved problems of crucial interest.

Let us mention for example the review paper by J. Droniou [98], 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 [98]. The first convergence proof for a positivity preserving and entropy diminishing method designed to approximate transient dissipative equation on general meshes was proposed very recently in [83]. The idea and the techniques introduced in [83] should be extended to practical applications.

In systems of PDEs, the values of physical parameters often change the qualitative behavior of the solution. 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 [107], are powerful tools as they permit 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 [79] for the drift-diffusion system, and based on the control of the numerical dissipation of entropy, to other dissipative systems in order 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 mixtures models. The team already developed such schemes for the variable density Navier–Stokes system [81] or [82]. 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 computation will have to be considered, in particular with the development of some *a posteriori* error estimators. Impressive progresses have been achieved in this field [94], 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 [90], the dead-oil model for porous media flows [84] or the Maxwell equations in their quasi-static approximation for some eddy current problems [88] and [89]. We aim to develop new *a posteriori* estimators for other dissipative systems, like fluid mixtures 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 numerical 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, the numerical methods dedicated to degenerate parabolic problems that the mathematicians are able to analyze almost all 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 & C. Guichard [83], [4] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness w.r.t. physical parameters,...).

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 [98] for an extensive 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 [85], [110]).

Recently, C. Chainais-Hillairet and co-authors [79], [86] and [87] 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 characteristic parameters, or in the long-time asymptotic. 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...) are required in [79], [86] and [87]. The schemes proposed in [83] and [4] 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* [83] with the methodology of [79], [86], [87] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would be also 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-M` software 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 [109] as a limiting 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 propose also 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 [83] 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) [99].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. 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 yield reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [111], [106], with high-order accuracy [66], [65], or for parabolic problems [63], [64] 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 Babuska and Rheinboldt more than thirty years ago [70], *a posteriori* error estimators have been widely studied. We will take advantage of the huge corresponding bibliography 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. [88] and [89]) 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 [81], [82] we developed combines features from Finite Elements and Finite Volumes. Fortunately, we do not start from scratch. Some recent references are devoted to the unsteady Navier–Stokes model in the Finite Element context [77], [114]. In the Finite Volume context, recent references deal with unsteady convection-diffusion equations [113], [68], [96] and [84]. 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 of punctual individuals (N) which interact pairwise which means $N(N-1)/2$ 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, swarming of fishes) or in the description of crowd motions. Building on the special structure of convolution-type of the interactions, the team develops computation methods based on the Non Uniform Fast Fourier Transform [102]. 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 resource management, nuclear waste repository management, or carbon dioxyde sequestration. We refer to [73], [72] 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 non-conformal 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 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 [67]) as the modeling of corrosion in an underground repository (DPCM model developed by Bataillon *et al.* [71]) 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 some 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 can not 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.

Kinetic theory of molecular gases models a gas as a system of elastically colliding spheres, conserving mechanical energy during impact. Once initialized, it takes a molecular gas not more than 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.

The 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 the 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 non-locality 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 knowledge 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 quote 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 non-destructive 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 as reliable as possible.

5. Highlights of the Year

5.1. Highlights of the Year

In 2019, RAPSODI members have been the laureates of several calls for projects.

- T. Rey has been awarded an ERC Generator grant (116 545 euros) from I-SITE Université Lille - Nord Europe for his project MANAKINEQO (R-ERCGEN-19-007-REY). Upon the next two years, T. Rey aims at investigating mathematical properties, as well as developing efficient numerical schemes, for multiscale collisional kinetic equations of the Boltzmann type. A 20-months post-doc will be funded using this grant, as well as an international conference. Following this ERC Generator grant, T. Rey will apply for an ERC Consolidator grant.
- S. Lemaire is the PI of the ADT project ParaSkel++, which is one of the funded Actions of Technological Development of the Inria Lille - Nord Europe 2019 campaign. The aim of the project is to develop an optimized C++ platform for the arbitrary-order numerical approximation of PDEs by skeletal methods on general 2D/3D meshes, with a particular emphasis on the implementation of HPC facilities. L. Beaude has been hired as a development engineer for this project. She will start in February 2020.
- C. Cancès, C. Chainais-Hillairet and B. Merlet are involved in the H2020 project EURAD (EUropean Joint Programme on RADioactive Waste Management). The aim of their project inside EURAD is to establish an energetic formulation of the Diffusion Poisson Coupled Model leading to new large-time robust numerical methods for the simulation of the corrosion processes in an underground repository. C. Cancès is the leader of the task "Numerical methods for high-performance computing of coupled processes" within the EURAD project.

One can also mention the obtention by T. Rey of a Young Researcher PEPS grant from CNRS's INSMI (3 500 euros, from March to November 2019). The granted project aimed at investigating high-order (in time and velocity) numerical methods for approximating the solutions to the granular gases equation.

6. New Software and Platforms

6.1. Platforms

6.1.1. Platform NS2DDV-M

NS2DDV-M [42] is a Matlab code, developed by C. Calgaro, E. Creusé, and A. Mouton (CNRS research engineer at Université de Lille), for the simulation of homogeneous and inhomogeneous fluid flows by a combined Finite Volume-Finite Element method. The code embeds parallel computation facilities, and is freely distributed, to allow for easy comparisons with concurrent codes on benchmark test-cases, and to promote new collaborations in the domain.

6.1.2. Platform KinDiff

`KinDiff` consists in a Python library and a Jupyter Notebook. It has been developed by M. Bessemoulin-Chatard (CNRS and Université de Nantes), M. Herda, and T. Rey. The `KinDiff` code approximates the solutions to the kinetic Fokker–Planck and linear BGK equations in a unidimensional periodic domain in space and a symmetric bounded unidimensional domain in velocity. Its outputs are the discretization of the distribution function in the phase space as well as the moments, along with some visualizations of these quantities. Kinetic equations display asymptotic behaviors such as return to equilibrium in large time, or convergence towards macroscopic equations in the diffusive limit. The finite volume method implemented within `KinDiff` reproduces these asymptotics at the discrete level. The presentation and numerical analysis of the scheme is available in the article [17]. The code is available at gitlab.com/thoma.rey/FV_HipoDiff.

7. New Results

7.1. Modeling and numerical simulation of complex fluids

In [38], N. Peton, C. Cancès *et al.* propose a new water flow driven forward stratigraphic model. Stratigraphy is a discipline of physics that aims at predicting the geological composition of the subsoil. The model enjoys the following particularities. First, the water surface flow is modelled at the continuous level, in opposition to what is currently done in this community. Second, the model incorporates a constraint on the erosion rate. A stable numerical scheme is proposed to simulate the model.

In [14], A. Ait Hammou Oulhaj and D. Maltese adapt the (positive) nonlinear Control Volume Finite Element scheme of [83] to the simulation of seawater intrusion in the subsoil nearby coastal regions. The proposed scheme is convergent even if the porous medium is anisotropic.

In [25], [41], C. Cancès *et al.* study an original model of degenerate Cahn–Hilliard type. Similarly to the classical degenerate Cahn–Hilliard model, the model can be interpreted as the gradient flow of a Ginzburg–Landau type energy, but the geometry considered here allows for more flexibility and the system thus dissipates faster than the usual degenerate Cahn–Hilliard system. Numerical evidences of this fact are given. Then, the existence of a solution to the model is established thanks to the convergence of a minimizing movement scheme.

In [19], I. Lacroix-Violet *et al.* generalize to the Navier–Stokes–Korteweg (with density-dependent viscosities satisfying the BD relation) and Euler–Korteweg systems a recent relative entropy proposed in [80]. As a concrete application, this helps justifying mathematically the convergence between global weak solutions of the quantum Navier–Stokes system and dissipative solutions of the quantum Euler system when the viscosity coefficient tends to zero. The results are based on the fact that Euler–Korteweg systems and corresponding Navier–Stokes–Korteweg systems can be reformulated through an augmented system. As a by-product of the analysis, I. Lacroix-Violet *et al.* show that this augmented formulation helps to define relative entropy estimates for the Euler–Korteweg systems in a simpler way and with less hypotheses compared to recent works [97], [100].

In [22], C. Calgaro, C. Colin, E. Creusé *et al.* investigate a specific low-Mach model for which the dynamic viscosity of the fluid is a specific function of the density. The model is reformulated in terms of the temperature and velocity, with nonlinear temperature equation, and strong solutions are considered. In addition to a local-in-time existence result for strong solutions, some convergence rates of the error between the approximation and the exact solution are obtained, following the same approach as Guillén-González *et al.* [103], [104].

In [21], C. Calgaro, C. Colin, and E. Creusé derive a combined Finite Volume-Finite Element scheme for a low-Mach model, in which a temperature field obeying an energy law is taken into account. The continuity equation is solved, whereas the state equation linking temperature, density, and thermodynamic pressure is imposed implicitly. Since the velocity field is not divergence-free, the projection method solving the momentum equation has to be adapted. This combined scheme preserves some steady-states, and ensures a discrete maximum principle on the density. Numerical results are provided and compared to other approaches

using purely Finite Element schemes, on a benchmark consisting in particular in a transient injection flow [74], [101], [69], as well as in the natural convection of a flow in a cavity [108], [105], [101], [69].

In [20], C. Calgaro, C. Colin, and E. Creusé propose a combined Finite Volume-Finite Element scheme for the solution of a specific low-Mach model expressed in the velocity, pressure and temperature variables. The dynamic viscosity of the fluid is given by an explicit function of the temperature, leading to the presence of a so-called Joule term in the mass conservation equation. First, they prove a discrete maximum principle for the temperature. Second, the numerical fluxes defined for the Finite Volume computation of the temperature are efficiently derived from the discrete Finite Element velocity field obtained by the solution of the momentum equation. Several numerical tests are presented to illustrate the theoretical results and to underline the efficiency of the scheme in terms of convergence rates.

In [46], C. Calgaro and E. Creusé introduce a Finite Volume method to approximate the solution of a convection-diffusion equation involving a Joule term. They propose a way to discretize this so-called "Joule effect" term in a consistent manner with respect to the nonlinear diffusion one, in order to ensure some maximum principle properties on the solution. They investigate the numerical behavior of the scheme on two original benchmarks.

7.2. Numerical simulation in low-frequency electromagnetism

In [32], [31], E. Creusé *et al.* investigate the behavior of some Finite Element error estimators in the context of low-frequency elecromagnetism simulations, to underline the main differences in some practical situations. A more theoretical contribution is also developed to prove the equivalence of some usual discrete gauge conditions. Once again, their numerical behaviors are compared on some characteristic benchmarks.

In [58], F. Chave, S. Lemaire *et al.* introduce a three-dimensional Hybrid High-Order (HHO) method for magnetostatic problems. The proposed method is easy to implement, supports general polyhedral meshes, and allows for arbitrary orders of approximation.

7.3. Structure-preserving numerical methods

In [54], 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 [55], C. Chainais-Hillairet and M. Herda apply an iterative energy method à la de Giorgi in order to establish L^∞ bounds for numerical solutions of noncoercive convection-diffusion equations with mixed Dirichlet-Neumann boundary conditions.

In [23], C. Cancès, C. Chainais-Hillairet *et al.* study a finite volume scheme for a degenerate cross-diffusion system describing the ion transport through biological membranes. The strongly coupled equations for the ion concentrations include drift terms involving the electric potential, which is coupled to the concentrations through the Poisson equation. The finite volume scheme is based on two-point flux approximations with "double" upwind mobilities. The existence of solutions to the fully discrete scheme is proven. When the particles are not distinguishable and the dynamics is driven by cross-diffusion only, it is shown that the scheme preserves the structure of the equations like nonnegativity, upper bounds, and entropy dissipation.

In [51], C. Cancès and B. Gaudeul propose a two-point flux approximation finite volume scheme for the approximation of the solutions to an entropy dissipative cross-diffusion system. The scheme is shown to preserve several key properties of the continuous system, among which positivity and decay of the entropy. Numerical experiments illustrate the behavior of the scheme.

In [48], 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 [24], C. Cancès *et al.* compare energy-stable finite volume schemes for multiphase flows in porous media with schemes based on the Wasserstein gradient flow structure of the equations, that has recently been highlighted in [3]. The model is approximated by means of the minimizing movement (or JKO) scheme, that C. Cancès *et al.* solve thanks to the ALG2-JKO scheme proposed in [76].

In [50], C. Cancès *et al.* propose a variational finite volume scheme for the computation of Wasserstein gradient flows. The discrete solution is the minimizer of a discrete action, keeping track at the discrete level of the optimal character of the gradient flow. The spatial discretization relies on upstream mobility fluxes, while an implicit linearization of the Wasserstein distance is used in order to reduce the computational cost by avoiding an inner time-stepping as in the related contributions of the literature.

In [61], T. Rey *et al.* present a new finite volume method for computing numerical approximations of a system of nonlocal transport equations modeling interacting species. In this work, the nonlocal continuity equations are treated as conservative transport equations with a nonlocal, nonlinear, rough velocity field. Some properties of the method are analyzed, and numerical simulations are performed.

In [15], I. Lacroix-Violet *et al.* are interested in 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 [78] 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 [36], S. Lemaire builds a bridge between the Hybrid High-Order [93] and Virtual Element [75] methods, which are the two main new-generation approaches to the arbitrary-order approximation of PDEs on meshes with general, polytopal cells. The Virtual Element method writes in functional terms and is naturally conforming; at the opposite, the Hybrid High-Order method writes in algebraic terms and is naturally nonconforming. It has been remarked a few years ago that the Hybrid High-Order method can be viewed as a nonconforming version of the Virtual Element method. Here, S. Lemaire ends up unifying the Hybrid High-Order and Virtual Element approaches by showing that the Virtual Element method can be reformulated as a (newborn) conforming Hybrid High-Order method. This parallel has interesting consequences as it sheds new light on the *a priori* analysis of Virtual Element methods, and on the differences between the conforming and nonconforming cases.

In [30], [40], S. Lemaire *et al.* design and analyze (in the periodic setting) arbitrary-order nonconforming multiscale methods for highly oscillatory elliptic problems, which are applicable on coarse grids that may feature general polytopal cells. The construction of these methods is based on the Hybrid High-Order framework [93]. As standard with such multiscale approaches, the general workflow of the method splits into an offline, massively parallelizable stage where all fine-scale computations are performed, and the online, fully coarse-scale stage.

In [52], C. Cancès and D. Maltese 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.

In [57], F. Chave proposes a new definition of the normal fracture diffusion-dispersion coefficient for a reduced model of passive transport in fractured porous media, and numerically studies the impact on the discrete solution on a few test-cases.

In [37], T. Rey *et al.* present high-order, fully explicit time integrators for nonlinear collisional kinetic equations, including the full Boltzmann equation. The methods, called projective integration, first take a few small steps with a simple, explicit method (forward Euler) to damp out the stiff components of the solution. Then, the time derivative is estimated and used in a Runge–Kutta method of arbitrary order. The procedure can be recursively repeated on a hierarchy of projective levels to construct telescopic projective integration methods. The method is illustrated with numerical results in one and two space dimensions.

In [60], I. Lacroix-Violet *et al.* 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.

7.5. Asymptotic analysis

In [18], C. Cancès *et al.* derive the porous medium equation as the hydrodynamic limit of an interacting particle system which belongs to the family of exclusion processes, with nearest neighbor exchanges. The particles follow a degenerate dynamics, in the sense that the jump rates can vanish for certain configurations, and there exist blocked configurations that cannot evolve. Our approach, which is based on the relative entropy method, is tailored to deal with vanishing initial densities.

In [13], A. Ait Hammou Oulhaj, C. Cancès, C. Chainais-Hillairet *et al.* study the large-time behavior of the solutions to a two-phase extension of the porous media equation, which models the seawater intrusion problem. Their goal is to identify the self-similar solutions that correspond to steady-states of a rescaled version of the problem. They fully characterize the unique steady-states that are identified as minimizers of a convex energy and shown to be radially symmetric. Moreover, they prove the convergence of the solution to the time-dependent model towards the unique stationary state as time goes to infinity. They also provide numerical illustrations of the stationary states and exhibit numerical convergence rates.

In [16], C. Chainais-Hillairet *et al.* propose a new proof of existence of a solution to the scheme introduced in [1] for drift-diffusion systems, which does not require any assumption on the time step. The result relies on the application of a topological degree argument which is based on the positivity and on uniform-in-time upper bounds of the approximate densities. They also establish uniform-in-time lower bounds satisfied by the approximate densities. These uniform-in-time upper and lower bounds ensure the exponential decay of the scheme towards the thermal equilibrium as shown in [1].

In [26], C. Chainais-Hillairet and M. Herda study the large-time behavior of the solutions to Finite Volume discretizations of convection-diffusion equations or systems endowed with non-homogeneous Dirichlet and Neumann type boundary conditions. Their results concern various linear and nonlinear models such as Fokker–Planck equations, porous media equations, or drift-diffusion systems for semiconductors. For all of these models, some relative entropy principle is satisfied and implies exponential decay to the stationary state. They show that in the framework of Finite Volume schemes on orthogonal meshes, a large class of two-point monotone fluxes preserve this exponential decay of the discrete solution to the discrete steady-state of the scheme.

In [49], C. Cancès, C. Chainais-Hillairet, M. Herda *et al.* analyze the large-time behavior of a family of nonlinear finite volume schemes for anisotropic convection-diffusion equations set in a bounded bidimensional domain and endowed with either Dirichlet and/or no-flux boundary conditions. They show that the solutions to the two-point flux approximation (TPFA) and discrete duality finite volume (DDFV) schemes under consideration converge exponentially fast toward their steady-state. The analysis relies on discrete entropy estimates and discrete functional inequalities. As a by-product of their analysis, they establish new discrete Poincaré–Wirtinger, Beckner and logarithmic Sobolev inequalities. Their theoretical results are illustrated by numerical simulations.

In [56], C. Chainais-Hillairet *et al.* introduce a nonlinear DDFV scheme for an anisotropic linear convection-diffusion equation with mixed boundary conditions and establish the exponential decay of the scheme towards its steady-state.

In [39], A. Zurek studies the large-time regime of the moving interface appearing in a concrete carbonation model. He proves that the approximate free boundary, given by an implicit-in-time Finite Volume scheme, propagates in time following a $\sqrt{t}$-law. This result is illustrated by numerical experiments.

In [17], M. Herda, T. Rey *et al.* are interested in the asymptotic analysis of a Finite Volume scheme for one-dimensional linear kinetic equations, with either Fokker–Planck or linearized BGK collision operator. Thanks to appropriate uniform estimates, they establish that the proposed scheme is asymptotic-preserving in the diffusive limit. Moreover, they adapt to the discrete framework the hypocoercivity method proposed in [95] to prove the exponential return to equilibrium of the approximate solution. They obtain decay estimates that are uniform in the diffusive limit. Finally, they present an efficient implementation of the proposed numerical schemes, and perform numerous numerical simulations assessing their accuracy and efficiency in capturing the correct asymptotic behaviors of the models.

In [44], M. Herda *et al.* are interested in the large-time behavior of linear kinetic equations with heavy-tailed local equilibria. Their main contribution concerns the kinetic Lévy–Fokker–Planck equation, for which they adapt hypocoercivity techniques in order to show that solutions converge exponentially fast to the global equilibrium. Compared to the classical kinetic Fokker–Planck equation, the issues here concern the lack of symmetry of the non-local Lévy–Fokker–Planck operator and the understanding of its regularization properties. As a complementary related result, they also treat the case of the heavy-tailed BGK equation.

In [35], M. Herda *et al.* consider various sets of Vlasov–Fokker–Planck equations modeling the dynamics of charged particles in a plasma under the effect of a strong magnetic field. For each of them, in a regime where the strength of the magnetic field is effectively stronger than that of collisions, they first formally derive asymptotically reduced models. In this regime, strong anisotropic phenomena occur; while equilibrium along magnetic field lines is asymptotically reached, the asymptotic models capture a nontrivial dynamics in the perpendicular directions. They do check that in any case the obtained asymptotic model defines a well-posed dynamical system and when self-consistent electric fields are neglected they provide a rigorous mathematical justification of the formally derived systems. In this last step they provide a complete control on solutions by developing anisotropic hypocoercive estimates.

In [45], T. Rey *et al.* propose a new mathematical model intended to describe dynamically the evolution of knowledge in structured societies of interacting individuals. This process, termed cumulative culture, has been extensively studied by evolutionary anthropologists, both theoretically and experimentally. Some of the mathematical properties of the new model are analyzed, and exponential convergence towards a global equilibrium is shown for a simplified model. A numerical method is finally proposed to simulate the complete model.

In [43], 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.

7.6. Applied calculus of variations

In [34], B. Merlet *et al.* study a variational problem which models the behavior of topological singularities on the surface of a biological membrane in P_β-phase (see [112]). The problem combines features of the Ginzburg–Landau model in 2D and of the Mumford–Shah functional. As in the classical Ginzburg–Landau theory, a prescribed number of point vortices appear in the moderate energy regime; the model allows for discontinuities, and the energy penalizes their length. The novel phenomenon here is that the vortices have

a fractional degree $1/m$ with m prescribed. Those vortices must be connected by line discontinuities to form clusters of total integer degrees. The vortices and line discontinuities are therefore coupled through a topological constraint. As in the Ginzburg–Landau model, the energy is parameterized by a small length scale $\varepsilon > 0$. B. Merlet *et al.* perform a complete Γ-convergence analysis of the model as $\varepsilon \downarrow 0$ in the moderate energy regime. Then, they study the structure of minimizers of the limit problem. In particular, the line discontinuities of a minimizer solve a variant of the Steiner problem.

In [27], B. Merlet *et al.* consider the branched transportation problem in 2D associated with a cost per unit length of the form $1 + \beta\theta$ where θ denotes the amount of transported mass and $\beta > 0$ is a fixed parameter (notice that the limit case $\beta = 0$ corresponds to the classical Steiner problem). Motivated by the numerical approximation of this problem, they introduce a family of functionals $(\{\mathcal{F}_\varepsilon\}_{\varepsilon>0})$ which approximate the above branched transport energy. They justify rigorously the approximation by establishing the equicoercivity and the Γ-convergence of $\{\mathcal{F}_\varepsilon\}$ as $\varepsilon \downarrow 0$. The functionals are modeled on the Ambrosio–Tortorelli functional and are easy to optimize in practice. Numerical evidences of the efficiency of the method are presented.

In [28], 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 [29].

In [29], B. Merlet *et al.* consider a generalization of branched transportation in arbitrary dimension and codimension: minimize the h-mass of some oriented k-dimensional branched surface in $\mathbf{R}^n$ with some prescribed boundary. Attached to the surface is a multiplicity $m(x)$ which is not necessarily an integer and is a conserved quantity (Kirchhoff current law is satisfied at branched points). The h-mass is defined as the integral of a cost $h(|m(x)|)$ over the branched surface. As usual in branched transportation, the cost function is a lower-semicontious, sublinear increasing function with $h(0) = 0$ (for instance $h(m) = \sqrt{1 + am^2}$ if $m \neq 0$ and $h(0) = 0$). For numerical purpose, it is convenient to approximate the measure defined by the k-dimensional surfaces by smooth functions in $\mathbf{R}^n$. In this spirit, B. Merlet *et al.* propose phase field approximations of the branched surfaces and of their energy in the spirit of the Ambrosio–Tortorelli functional. The convergence of these approximations towards the original k-dimensional branched transportation problem is established in the sense of Γ-convergence. Next, considering the cost $h(m) = \sqrt{1 + am^2}$ and sending a to 0, a phase field approximation of the Plateau problem is obtained. Numerical experiments show the efficiency of the method. These numerical results are exceptional as they are obtained without any guess on the topology of the minimizing k-surface (as opposed to methods based on parameterizations of the k-surface).

In [33], [62], B. Merlet *et al.* 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 we consider vanishes if u is of the form $u(x_1)$ or $u(x_2)$. We prove the converse property and related quantitative results. In particular, we 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.

7.7. Approximation theory

In [59], M. Herda *et al.* propose an iterative algorithm for the numerical computation of sums of squares of polynomials approximating given data at prescribed interpolation points. The method is based on the definition of a convex functional G arising from the dualization of a quadratic regression over the Cholesky factors of the sum of squares decomposition. In order to justify the construction, the domain of G, the boundary of the domain and the behavior at infinity are analyzed in details. When the data interpolate a positive univariate polynomial, we show that in the context of the Lukacs sum of squares representation, G is coercive and strictly convex which yields a unique critical point and a corresponding decomposition in sum of squares. For multivariate polynomials which admit a decomposition in sum of squares and up to a small perturbation of

size ε, G^ε is always coercive and so its minimum yields an approximate decomposition in sum of squares. Various unconstrained descent algorithms are proposed to minimize G. Numerical examples are provided, for univariate and bivariate polynomials.

In [47], M. Herda *et al.* investigate the numerical approximation of bounded functions by polynomials satisfying the same bounds. The contribution makes use of the recent algebraic characterization found in [91] and [92] where an interpretation of monovariate polynomials with two bounds is provided in terms of a quaternion algebra and the Euler four-squares formulas. Thanks to this structure, the authors generate a new nonlinear projection algorithm onto the set of polynomials with two bounds. The numerical analysis of the method provides theoretical error estimates showing stability and continuity of the projection. Some numerical tests illustrate this novel algorithm for constrained polynomial approximation.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

A new contractual collaboration between C. Cancès and IFPEN corresponding to the supervision of the PhD thesis of S. Bassetto started in January 2019. This contract is part of the Inria-IFPEN framework agreement.

8.2. Bilateral Grants with Industry

C. Bataillon (CEA) and L. Trenty (ANDRA) are involved in the `EURAD` project on corrosion modeling together with C. Cancès, C. Chainais-Hillairet, and B. Merlet. More details in Section 9.3.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. ERC Generator

T. Rey has been awarded an ERC Generator grant (116 545 euros) from I-SITE Université Lille - Nord Europe for his project `MANAKINEQO` (R-ERCGEN-19-007-REY). In the next two years, T. Rey aims at investigating mathematical properties, as well as developing efficient numerical schemes, for multiscale collisional kinetic equations of the Boltzmann type. A 20-months post-doc will be funded using this grant, as well as an international conference. Following this ERC Generator grant, T. Rey will apply for an ERC Consolidator grant.

9.1.2. Actions of Technological Development (ADT)

S. Lemaire is the PI of the ADT project `ParaSkel++`, which is one of the funded ADT of the Inria Lille - Nord Europe 2019 campaign. The aim of the project is to develop an optimized C++ platform for the arbitrary-order numerical approximation of PDEs by skeletal methods on general 2D/3D meshes, with a particular emphasis on the implementation of HPC facilities. L. Beaude has been hired as a development engineer for this project. She will start in February 2020.

In the same vein, T. Rey is part of the ADT project `SIMPAPH` led by the MEPHYSTO-POST team, that has as well been funded as a result of the Inria Lille - Nord Europe 2019 campaign. The aim is to develop robust numerical methods to solve large systems of stochastic differential equations describing (among others) particles in an optic fiber, schools of fish, or microscopic particles. The expected code will attempt to solve these multiscale problems using different approaches, and to be versatile enough to act as an industrial benchmark. A. Roget has been hired as a development engineer for this project.

9.2. National Initiatives

9.2.1. ANR

C. Chainais-Hillairet has been a member of the ANR MOONRISE project. The MOONRISE project aimed at exploring modeling, mathematical, and numerical issues originating from the presence of high oscillations in nonlinear PDEs mainly from the physics of nanotechnologies and from the physics of plasmas.

Title: MOdels, Oscillations, and NumeRIcal SchEmes

Type: Fondements du numérique (DS0705) - 2014

ANR reference: ANR-14-CE23-0007

Coordinator: F. Méhats (Université de Rennes 1)

Duration: October 2014 - June 2019

C. Chainais-Hillairet and T. Rey are members of the ANR MOHYCON project. The MOHYCON 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: Société de l'information et de la communication (DS07) - 2017

ANR reference: ANR-17-CE40-0027

Coordinator: M. Bessemoulin-Chatard (CNRS and Université de Nantes)

Duration: January 2018 - December 2020

C. Cancès is a member of the ANR COMODO project. The COMODO project focuses on the mathematical and numerical study of cross-diffusion systems in moving domains. The targeted application is the simulation of the building of solar plants by the vapour deposition process.

Title: CrOss-diffusion equations in MOving DOmains

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

ANR reference: ANR-19-CE46-0002

Coordinator: V. Ehrlacher (École des Ponts ParisTech and Inria Paris)

Duration: January 2020 - December 2023

M. Herda is a member of the ANR JCJC MICMOV project. The MICMOV 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

Coordinator: M. Simon (Inria Lille - Nord Europe)

9.2.2. LabEx CEMPI

Title: Centre Européen pour les Mathématiques, la Physique et leurs Interactions

Coordinator: S. De Bièvre (LPP, Université de Lille)

Duration: January 2012 - December 2019, extended in 2019

Partners: Laboratoire Paul Painlevé (LPP) and Laser Physics department (PhLAM), Université de Lille

The "Laboratoire d'Excellence" Centre Européen pour les Mathématiques, la Physique et leurs Interactions (CEMPI), 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.

One of the three focus areas of CEMPI research is the interface between mathematics and physics. This focus area encompasses three themes. The first is concerned with key problems of a mathematical, physical and technological nature coming from the study of complex behavior in cold atoms physics and nonlinear optics, in particular fiber optics. The two other themes deal 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.

9.2.3. PEPS

T. Rey has been the laureate in 2019 of a Young Researcher PEPS grant from CNRS's INSMI (3 500 euros, from March to November 2019). The granted project aimed at investigating high-order (in time and velocity) numerical methods for approximating the solutions to the granular gases equation.

9.3. European Initiatives

C. Cancès, C. Chainais-Hillairet and B. Merlet are involved in the H2020 project EURAD (EUropean Joint Programme on RADioactive Waste Management). The aim of their project inside EURAD is to establish an energetic formulation of the Diffusion Poisson Coupled Model leading to new large-time robust numerical methods for the simulation of the corrosion processes in an underground repository.

C. Cancès is the leader of the task "Numerical methods for high-performance computing of coupled processes" within the EURAD project.

9.4. International Initiatives

C. Cancès is a member of the Indo-French Center for Applied Mathematics (IFCAM) project "Conservation laws: BV^s, control, interfaces" (PIs: S. Ghoshal, TIFR Centre For Applicable Mathematics, India and S. Junca, Université de Nice).

9.5. International Research Visitors

9.5.1. Visits of International Scientists

In January-February, E. Daus (TU Vienna, Austria) visited C. Cancès and C. Chainais-Hillairet during two weeks.

In 2019, RAPSODI members also invited several researchers for short visits (a week or less) in Lille.

- R. Bailo (Imperial College London, UK) came in November to work with T. Rey (funded by his Young Researcher PEPS grant).
- R. V. Sabariego (KU Leuven, Electrical Engineering ESAT/Electa, EnergyVille, Belgium) came in May to work with E. Creusé.
- E. Bretin and S. Masnou (Institut Camille Jordan, Lyon) and M. Goldman (CNRS and LJLL/Université Paris Diderot) came in June and December to work with B. Merlet.
- A. Trescases (CNRS and Institut de Mathématiques de Toulouse) came in September to work with M. Herda.
- C. Bataillon (CEA), V. Ehrlacher (École des Ponts ParisTech and Inria Paris) and C. Perrin (CNRS and Université d'Aix-Marseille) came to work with C. Cancès.
- M. Cassier (CNRS and Institut Fresnel, Marseille) came in February-March to work with S. Lemaire.

On a slightly different note, from March to October, G. Robillard has been an AIRLab resident (Artiste en Immersion Recherche dans un Laboratoire) in order to work with C. Calgaro and E. Creusé (with a support from the Communauté d'Universités et d'Établissements Lille Nord-de-France).

9.5.2. Visits to International Teams

B. Gaudeul spent two weeks in WIAS Berlin, Germany in November in order to work with J. Fuhrmann on the extension of the results obtained in [48] to Nernst–Planck–Poisson systems with ion size and solvation effects.

M. Herda spent one week at Imperial College London, UK in February to work with P. Degond on a Fokker–Planck approach to the study of robustness in gene expression.

T. Rey visited 3 times J. A. Carrillo and J. Hu at Imperial College London, UK between February and March, for 3 days long stays funded by his Young Researcher PEPS grant, to work (in particular) on the development of a new high-order numerical method for solving the granular gases equation.

C. Cancès and B. Merlet spent one week at the University of Lisbon, Portugal in December to work with L. Monsaingeon.

C. Cancès spent one week at Université de Tours to work with B. Andreianov.

B. Merlet visited E. Bretin and S. Masnou at Institut Camille Jordan in Lyon in February, and visited several times M. Goldman at LJLL/Université Paris Diderot in March, May, October, and November.

F. Chave and S. Lemaire spent 3 days at Université de Montpellier in September to work with D. A. Di Pietro on arbitrary-order polytopal methods for electromagnetism.

9.5.3. Research Stays Abroad

M. Herda was in residence at the Hausdorff Research Institute for Mathematics (University of Bonn, Germany) from May 19 to July 7 in the framework of the Junior Trimester Program in Kinetic Theory, that gave young mathematicians the opportunity to carry out collaborative research in kinetic theory. M. Herda was part of a project in collaboration with N. Ayi (Sorbonne Université), M. Breden (École Polytechnique), J. Guerand (University of Cambridge, UK), H. Hivert (Centrale Lyon), and I. Tristani (ENS Paris) on the study of a fractional kinetic Fokker–Planck equation. This collaboration has already led to the article [44], and a second article is in preparation. A collaboration was also initiated with M. Breden and A. Trescases (CNRS and Institut de Mathématiques de Toulouse) on the derivation of cross-diffusion systems from kinetic models.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

M. Herda co-organized the yearly Journée de la Fédération de Recherche Mathématique du Nord-Pas-de-Calais which took place on October 15 in Lille. This one-day conference brought together all the maths research laboratories from the Hauts-de-France region and gave the opportunity to new permanent members to present their research.

E. Creusé was part of the organizing committee of the first Rencontres Mathématiques Valenciennoises, that were held on March 13. This meeting was organized for maths students at Université Polytechnique Hauts-de-France as well as for high-school students of Lycée Wallon in Valenciennes. Several researchers presented some applications of mathematics in industry as well as in academic research. This meeting gathered around 500 participants.

T. Rey organized the yearly ANEDP team day at Laboratoire Paul Painlevé on December 17.

C. Cancès and T. Rey co-organized mini-symposia on, respectively, (i) cross-diffusion systems and (ii) novel time discretization methods and moment models for kinetic equations at ICIAM 2019 in Valencia. S. Lemaire co-organized a mini-symposium on polytopal methods at MAFELAP 2019 in Brunel University, London.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

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

10.1.2.2. Reviewer - Reviewing Activities

RAPSODI team members are regular reviewers for all the main international journals in numerical analysis/scientific computing and PDEs.

10.1.3. Invited Talks

C. Calgaro was one of the speakers of the seventh Amarena Days held in Amiens.

C. Cancès was invited to give a talk in Paris during the closure workshop of the MANON common laboratory (CEA Saclay / LJLL Sorbonne Université). He was also invited to give a talk in Kalvåg (Norway) during the workshop Analysis and Computation of Coupled Systems. He finally gave seminars in Compiègne and at the University of Lisbon.

C. Chainais-Hillairet was an invited plenary speaker at the POEMs conference held at CIRM in Marseille, and for the Journées Corrosion `MaNu` 2019 held in Orsay. She also gave a talk at ENUMATH 2019 that was held in Egmond aan Zee. She finally gave seminars in Nice, Orsay and Paris (Laboratoire Jacques-Louis Lions), as well as a talk for the ANEDP team day.

F. Chave was an invited speaker in ENUMATH 2019 that was held in Egmond aan Zee. He also presented a poster at the POEMs conference held at CIRM in Marseille. He finally gave a seminar for the ANEDP team at Laboratoire Paul Painlevé.

B. Gaudeul was an invited speaker of the Journées Corrosion `MaNu` 2019 held in Orsay. He also presented a poster at the conference Numerical Methods for Multiscale Models arising in Physics and Biology held in Nantes. He finally gave a seminar at WIAS Berlin, as well as a talk for the PhD students seminar in Lille.

M. Herda was an invited speaker in the workshop Analytical and Computational Problems for Mixtures and Plasma Dynamics which took place at the Hausdorff Research Institute for Mathematics in Bonn in the framework of the Junior Trimester Program in Kinetic Theory. He was also one of the speakers of the mini-symposium “Novel time discretization methods and moment models for kinetic equations” co-organized by T. Rey at ICIAM 2019 in Valencia. Finally, he gave a talk in the Applied PDEs seminar of Imperial College London.

I. Lacroix-Violet was an invited speaker in the workshop Women in PDEs that was held in Vienna. She also gave several seminars in Université Paris-Est Créteil, Nancy, Dijon, and Lyon, as well as a talk for the ANEDP team day.

S. Lemaire was an invited speaker at the GAMM 2019 conference held in Vienna, and for the POEMs conference held at CIRM in Marseille. He also gave a talk for the yearly Journée de la Fédération de Recherche Mathématique du Nord-Pas-de-Calais held in Lille, and a seminar at ENSTA ParisTech.

B. Merlet was an invited speaker of the fourth Journées Optimisation de Formes et Applications held in Palaiseau. He also gave two seminars in École Polytechnique and at the University of Lisbon, as well as a talk for the ANEDP team day.

T. Rey was an invited plenary speaker in the Summer School Trails in kinetic theory: foundational aspects and numerical methods from the Junior Trimester Program in Kinetic Theory of the Hausdorff Research Institute for Mathematics, held in Bonn. He was also one of the speakers of the conference Numerical Methods for Multiscale Models arising in Physics and Biology held in Nantes. He finally gave a colloquium in the mathematics department of Université Paris-Est Créteil, and a seminar at ENS Ker Lann in Rennes.

A. Zurek was an invited speaker of the Journée EDP held in Calais. He was also a contributed speaker in the conference Numerical Methods for Multiscale Models arising in Physics and Biology held in Nantes. He finally gave a talk during the thirteenth Journée des Doctorants en Mathématiques du Nord-Pas-de-Calais in Lens.

10.1.4. Leadership within the Scientific Community

C. Cancès is the head of the French Research Group GdR MaNu on Mathematics for Nuclear Energy (funded by CNRS's INSMI).

He is also the leader of the task "Numerical methods for high-performance computing of coupled processes" within the EURAD project (H2020, EJP COFUND); cf. Section 9.3.

10.1.5. Research Administration

C. Calgaro is a member of the Conseil de Département de Mathématiques. She has been a member of the CNU 26 until September.

C. Cancès is a member of the Scientific Board of the Inria Lille - Nord Europe research center.

Until September, C. Chainais-Hillairet has been a member of the Conseil de Département de Mathématiques. Since September, she is a member of the Conseil de la Faculté des Sciences et Technologies of Université de Lille. She also joined in January the CNRS evaluation committee of the Laboratoire de Mathématiques de Reims.

B. Gaudeul is the delegate of the PhD students at the Commission Mixte in Mathematics of Université de Lille.

I. Lacroix-Violet is an elected member of the Conseil du Laboratoire Paul Painlevé. She is also a member of the Comité d'Éthique de la Recherche.

S. Lemaire is a member of the Commission de Développement Technologique of the Inria Lille - Nord Europe research center.

B. Merlet is an elected member of the Conseil du Laboratoire Paul Painlevé.

T. Rey is also an elected member of the Conseil du Laboratoire Paul Painlevé. T. Rey and M. Herda (since September) are in charge of the organization of the weekly seminar of the ANEDP team at the Laboratoire Paul Painlevé. T. Rey is a member of the team of Opération Postes.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

RAPSODI team members are strongly involved in teaching at Université de Lille. C. Calgaro is in charge of the Master of Mathematical Engineering. I. Lacroix-Violet is responsible of the IESP2A's third year at Polytech Lille. B. Merlet is in charge of the Master 2 of Scientific Computing. E. Creusé is the director of the Mathematics Department of the Université Polytechnique Hauts-de-France.

In 2019, C. Cancès gave practicals (16h) of scientific computing at the École Centrale de Lille. He also gave lectures (32h) on fundamental notions in mathematics in the framework of the newly created Master on Data Sciences of the Université de Lille and the École Centrale de Lille. F. Chave gave practicals to first-year students at Polytech Lille. M. Herda gave lectures (26h) on mathematical methods for signal processing in the Master of Numerical and Statistical Engineering of Université de Lille. S. Lemaire gave lectures (32h) on mathematical tools for simulation in the Master 2 of Scientific Computing at Université de Lille.

C. Chainais-Hillairet gave lectures about "Finite volume methods, dissipative problems, and long-time behavior" in 2 Summer Schools, at Le Lioran (GdR EGRIN) in June, and at CIRM in Marseille (CEMRACS 2019) in July.

10.2.2. Supervision

Post-doc in progress: F. Chave, on "High-order polytopal discretization methods for electromagnetism", since 12/01/2018; supervisors: S. Lemaire and E. Creusé.

PhD in progress: A. Nahas, on "Vortices in Bose–Einstein condensates", since 09/01/2019; advisors: I. Lacroix-Violet and G. Dujardin (Inria Lille - Nord Europe). The thesis is half funded by the LabEx CEMPI.

PhD in progress: S. Bassetto, on "Towards a more robust and accurate treatment of capillary effects in multiphase flow simulations in porous media", since 01/01/2019; advisors: C. Cancès, G. Enchéry and Q.-H. Tran (IFPEN).

PhD in progress: B. Gaudeul, on the "Numerical approximation of cross-diffusion systems arising in physics and biology", since 09/01/2018; advisors: C. Chainais-Hillairet and C. Cancès.

PhD: A. Zurek defended his PhD thesis [11] entitled "Problèmes à interface mobile pour la dégradation de matériaux et la croissance de biofilms : analyse numérique et modélisation" on September 26; advisors: C. Chainais-Hillairet and B. Merlet.

PhD: C. Colin defended her PhD thesis [12] entitled "Analyse et simulation numérique par méthode combinée Volumes Finis - Éléments Finis de modèles de type faible Mach" on May 10; advisors: E. Creusé and C. Calgaro.

M2 Modélisation - Optimisation - Sécurité group research in progress (Université Polytechnique Hauts-de-France): L. Romanowicz and A. Violet, on the "Numerical study of the rise of a suspension bridge", 2019-2020; advisor: E. Creusé.

M2 internship: L. Maisonneuve, on the "Mathematical modeling of a knowledge model in structured populations", from April to September; advisors: T. Rey, S. Billiard and M. Derex.

M2 internship: A. Nahas, on the "Numerical study of the local minimizers of a Bose–Einstein energy functional in 2D", from January to July; advisors: I. Lacroix-Violet and G. Dujardin (Inria Lille - Nord Europe).

M2 internship: N. Aghouzzaf, on "Keller–Segel equations for chemotaxis", from December 2018 to July; advisor: T. Rey.

M1 internship: Q. Fourche, on "Spectral moment methods for linear kinetic equations", from June to July; advisor: T. Rey.

M1 internship: M. Jonval, on "Nonlinear numerical schemes for drift-diffusion equations", from June to July; advisor: C. Chainais-Hillairet.

M1 CHPS group research (Université de Lille): M. Ghestin and A. Rotolo, on "Systems of interacting particles and their mean-field limits", from February to May; advisor: T. Rey.

M1 MAS group research (Université de Lille): C. Germain and A. Jossien, on "Deterministic predictive models of the average annual temperature in Morocco in 2019", 2019; advisor: C. Calgaro.

M1 Modélisation - Optimisation - Sécurité group research (Université Polytechnique Hauts-de-France): I. Kahiyehmoumin, A. Ndao and M. Fall, on a "Domain decomposition method for the finite difference approximation of a diffusion problem", 2019; advisor: E. Creusé.

L3 internship: G. Helbecque, on the "Numerical simulation of charged particles in a strong magnetic field", from April to May; advisor: M. Herda.

10.2.3. Juries

C. Calgaro was a jury member for the PhD defense of M. Tsegmid (Université du Littoral-Côte-d'Opale). She is also a member of the Jury de l'Agrégation de Mathématiques, which is a national hiring committee for the highest level of high-school teachers.

C. Cancès reported on T. Beltzung's (CEA / UVSQ), J. W. Both's (University of Bergen, Norway), and D. Shylaja's (Monash University / ITT Bombay, Australia / India) PhD theses. He is also a member of the Jury de l'Agrégation de Mathématiques.

C. Chainais-Hillairet reported on A. Gerstenmayer's (T.U. Vienna) PhD thesis. She was also a jury member for the PhD defenses of L. Boittin (Paris), C. Colin (Lille), R. Chalayer (Clermont-Ferrand), P. Mennuni (Lille), and M. Id Moulay (Pau). She finally was part of the selection committee for an associate professor (MCF) position at Orsay.

E. Creusé reported on P. Daniel's PhD thesis, defended on March 22 at Sorbonne Université, and entitled "Éléments finis hp-adaptatifs avec contraction d'erreur garantie et solveurs multi-niveaux inexacts". He was also a jury member for the PhD defenses of J. Tomezyk (Université Polytechnique Hauts-de-France) and G. Jeanmasson (Université de Bordeaux). He finally was part of the selection committee for an associate professor (MCF) position at Université Polytechnique Hauts-de-France.

B. Gaudeul was a jury member for the Tournoi Français des Jeunes Mathématiciennes et Mathématiciens.

I. Lacroix-Violet was a jury member for the PhD defense of I. Bensouilah (Lille), and for the habilitation of D. Sanchez (Toulouse).

B. Merlet reported on M. Bonafini's PhD thesis, defended on April 11 at the University of Trento (Italy), and entitled "Variational and convex approximations of 1-dimensional optimal networks and hyperbolic obstacle problems".

10.3. Popularization

C. Calgaro is in charge of the communication of the Laboratoire Paul Painlevé. She organized in 2019 various events to promote mathematics among young people:

- "Les mathématiciens de Lille fêtent les 80 ans du CNRS" (about 600 participants from high-school or Classes Préparatoires);
- a conference of E. Ghys for the presence of the Jury de l'Agrégation de Mathématiques in Lille (about 200 participants);
- les "Mathématiques itinérantes", a series of conferences in high-schools.

E. Creusé gave two popularization talks at Université Polytechnique Hauts-de-France:

- "Le calcul scientifique pour la simulation et le contrôle des écoulements" for the first Rencontres Mathématiques Valenciennoises in March;
- "Comment prévoir la population de poissons dans l'océan ou le déplacement d'oiseaux migrateurs dans le ciel ? Les maths nous répondent !" for the Semaine des Mathématiques 2019 in March.

M. Herda gave a talk at Inria Lille - Nord Europe for the internal scientific popularization event "30 minutes of Science" in January.

T. Rey was one of the four speakers of the event "Les mathématiciens de Lille fêtent les 80 ans du CNRS".

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Major publications by the team in recent years

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