RESEARCH CENTRE

Inria Center at the University of Lille

IN PARTNERSHIP WITH:

Université de Lille

2022

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

Inria

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Project-Team RAPSODI

Creation of the Project-Team: 2017 November 01

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2 Overall objectives

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

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

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

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

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

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

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

Some technological bottlenecks related to points (a)–(c) mentioned above are well identified. In particular, it appears that a good numerical method should handle general meshes, so that dynamic mesh adaptation strategies can be used in order to achieve (b). But it should also be of the highest possible order while remaining stable in the sense of (a), and robust in the sense of (c). There have been numerous research contributions on each point of (a)–(c) in the last decades, in particular for solving each difficulty separately, but combining them still leads to unsolved problems of crucial interest. Yet, before addressing the above points (a)–(c) concerning the design of nice numerical methods, one has to identify the structural properties of (and possibly modify) the continuous model to be discretized.

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

1. Study of the structural properties of continuous PDE models.

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

3. Computational optimization of the numerical methods.

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

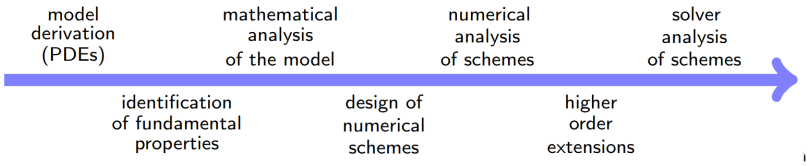

Figure 1: We consider the problem resolution in a global manner, starting from the model derivation (for instance based on physical principles) to the practical development of efficient numerical methods.

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

3 Research program

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

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

3.1.1 Thermodynamically consistent models for multi-component systems

Mathematical tools for the derivation and the mathematical analysis of models which are compatible with the second principle of thermodynamics and more specifically with Onsager's reciprocal principle [121] widely developed in the last decade. The general setting proposed in [115, 123] offers a powerful and robust framework for obtaining such models in configurations where inertia can be neglected.

This situation is typical of porous media flows in the Darcy regime. When rich physics are considered, like in presence of multiple phases and components within deformable and fractured matrices, the derivation of such thermodynamically consistent models is a timely problem [129, 130, 132]. One of the goals of the RAPSODI project-team is to contribute to the mathematical understanding of such models [4].

Inertia is also commonly neglected in models for semi-conductors of van Roosbroeck type, as for instance in models for the corrosion of iron [60]. In the latter framework, the geometry of the domain varies along time and is one of the unknowns of the problem. The reference model proposed in [60] is not built from thermodynamical considerations. The design, the simulation and the calibration of a mathematical model which is consistent with the second principle is an ongoing task addressed by our team (see [32] for preliminary results).

3.1.2 Variational models and optimal transport

Optimal transport has a long history. In Monge's seminal work "Théorie des déblais et des remblais" dating back to 1781 [131], the problem was roughly stated the following way: how should one proceed to move piles of sand from one point to another in order to minimize the workload? This problem is now often referred to as "Monge problem". It has stayed with no solution in the general case until the 1940s, when Kantorovich inserted it into a proper framework [107], which allowed eventually to tackle it and provide solutions. A major breakthrough was obtained by Brenier [69], who showed that under very broad assumptions, the general solution to the optimal transport problem had a very specific form and could be linked with the famous Monge–Ampère equation.

In recent years, optimal transport has become a very active field of research, due to the discovery of new and efficient algorithms [92] and to its wide range of applications, to economy, image processing, analysis of partial differential equations or data sciences (see e.g. references in [125]).

One of the focus of the team is the use of optimal transport for understanding the formation of bi-layer cellular membranes thanks to a model introduced in [124]. In this model, the global shape of micelles or liposomes should be the result of competing forces: a short-range attractive force given by the area of the boundary, and a non-local repulsive force of Wasserstein-type (that is, an optimal transport cost). Our aim is to explore numerically this problem and obtain theoretically the shape of the solutions in some asymptotic regimes.

3.1.3 Kinetic models of large particle systems and their asymptotic regimes

Nearly 150 years after Boltzmann paved the way to the kinetic representation of complex phenomena [68], this approach for modeling is more than ever active. This increasing interest is partially due to the development of computational facilities that make the numerical approximation of such models possible, but also to the great flexibility of the approach which can be applied in biology [128], economics [94] or social sciences [70], way beyond its original scope in physics of gases.

One focus of the team is the asymptotic analysis of these equations. The large-time limit of kinetic equations has been dealt with thanks to hypocoercivity techniques in [58] and new hydrodynamic limits have been derived from kinetic models for gases composed of macroscopic particles interacting via energy dissipative collisions [105, 85] and plasmas [104]. A future concern will be the study of the long time dynamics of a kinetic model for relativistic electron bunches in storage rings [126] (see Section 4.6).

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

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

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

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

In this regard, two-point flux approximation (TPFA) finite volume schemes are very popular in industrial codes since they enjoy remarkable stability properties at a moderate computational price. The team has a strong experience in the design of provably convergent entropy stable TPFA finite volume schemes for complex problems [51, 76, 81, 101, 19, 33, 75, 88, 79, 82, 19]. Ongoing [80, 119] and future research directions are based on the discretization of some action functionals and their optimization to obtain so-called variational schemes based on TPFA finite volumes. We also mention the Lagrangian

approach [26], for which the computation of some optimal tessellation based on semi-discrete optimal transportation shows subtle but deep similarities with Eulerian TPFA based methods.

The main drawback of TPFA finite volume schemes is that they (essentially) restrict to isotropic diffusion problems and to regular grids [97, 100]. The strong constraints on the meshes and on the isotropic nature of the problems under consideration for TPFA schemes motivated in the last decades the development of more robust finite volume schemes, see for instance [95] for a review on this topic. These developments were particularly motivated by applications in geosciences, where anisotropic porous media are common and where (possibly poorly regular) meshes are often prescribed by data. Tuning such advanced methods, which do not enjoy monotonicity properties in general, to make them thermodynamically consistent is a key challenge for our team. An active research topic of the team is to propose new structure-preserving numerical schemes beyond TPFA. The team has made important preliminary contributions on this topic through the design of structure-preserving control volume finite elements schemes [52, 53], vertex centered finite volume schemes [5], discrete duality finite volume schemes [78], finite element schemes [83] and hybrid finite volume schemes [20]. The latter numerical method also constitutes a first step towards high-order methods (see Section 3.2.2).

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

3.2.2 High-order structure-preserving numerical methods

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

There are important contributors in the community in these topics. For instance, the development of high-order in space methods allowing for general grids for diffusion problems was pushed forward in the last decade by several groups, for instance around Lourenço Beirão da Veiga and Franco Brezzi [63] for the Virtual Element Methods (VEM), around Daniele A. Di Pietro and Alexandre Ern [8, 93] for the Hybrid High-Order (HHO) methods, or around Bernardo Cockburn [90] for the Hybridizable Discontinuous Galerkin (HDG) methods.

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

Concerning the time discretization strategies, we take inspiration in the works by Giovanni Samaey [108] for projective integration schemes, and those by Christophe Besse [65] and Jie Shen [71] for relaxation methods. It appears that (explicit) Strong Stability Preserving high-order time discretizations [103], which are very popular in the community working on hyperbolic systems, are not suitable for solving dissipation driven (and typically parabolic) systems for which implicit methods are commonly used.

At the moment most of our energy stable methods rely on merely first-order time discretizations, typically Backward Euler or minimizing movement schemes [106]. The extension to higher order time discretizations is already the purpose of ongoing studies in the team. Two tracks have been identified so far and are already studied: (i) the variational BDF2 scheme [113] which generalizes to second order in time the minimizing movement scheme, and (ii) Runge-Kutta type schemes obtained after having changed of main unknowns. Both approaches have their pros and their cons: (i) is difficult to implement, whereas (ii) might lead to non-conservative methods. Our goal for the next years on this topic is to be able to overpass the difficulties of (at least one of) these methods and to get efficient implementation strategies as well as theoretical foundations.

3.2.3 Asymptotic-preserving and multiscale numerical methods

It has been understood around year 2000 that the fine quantification of the entropy dissipation allows to deduce fine properties on the asymptotic behavior of the solutions to dissipative PDEs [56, 84]. The extension to the discrete setting of this type of tools is more recent, see for instance [86, 66, 87]. The team

is involved in the study of the long-time behavior of numerical schemes for drift-diffusion models [67, 77, 6, 20] and kinetic equations [2, 12]. A future challenge is the study of the long time behavior properties for numerical schemes which can handle general meshes and high order accuracy (see Section 3.2.1 and Section 3.2.2).

We also contribute actively to the design and analysis of multiscale methods for highly heterogeneous (or highly oscillatory) diffusion problems. We have extended in [89] within the HHO framework the nonconforming multiscale method of [109] to arbitrary approximation orders (and its analysis also to the case of general meshes). We have also established in [21] an equivalence result between our multiscale HHO method and the MHM method of [55], improving in passing on both methods.

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

3.2.4 Numerical methods for optimal transport

In the last years optimal transport and its generalisations have proven to be a powerful tool to analyse a large class of models, exposing useful mathematical structures which are responsible of their properties [54], and guiding the conception of novel numerical schemes. Due to its geometric and physical meaning, optimal transport has also emerged as a useful modelling tool in different contexts including economics, biology or social sciences [127].

Transportation problems can often be cast as global space-time optimisation problems such as in variational mean field games or optimal planning problems [64]. Part of the activity of the team in this area is concerned with the analysis of such models in the discrete setting, which poses significant difficulties both in terms of conception of schemes (which often passes through the definition discrete variational problems) [119][118], and construction of efficient optimization algorithms to compute their solutions [37].

As currently many of these problems are still intractable at the numerical level (due to their high dimensionality and lack of smoothness), our aim is to further improve the current approaches, for example by using unstructured meshes in space-time, which would pave the way for the development of adaptive refinement techniques. Importantly, such new schemes could be used as a building block to construct new discretisations for PDEs with a variational structure related to optimal transport (such as Wasserstein gradient flows [120][38]). In particular, this could represent an additional research path to reach our objectives mentioned in Section 3.2.1.

3.3 Axis 3: Computational optimization of the numerical methods

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

To increase the efficiency and applicability of our methods, we work on three tracks. First, we aim at building a unified and optimized software platform to implement, test and diffuse our numerical methods. Second, since our methods often yield nonlinear systems, the improvement of the nonlinear solvers is also key to increase the efficiency of our methods. Finally, for high-dimensional models such as kinetic and particles systems, the curse of dimensionality makes numerical computations realistically feasible only if specific computationally efficient numerical strategies are used.

3.3.1 Development of the platform `ParaSkel++`

`ParaSkel++` [62] is a C++ platform, conceived by S. Lemaire and mainly developed since December 2022 by T. Zoto (succeeding L. Beaude), which is freely distributed under LGPL v3.0. The `ParaSkel++` platform aims at the high-performance, arbitrary-order, 2/3D numerical approximation of PDEs on general polytopal meshes using skeletal Galerkin methods (see [111]).

A first version (v1, August 2021) of the platform is operational, featuring a sequential implementation of all the main skeletal methods (Lagrange FE, VEM and HHO). The next 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 capabilities.

3.3.2 Design of robust nonlinear solvers

The entropy stable methods we build often yield nonlinear systems to be solved at each time step. It is therefore of paramount importance to have fast and robust nonlinear solvers at hand to address them, hence the increasing interest for so-called nonlinear preconditioning techniques. In [3], we proposed a strategy which consists in expressing the problem in terms of a new primary variable which, if well chosen, allows to remove the degeneracies of the system under consideration. This strategy has then been extended to the case of more complex systems arising in the context of porous media flows [59, 14]. In the framework of the collaboration with IFPEn, we develop new solvers for the computation of chemical equilibria, with application to reactive transport. The methodology being developed in this framework will then be transposed to other contexts in an as generic as possible way.

3.3.3 Efficient numerical methods for high-dimensional systems

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

A robust and fully explicit method that was developed and allows for time integration of (two-scale) stiff systems with arbitrary order of accuracy in time is called projective integration (PInt). It was proposed in [102] for stiff systems of ordinary differential equations with a clear gap in their eigenvalue spectrum. In [108], PInt was introduced and analyzed for linear kinetic equations with a diffusive scaling. It was then extended to the nonlinear Boltzmann equation in [114] and to gas mixtures in [13].

Moreover, having robust numerical methods is not enough: one also needs these methods to be extremely accurate and implemented efficiently, in order to obtain relevant numerical results in reasonable time. Spectral methods based on the fast Fourier transform have been developed in this sense in the last two decades, and reached enough maturity to be incorporated in high performance computing codes [9]. Equilibrium preserving extensions were also introduced and analyzed in the series of papers [122, 28]. Finally, an extension to the more mathematically intricated quantum Boltzmann operator has been achieved in the code `KINEBEC` [116], which has been used to show Bose–Einstein condensation and Fermi–Dirac relaxation in [47].

A major effort of the team will be aimed at extending model adaptation strategies to more complex kinetic models (complex plasmas with electron-ion interactions, space shuttle atmospheric reentries). The use of hybridized kinetic/fluid strategies as in [98] will allow us to benefit from the best of both fluid (efficiency of solvers) and kinetic (relevancy with the physics) approaches. This work will also benefit of collaborations with CENAERO, a private non-profit applied research center specialized in aerospace engineering, through the framework of the European Project DATAHYKING.

4 Application domains

4.1 Subsurface CO2 storage

The capture and storage in the subsurface of carbon dioxide is commonly acknowledged as a promising solution to mitigate the emission of greenhouse gas from localized production sites, as for instance cement plants. The safety assessment of the subsurface sequestration sites requires advanced numerical tools building on theoretically assessed numerical models and algorithms which remain valid in the long time limit. Among the numerous difficulties encountered in such a setting, let us mention the high level of coupling between the mechanics of the (solid) porous matrix [91], the multiphase and multicomponent character of the fluid which flows therein [61], and chemical reactions with a wide range of characteristic times [110]. Despite important differences (at the level of chemistry especially), similar problems occur in the emerging topic of dihydrogen subsurface storage, or native dihydrogen (generated by the corrosion of iron in an aqueous environment) migration in the context of nuclear waste repository management.

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

4.2 Material sciences

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

4.3 Complex fluid flows

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

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

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

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

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

4.4 Electromagnetism for non-invasive control

The RAPSODI team works on the development of high-order polyhedral methods for electromagnetism. A well-known specificity in electromagnetism is that topology plays a crucial role in the well-posedness of the models. Dedicated analysis tools must then be deployed for their study [57]. We are interested in the devising of HHO methods in the curl/curl setting [22]. The mathematical analysis of HHO methods in this setting is particularly involved, as most of the needed discrete functional analysis tools are currently lacking. The design of (efficient and robust) multilevel linear solvers for statically condensed HHO approximations of electromagnetic models, as well as of computable (reliable and locally efficient) a posteriori error estimators on polyhedral cells are two other, still largely unexplored, aspects we are interested in. Our main target application, in the framework of a recently initiated collaboration with EDF, is the simulation of eddy current testing (ECT). ECT is used by EDF as a non-invasive control technique to assess the integrity of heat exchanger tubes in nuclear plants. The forward problem consists in solving the time-harmonic 3D Maxwell's equations in domains featuring more or less complex flaws. The use of high-order polyhedral methods is expected to yield improvements on two aspects. First, the support of polyhedral cells is expected to ease the full meshing process, and in particular enable to account for defects with complex geometries/topologies. Second, the increase in the approximation order is expected to yield a reduction of the noise on the computed control signal, based on which the presence of a defect is inferred.

4.5 Large population models in epidemiology

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

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

4.6 Particle accelerators

Relativistic electron bunches are used in storage rings to produce intense radiation in various ranges of frequencies. The dynamics of these bunches is nonlinear because of interactions between electrons in the bunch. Moreover, these interactions occur in an asymmetric fashion because of the relativistic nature of the dynamics. The stability properties of the bunch (and thus the long-time properties of the dynamics) have been shown, both theoretically and experimentally, to be crucial in the understanding of the intensity of the emitted radiation [72, 96].

From a mathematical point of view, the dynamics of the electron density in the phase space can be described by a Vlasov–Fokker–Planck type equation [72] with a well suited mean-field self-interaction term [117]. The mathematical understanding of the long time behavior of solutions to this equation and the design of adapted numerical schemes constitutes a challenging and physically important problem.

5 New software and platforms

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

5.1 Platform `ParaSkel++`

Family={research, vehicle}; Audience={partners}; Evolution={lts}; Duration={2}; Contribution={leader}; URL={gitlab.inria.fr/simlemai/paraskel}

`ParaSkel++` [62] is a C++ platform, conceived by S. Lemaire and mainly developed since December 2022 by T. Zoto (succeeding L. Beaude), which is freely distributed under LGPL v3.0. The `ParaSkel++` platform aims at the high-performance, arbitrary-order, 2/3D numerical approximation of PDEs on general polytopal meshes using skeletal Galerkin methods. Skeletal Galerkin methods form a vast family of numerical methods for the approximation of PDE-based models that satisfy the following two building principles (see [111]):

- 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, HDG, HHO…). 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.

5.2 Code `KINEBEC`

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

`KINEBEC` (Kinetic Bose–Einstein Condensates) [116] 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.

5.3 Other codes

5.3.1 Code `Nonlocal SKT`

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

The Matlab code `Nonlocal SKT`, developed by M. Herda, was used to produce the numerical simulations of the article "Study of a structure preserving finite volume scheme for a nonlocal cross-diffusion system" [43].

5.3.2 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" [12].

6 New results

6.1 Modeling and numerical simulation of multi-component systems

The mathematical and numerical modeling of corrosion is a longstanding topic shared by several members of the RAPSODI research team. In the framework of the H2020 European program EURAD on the management of nuclear wastes, C. Cancès, C. Chainais-Hillairet, B. Merlet, F. Raimondi and J. Venel proposed in [32] a modification of a reduced model for the corrosion of the iron to make it compatible with the second principle of the thermodynamics, in the sense that the free energy is decaying along time. This remarkable stability property and uniform bounds derived thanks to the Moser iteration technique allow to rigorously establish the global in time existence of solutions to the model. In particular, and as highlighted by numerical results presented in [32], the new model preserves some physical bounds that are sometimes overpassed by the preceding models of the literature. The presence of moving interfaces is a characteristic of corrosion phenomena. The evolution of these interfaces is governed by nonlinear laws and poses significant difficulties in the theoretical and numerical treatment of the models. B. Merlet, J. Venel *et al.* attack these difficulties in [45] where they show the existence of solutions to a 1D reduced corrosion model with a moving interface. Their method is based on a minimizing movement scheme for some modified Wasserstein metric.

One of the key modifications proposed in [32] to make the model compatible with thermodynamics is the fact that the evolution of the iron cations follows a vacancy diffusion process, leading to nonlinear convection, while diffusion remains linear. As a consequence, Scharfetter–Gummel fluxes can no longer be used to compute a finite volume approximation of the iron cation concentration. In [18], C. Cancès and J. Venel proposed a new finite volume scheme to compute approximate solutions to such nonlinear convection diffusion equations. The scheme, which extends to the nonlinear mobility setting the so-called square-root approximation finite volume scheme [112], enjoys several remarkable properties, among which the decay at the discrete level of the free energy. By properly quantifying the dissipation of the free energy, C. Cancès and J. Venel show the convergence of the scheme when the discretization parameters (mesh size and time step) tend to 0 in the case of a scalar nonlinear convection diffusion equation. Numerical experiments show that the scheme is very efficient, justifying its use in the more complex setting of [32].

In [17], C. Cancès *et al.* 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 [74] is the nonlinearity of the energy density in the gradient part, which becomes singular at the interface between pure and mixed phases.

In [15], T.Rey *et al.* study a stochastic individual-based model of interacting plant and pollinator species through a bipartite graph: each species is a node of the graph, an edge representing interactions between a pair of species. The dynamics of the system depends on the between- and within-species interactions: pollination by insects increases plant reproduction rate but has a cost which can increase plant death rate, depending on pollinators density. Pollinators reproduction is increased by the resources harvested on plants. Each species is characterized by a trait corresponding to its degree of generalism. This trait determines the structure of the interactions graph and the quantity of resources exchanged between species. Their model includes in particular nested or modular networks. Deterministic approximations of the stochastic measure-valued process by systems of ordinary differential equations or integro-differential equations are established and studied as in [99], when the population is large or when the graph is dense and can be replaced with a graphon. The long-time behaviors of these limits are studied and central limit theorems are established to quantify the difference between the discrete stochastic individual-based model and the deterministic approximations. Finally, studying the continuous limits of the interaction network and the resulting PDEs, they show that nested plant-pollinator communities are expected to collapse towards a coexistence between a single pair of species of plants and pollinators.

In [48], J. Moatti *et al.* consider an (In,Ga)N/GaN semiconductor system with quantum wells. They introduce a model with accounts for random alloy fluctuations through an atomistic tight-binding model, where quantum corrections are introduced via a localization landscape theory and propose a numerical method to simulate the model at hand. They investigate the impact of the order of the wells on the device behaviour and compare the results of the simulations with existing simulation codes as well as with physical experimentations.

6.2 Analysis and numerical simulation in electromagnetism

In [23], 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 [22], 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.

6.3 Structural properties of dissipative models and their discretization

In [30] C. Chainais-Hillairet, M. Herda *et al.* consider a drift-diffusion charge transport model for perovskite solar cells, where electrons and holes may diffuse linearly (Boltzmann approximation) or nonlinearly (e.g. due to Fermi-Dirac statistics). To incorporate volume exclusion effects, they rely on the Fermi-Dirac integral of order -1 when modeling moving anionic vacancies within the perovskite layer which is sandwiched between electron and hole transport layers. After non-dimensionalization, they first prove a continuous entropy-dissipation inequality for the model. Then, they formulate a corresponding two-point flux finite volume scheme on Voronoi meshes and show an analogous discrete

entropy-dissipation inequality. This inequality helps them to show the existence of a discrete solution of the nonlinear discrete system with the help of a corollary of Brouwer's fixed point theorem and the minimization of a convex functional. Finally, they verify their theoretically proven properties numerically, simulate a realistic device setup and show exponential decay in time with respect to the L^2 error as well as a physically and analytically meaningful relative entropy.

In [12] M. Herda *et al.* introduce and analyse 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 scheme and show exponential stability and convergence of the scheme. 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 [19], C. Cancès *et al.* 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 [13], T. Rey *et al.* 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 [35], C. Chainais-Hillairet *et al.* propose a new numerical 2-point flux for a quasilinear convection-diffusion equation. This numerical flux is shown to be an approximation of the numerical flux derived from the solution of a two-point Dirichlet boundary value problem for the projection of the continuous flux onto the line connecting neighboring collocation points. The later approach generalizes an idea first proposed by Scharfetter and Gummel for linear drift-diffusion equations. Convergence of the scheme is established, as relative entropy decay properties.

In [20], 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 [46], J. Moatti considers an anisotropic drift-diffusion system for semiconductors models in exterior magnetic fields. Following the methodology introduced in [20], he introduces an Hybrid Finite Volume scheme and proves the existence of discrete solutions with bounds on the densities, as well as a long-time behaviour result. Numerical experiments illustrate the behaviour of the scheme.

In [43] M. Herda *et. al.* analyse a finite volume scheme for a nonlocal version of the Shigesada-Kawazaki-Teramoto (SKT) cross-diffusion system. They prove the existence of solutions to the scheme, derive qualitative properties of the solutions and prove its convergence. The proofs rely on a discrete entropy-dissipation inequality, discrete compactness arguments, and on the novel adaptation of the so-

called duality method at the discrete level. Finally, thanks to numerical experiments, they investigate the influence of the nonlocality in the system: on convergence properties of the scheme, as an approximation of the local system and on the development of diffusive instabilities.

In [29], 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.

In [33], 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.

6.4 Assessment and improvement of the efficiency of numerical methods

In [44], T. Laidin presents a hybrid numerical method that allows to reduce the computational cost of linear collisional kinetic equations. The method relies on an accurate dynamic domain decomposition technique. In addition to a rigorous study of the conservation of mass, he shows that the method is very efficient. Several numerical experiments also illustrate the properties of the method such as the conservation of mass and the long-time behaviour of discrete solutions.

In [36], E. Creusé *et al.* present unified frameworks for goal-oriented estimates for elliptic and parabolic problems that combine the dual-weighted residual method with equilibrated flux reconstruction. These frameworks allow to analyze simultaneously different approximation schemes for the space discretization of the primal and the dual problems, as conforming or nonconforming finite element method, discontinuous Galerkin methods, or finite volume method. Their main contribution is the splitting of the error on the quantity of interest into a fully computable estimator and a remainder that is bounded, up to an explicit constant, by the product of the fully computable estimators of the primal and dual problems. Some illustrative numerical examples that validate their theoretical results are presented.

In [31], C. Calgaro, C. Cancès and E. Creusé performed the convergence analysis of a finite volume scheme for a convection diffusion equation involving a Joule effect term which was introduced in the former contribution [73] emanating from the team. The proof proposed in [31] relies on compactness arguments. In order to treat the Joule effect term, a second order discrete Gagliardo-Nirenberg inequality has been established by the authors. By going beyond the (nowadays usual) framework of discrete functional inequalities involving first order discrete differential operators, this contribution seems to be a genuine novelty in the field of discrete functional analysis.

In [21], S. Lemaire *et al.* establish the equivalence between the Multiscale Hybrid-Mixed (MHM) [55] and the Multiscale Hybrid High-Order (MsHHO) [89] 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], T. Rey *et al.* 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 [14], S. Bassetto, C. Cancès *et al.* 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 [37] E. Facca, A. Natale *et al.* address the numerical solution of the quadratic optimal transport problem in its dynamical form, the so-called Benamou-Brenier formulation. When solved using interior point methods, the main computational bottleneck is the solution of large saddle point linear systems arising from the associated Newton-Raphson scheme. The main purpose of this paper is to design efficient preconditioners to solve these linear systems via iterative methods. Among the proposed preconditioners, they introduce one based on the partial commutation of the operators that compose the dual Schur complement of these saddle point linear systems, which they refer as $\mathscr{BB}$-preconditioner. A series of numerical tests show that the $\mathscr{BB}$-preconditioner is the most efficient among those presented, with a CPU-time scaling only slightly more than linearly with respect to the number of unknowns used to discretize the problem.

In [28], T. Rey *et al.* 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.

Volume integral methods for the solution of eddy current problems are very appealing in practice since they require meshing only the conducting regions. However, they require the assembly and storage of a dense stiffness matrix. With the objective of cutting down assembly time and memory occupation, low-rank approximation techniques like the Adaptive Cross Approximation (ACA) have been considered a major breakthrough. Recently, the VINCO framework has been introduced to reduce significantly memory occupation and computational time thanks to a novel factorization of the dense stiffness matrix. In [49] S. Pitassi *et al.* introduce a new matrix compression technique enabled by the VINCO framework. They compare the performance of VINCO framework approaches with state-of-the-art alternatives in terms of memory occupation, computational time and accuracy by solving benchmark eddy current problems at increasing mesh sizes; the comparisons are carried out using both direct and iterative solvers. The results clearly indicate that the so-called VINCO-FAIME approach which exploits the Fast Multipole Method (FMM) has the best performance.

6.5 Analysis and numerical simulation of variational models

In [34], C. Cancès *et al.* consider the convergence of a finite element discretization of a degenerate parabolic equation of q-Laplace type with an additional external potential. The main novelty of the approach presented therein is that the authors use the underlying gradient flow structure in the L^p-Wasserstein metric: from the abstract machinery of metric gradient flows, convergence of scheme is obtained solely on the basis of estimates that result naturally from the equation's variational structure. In particular, the limit is identified as the unique gradient flow solution without reference to monotonicity methods.

In [26], 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 [38], A. Natale *et al.* introduce a time discretization for Wasserstein gradient flows based on the

classical Backward Differentiation Formula of order two. The main building block of the scheme is the notion of geodesic extrapolation in the Wasserstein space, which in general is not uniquely defined. They propose several possible definitions for such an operation, and prove convergence of the resulting scheme to the limit PDE, in the case of the Fokker-Planck equation. For a specific choice of extrapolation they also prove a more general result, that is convergence towards EVI flows. Finally, they propose a variational finite volume discretization of the scheme which numerically achieves second order accuracy in both space and time.

In [24], 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 wet-lab experiments, the slime mold Physarum polycephalum has demonstrated its ability to tackle a variety of computing tasks, among them the computation of shortest paths and the design of efficient networks. For the shortest path problem, a mathematical model for the evolution of the slime is available and it has been shown in computer experiments and through mathematical analysis that the dynamics solves the shortest path problem. In [16], E. Facca *et al.* generalize the dynamics to the network design problem. They formulate network design as the problem of constructing a network that efficiently supports a multi-commodity flow problem. They investigate the dynamics in computer simulations and analytically. The simulations show that the dynamics is able to construct efficient and elegant networks. In the theoretical part they show that the dynamics minimizes an objective combining the cost of the network and the cost of routing the demands through the network. They also give alternative characterizations of the optimum solution.

In[25] E. Facca *et al.* introduce the *transport energy* functional $\mathscr{E}$ (a variant of the Bouchitté-Buttazzo-Seppecher shape optimization functional) and they prove that its unique minimizer is the optimal transport density μ^*, i.e., the solution of Monge-Kantorovich partial differential equations. They study the gradient flow of $\mathscr{E}$ and show that μ^* is the unique global attractor of the flow. Next they introduce a two parameter family $\{\mathscr{E}_{\lambda,\delta}\}_{\lambda,\delta>0}$ of strictly convex regularized functionals approximating $\mathscr{E}$ and they prove the convergence of the minimizers $\mu^*_{\lambda,\delta}$ of $\mathscr{E}_{\lambda,\delta}$ to μ^* as they let $\delta \to 0^+$ and $\lambda \to 0^+$. They derive an evolution system of fully non-linear PDEs as the gradient flow of $\mathscr{E}_{\lambda,\delta}$ in L^2, showing existence and uniqueness of the solution for all times. They are able to prove that the trajectories of the flow converge in $W_0^{1,p}$ to the unique minimizer $\mu^*_{\lambda,\delta}$ of $\mathscr{E}_{\lambda,\delta}$. This allows them to characterize $\mu^*_{\lambda,\delta}$ by a non-linear system of PDEs which turns out to be a perturbation of Monge-Kantorovich equations by a p-Laplacian.

B. Merlet *et al.* continued their work about the characterization of objects which split as cartesian products. Their previous work leads to the study of generalized surfaces of dimension $k = k_1 + k_2$ in $\mathbb{R}^n = \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$ which write as cartesian products $\Sigma_1 \times \Sigma_2$ with $\Sigma_1 \subset \mathbb{R}^{n_1}$ of dimension k_1 and $\Sigma_2 \subset \mathbb{R}^{n_2}$ of dimension k_2. The generalized surface they consider are the so called *normal rectifiable k-chains*. In [41] they establish a rigidity result for such objects, namely given some normal rectifiable k-chain A, they show that if at almost every x, the tangent k-plane to A at x splits as a cartesian product $L^1(x) \times L^2(x)$ with $L^1(x) \subset \mathbb{R}^{n_1}$ of dimension k_1 and $L^2(x) \subset \mathbb{R}^{n_2}$ of dimension k_2 then A is supported in a countable union of cartesian products of the form described above: $\cup_j \Sigma_1^j \times \Sigma_2^j$.

As a preliminary work, B. Merlet *et al.* establish in [40] that normal rectifiable chains admit a decomposition in a (at most) countable number of connected components.

In [41] B. Merlet *et al.* introduce and study the notion of *tensor rectifiable chains* which form a two dimensional chain complex of normed groups. They complete the theory of tensor flat chains in [39] by establishing a deformation theorem in this setting and by identifying isometrically some subgroups of tensor flat chains with corresponding subgroups of classical chains.

In [42], B. Merlet, M. Pegon *et al.* establish a $C^{1,\alpha}$-regularity theorem for almost-minimizers of the functional $\mathscr{F}_{\varepsilon,\gamma} = P - \gamma P_\varepsilon$, where $\gamma \in (0,1)$, P is the standard perimeter for Caccioppoli sets and P_ε is a nonlocal energy converging to the perimeter as ε vanishes. Their theorem provides a criterion for $C^{1,\alpha}$-regularity at a point of the boundary which is *uniform* as the parameter ε goes to 0. As a consequence they obtain that volume-constrained minimizers of $\mathscr{F}_{\varepsilon,\gamma}$ are balls for any ε small enough. For small ε,

this minimization problem corresponds to the large mass regime for a Gamow-type problem where the nonlocal repulsive term is given by an integrable kernel G with sufficiently fast decay at infinity.

In [27], 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.

7 Bilateral contracts and grants with industry

7.1 Bilateral contracts with industry

A research collaboration contract has been signed in 2022 between RAPSODI and EDF R&D in the framework of the ANR France Relance funding plan. The contract follows the lines of the bilateral agreement between Inria and EDF. The collaboration involves S. Lemaire and S. Pitassi, and concerns the development of high-order polyhedral methods for the numerical simulation of eddy current testing. The 2-year post-doc position of S. Pitassi, which started in October 2022, is funded by this grant ("Dispositif 4"). It has also been agreed that the `ParaSkel++` code will be the prototyping platform for this project.

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.

7.2 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 8.3.1.

In the framework of the MSCA's DATAHYKING project led by T. Rey, the Lille pole will work with a Wallonian private for non-profit research center called Cenaero, which "provides to companies, involved in a technology innovation process, numerical simulation methods and tools to invent and design more competitive products. Internationally recognized, Cenaero is mainly active in the fields of aeronautical design, spacecrafts, manufacturing processes, and buildings and smart cities". More details on the project can be found in Section 8.3.2.

8 Partnerships and cooperations

8.1 International initiatives

8.1.1 PHC (Partenariats Hubert Curien)

C. Cancès is co-PI with Jakub Wiktor Both (Univ. Bergen, Norway) of the 2022-2023 Franco-Norwegian Aurora project GradFlowPoro funded (~ 4.5k€/year) by Campus France. M. Jonval also takes part to the project.

M. Herda was the co-PI with Ansgar Jungel (TU Vienna, Austria) of a 2021-2022 Franco-Austrian Amadeus project funded (~ 2.5k€/year) by Campus France. The project is entitled "Design and analysis of structure-preserving numerical schemes for cross-diffusion systems". C. Cancès also took part to the project.

8.2 International research visitors

8.2.1 Visits of international scientists

Jakub Wiktor Both

Status: Researcher

Institution of origin: University of Bergen

Country: Norway

Dates: September 26-30

Context of the visit: The goal of this collaboration is to formalize from a mathematical point of view the equations governing multiphase flows in deformable porous media.

Mobility program/type of mobility: Research stay in the framework of the Aurora Franco-Norwegian project GradFlowPoro (2022–2023) supported by Campus France.

8.2.2 Visits to international teams

C. Cancès and M. Jonval

Visited institution: University of Bergen

Country: Norway

Dates: May 2-6

Context of the visit: The goal of this collaboration is to formalize from a mathematical point of view the equations governing multiphase flows in deformable porous media.

Mobility program/type of mobility: Research stay in the framework of the Aurora Franco-Norwegian project GradFlowPoro (2022–2023) supported by Campus France.

T. Rey

Visited institution: University of Cambridge

Country: Great Britain

Dates: May 25 - June 15

Context of the visit: Participation in the thematic semester Frontiers in kinetic theory

Mobility program/type of mobility: Research stay and workshop

J. Moatti

Visited institution: Weierstrass Institute, Berlin (WIAS)

Country: Germany

Dates: May – July

Context of the visit: Collaboration with P. Farrell and his research team Numerical Methods for Innovative Semiconductor Devices. The goal was to work on the numerical simulation of semiconductor models with random alloy fluctuations and quantum effects

Mobility program/type of mobility: Research stay supported by the Collège Doctoral de l'Université de Lille (PhD Mobility Program) and the WIAS.

M. Herda

Visited institution: Vienna University of Technology

Country: Austria

Dates: November 14-18

Context of the visit: Collaboration with A. Jungel on the numerical discretization of nonlocal cross-diffusion systems.

Mobility program/type of mobility: Research stay in the framework of an Amadeus Franco-Austrian project (2021–2022) supported by Campus France.

8.3 European initiatives

8.3.1 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 [50]. The postdoc position of F. Raimondi is funded by EURAD.

8.3.2 Marie Skłodowska-Curie Actions

T. Rey is the co-PI of the DATAHYKING project which aims to create a data-driven simulation framework for kinetic models of interacting particle systems, and define a common methodology for training future modeling and simulation experts. The network focuses on

- reliable and efficient simulation;
- robust consensus-based optimisation, also for machine learning;
- multifidelity methods for uncertainty quantification and Bayesian inference;
- applications in fluid flow, traffic flow, and finance.

All these topics will be collaborations between academic and industrial partners.

- Title: Data-driven simulation, uncertainty quantification and optimization for hyperbolic and kinetic models
- Duration: March 2023 - March 2027
- Poles: Lille, Leuven, Aachen, Kaiserslauter, Roma, Ferrara, Nice + 11 industrial partnerships
- Budget: 428 k€ (total of 3.45 M€ for the 7 poles)
- Coordinator of the Lille pole: T. Rey
- Industrial partner in the Lille pole: Cenaero

8.4 National initiatives

8.4.1 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 (University of Lyon)

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 were members of the ANR JCJC project MOHYCON. This project was related to the analysis and simulation of multiscale models of semiconductors. As almost all current electronic technology involves the use of semiconductors, there was 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)

8.4.2 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 was funded by the LabEx CEMPI.

8.5 Regional initiatives

8.5.1 Technological Development Action (ADT)

S. Lemaire is the P.I. of the ADT project ParaSkel++, funded by Inria and the Hauts-de-France region, which started in February 2020 and was renewed for two more years in 2022. The aim of the project is to develop an optimized parallel C++ platform for the arbitrary-order numerical approximation of PDEs by skeletal methods on general 2/3D polytopal meshes (more details can be found in Section 5.1). T. Zoto was hired in December 2022 to become the new lead developer of the platform.

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

C. Cancès was part of the organizing committee of the DONUT progress meeting (see Section 8.3.1) held online on February 2-3.

T. Rey was part of the organizing committee of the symposium Challenges in the Kinetic Modeling of Complex Systems during the congress SIAM PD 22. He also co-organized the *Journée d'équipe* of the PDE and numerical analysis team of the Laboratoire Paul Painlevé.

J. Candau-Tilh, B. Merlet, A. Natale and M. Pegon organized the 3rd edition of the Conference on Calculus of Variations in Lille which took place from July 4 to July 6. It was held at the Laboratoire Paul Painlevé (Université de Lille). The aim of this 3-day conference was to bring together experts and young researchers in Calculus of Variations with applications in different areas of physics, mechanics and image processing. This event gathered around 50 participants.

M. Herda co-organized with C. Calgaro the regional one-day conference Applied Analysis day in Hauts-de-France which gathered around 40 participants and was held on November 10.

9.1.2 Member of the editorial boards

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

9.1.3 Reviewer - reviewing activities

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

9.1.4 Invited talks

C. Cancès was an invited plenary speaker at the CANUM2020 conference held in Evian-les-Bains, postponed to June 13-17, 2022 for sanitary reasons, as well as in the NEEA workshop held in Chemnitz on September 2-9. He was also invited to give a talk during the CEMPI scientific days (March 31-April 1, Lille), and an online talk in a minisymposium of the SIAM PD 22 conference (March 14-18) held online. Moreover, C. Cancès gave an online talk at the meeting of the mechanical chapter of the French Academy of Science on February 8, as well as seminars at the universities of Lyon, Bergen (Norway) and in the CEA at Bruyères-le-Chatel. Eventually, he was invited to speak at the colloquium of the LJAD in Nice.

C. Chainais-Hillairet gave a talk at the conference New trends in complex flows, held at Institut Henri Poincaré (Paris) on September 19-21. She also gave a colloquium at the Institut de recherche mathématique de Rennes.

B. Merlet was an invited speaker of the *Journée EDP* held on May 9 at the Université Libre de Bruxelles (Belgique). He also was an invited speaker of the closing session day of the seminar Calva held on June 20.

C. Calgaro gave several seminars in Université Picardie Jules Verne (Amiens), Université Technologique de Compiègne and Université de Lille.

M. Herda gave an online talk at the SIAM Conference on Analysis and PDEs during the mini-symposium "Challenges in the Kinetic Modelling of Complex Systems part III" on March 18. He also gave a talk at the ANR MoHyCon workshop: Numerical methods for multiscale problems, that was held in Pornichet on March 9-11. Finally he gave several seminars in Université Littoral Côte d'Opale (Calais), Université de Picardie Jules Verne (Amiens), École Polytechnique (Palaiseau) and in the BIOEPAR lab (INRAE Nantes).

S. Lemaire gave an invited talk in the conference on "Herglotz-Nevanlinna functions and their applications to dispersive systems and composite materials", that was held in CIRM (Marseille) on May 23-27. He also gave an online talk in the WCCM XV conference that was held remotely on August 1-5, as well as an invited talk in the POEMs IV conference on "POlytopal Element Methods in Mathematics and Engineering", that was held in Milan (Italy) on December 12-14. Finally, he gave several seminars in French research labs, at UTC (Compiègne) in September, at ULCO (Calais) in October, at UCB (Lyon) in November, and in the ERMES department at EDF R&D (Palaiseau) in October.

A. Natale gave a talk in the seminar of the team Modélisation & Contrôle at the IRMA in Strasbourg, at the Journées ANR MAGA in Autrans, and in the seminar of the team INRAE Dynamo in Nantes.

M. Pegon gave several seminars in Université Paris-Saclay (twice), Université Toulouse III - Paul Sabatier, Sapienza Università di Roma and CentraleSupélec.

T. Rey gave an online talk at the Workshop Modelling and Numerical Simulation of Non-Equilibrium Processes Part 2 (originally planned to be held in the National University of Singapore). He gave an online talk at the Minisymposium Challenges in the Kinetic Modelling of Complex Systems in March 2022, part of the SIAM PD 22 conference. He also gave a plenary lecture at the conference Frontiers in Numerical Analysis of Kinetic Equations, held in the University of Cambridge in May 2022. T. Rey also gave several lab seminars in Université de Montpellier (January 2022), Oak Ridge National Laboratory, Tenessee, USA (April 2022), Université d'Amiens (November 2022) and Université Claude Bernard Lyon 1 (November 2022).

J. Venel gave seminars in Université de Lorraine and Université de Lyon as well as a talk for the Journée d'équipe ANEDP held on June 23 at Université de Lille.

E. Facca presented the result described in [37] in the following conferences: the 17th Copper Mountain Conference on Iterative Methods (held online on April 4-8), the 7th IMA Conference on Numerical Linear

Algebra and Optimization (held in Birmingham, UK, on June 29-July 01), and the Optimal Transportation and Applications conference (held in Pisa, IT, on October 24-28).

F. Raimondi presented a poster at the CANUM2020 conference, held at Evian-les-Bains on June 13 -17.

J. Candau-Tilh attended the Conference on Calculus of Variations held in Lille on July 4-6. He also attended a summer school on non-linear partial differential equations, held in Bonn on August 7-12. Additionally, he gave a talk at the workshop *Théorie géométrique de la mesure et calcul des variations*, held in Nancy on December 13-14 2022.

M. Jonval gave a talk during the kick-off meeting of the Campus France AURORA project at the University of Bergen (Norway) on May 2. He presented a poster at the Canum 2020 conference in Evian-les-Bains on June 13-17. He also gave an online talk at the doctoral seminar of IFP Énergies Nouvelles on June 20, a talk at the ANEDP team day in the University of Lille on June 23 and also a talk at the doctoral seminar of the Painlevé laboratory in Lille on Novembre 23.

T. Laidin presented posters at ANR MoHyCon conference (9-11 March), CANUM 2020 conference (13-17 June) and Kinetic Theory research school at CIRM (14-18 November). He also gave talks at the PhD students' seminar in laboratoire Paul Painlevé in Lille and PhD students' day in Valenciennes.

J. Moatti presented a poster at the closure conference of ANR MoHyCon held in Pornichet on March 9-11. He gave talks at PhD seminars in Séminaire Compréhensible at the Institut Fourrier (Grenoble), in Laboratoire Paul Painlevé (Lille) and in Institut de Mathématiques de Bourgogne (Dijon). He also gave a talk at the Numerische Mathematik Seminar in the WIAS (Berlin, Germany), as well as an online talk at the NUSOD 2022 conference, held remotely on September 12-16 and a talk at the POEMS 2022 workshop, held on December 12-14.

9.1.5 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 8.3.1).

9.1.6 Scientific expertise

C. Cancès, T. Rey and C. Calgaro were part of the hiring committee for a tenured assistant professor position (MCF) at Polytech Lille and the Laboratoire Paul Painlevé.

J. Venel was part of the selection committee for a tenured assistant professor position (MCF) at Université Polytechnique Hauts-de-France.

C. Chainais-Hillairet was part of the selection committee for junior researchers (CR and ISFP) at the Inria centre at the University of Bordeaux, as well as of the selection committee for a full professor (PR) position at Université Lyon 1. She is also member of the Section 26 (Mathématiques appliquées et application des mathématiques) of the Conseil National des Universités. Finally she was a member of the jury for the SMAI-GAMNI Blaise Pascal prize in 2022.

9.1.7 Research administration

C. Cancès is a member of the council of the graduate school MADIS, of the *Conseil d'Administration* of the SMAI, and of the *Bureau Scientifique* of the Inria centre at the University of Lille.

C. Chainais-Hillairet is vice-director of the Laboratoire Paul Painlevé, in charge of human resources for researchers, professors and assistant professors. She is also a member of the mathematics scientific board of the graduate school MADIS. She is a member of the *Commission égalité* and of the COREGAL (correspondent on equality) for the CNRS at Laboratoire Paul Painlevé.

J. Candau-Tilh is a member of the *Commission égalité* of the Laboratoire Paul Painlevé.

T. Rey was a member of the Opération Postes, the local correspondent of the biomath-oriented research group GdR MathSAV and *0 carbon referent* in charge of the evaluation and communication on the environmental footprint of the activities of the Laboratoire Paul Painlevé.

T. Laidin is a member of the *Commission Mixte* of the Laboratoire Paul Painlevé.

M. Jonval is the PhD students representative at the MADIS doctoral school council.

C. Calgaro is a member of the management team of the Faculté des Sciences et Technologies of the Université de Lille and is a member of the Conseil de Deépartement de Matheématiques at Université de Lille.

B. Merlet is an elected member of the council of the Faculty of Sciences and Technology of Lille. He represents the team Numerical Analysis and PDE in the Laboratoire Paul Painlevé. He is a member of the *Commission Mixte* of this laboratory and of the department of Mathematics of the University.

S. Lemaire is responsible, for the Inria Lille research center (15 research teams), of the yearly activity reports campaign. He is also a member of the Commission de Développement Technologique (CDT) of the Inria Lille research center. Finally, he is the webmaster of the RAPSODI website.

M. Herda was the co-organizer of the weekly Numerical Analysis and PDEs (ANEDP) seminar of the Laboratoire Paul Painlevé until August 2022. He is also an elected member of the *Conseil de Laboratoire* and of the *Commission Mixte* related to the math laboratory and the math department. M. Herda is also substitute member of the Inria Lille *Comité de Centre*.

T. Laidin has been co-organising the PhD students' seminar at the Paul Painlevé Laboratory in Lille since September 2022.

A. Natale is the co-organizer of Numerical Analysis and PDEs (ANEDP) seminar of the Laboratoire Paul Painlevé since September 2022.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

RAPSODI team members are strongly involved in teaching at University of Lille, in the engineering schools Centrale Lille and Polytech Lille, SKEMA business school 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 was in charge of the Master "Mathematics and Applications » until August 2022. E. Creusé is the head of the mathematics department of the CERAMATHS laboratory in the Université Polytechnique des Hauts-de-France. T. Rey is in charge of the Master 2 "Scientific Computing" since September 2021.

Inria members of the project-team also take an important part in teaching activities. C. Cancès was in charge of the course on Scientific Computing for the *1st year of Engineering school* (≡ L3) students in Centrale Lille (24h), of the course on Fundamental Notions in Mathematics (24h) in the *M1 "Data science"* of the University of Lille and Centrale Lille, and of the course on Nonlinear PDEs (24h) of the *M2 Recherche* of the Mathematics department of the University of Lille. A. Natale taught the course "Refresher in Mathematics" (20h) in the framework of the *M2 "Data Science"* of Université de Lille and Centrale Lille. He also taught the course "Numerical solution of nonlinear problems" (49h) in the framework of the Master 1 "Scientific Computing" at Université de Lille. S. Lemaire taught the course "Mathematical Tools for Simulation" (44h) in the framework of the *M2 "Scientific Computing"* at Université de Lille. M. Herda taught part (32h) of the *M2 Recherche* speciality course "Mathematical and numerical topics in kinetic theory" between January and March. He also taught part (15h) of the *M2 "Scientific Computing"* refresher course "Modeling" between September and October.

Finally, PhD students also contribute in the teaching activities (up to 64h yearly), either at the University of Lille (J. Candau-Tilh, J. Moatti, T. Laidin) or in SKEMA business school and Centrale Lille (M. Jonval).

9.2.2 Supervision - Mentoring

Post-docs

- Post-doc of S. Pitassi (Inria/EDF): *High-order polyhedral methods for eddy current testing simulation*, co-advised by Jérémy Dalphin (EDF), Jean-Pierre Ducreux (EDF) and S. Lemaire, since October 2022, funded through the research collaboration contract between RAPSODI and EDF R&D in the framework of the ANR France Relance funding plan.
- 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, October 2020 - July 2022, funded by the H2020 project EURAD.

Engineer

- Software engineer position of T. Zoto (Inria) on the development of the ParaSkel++ platform, supervised by S. Lemaire, since December 2022, funded by Inria & HdF region (ADT ParaSkel++).

PhD students

- 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.
- 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) 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.

Interns

- M2 internship of Robin Colombier (M2 MATMECA Bordeaux), supervised by T. Rey and Ingrid Lacroix-Violet (Univ. Lorraine): *Asymptotic preserving numerical scheme for the Wigner-BGK equation.* March-Sept. 2022.
- M2 internship of Jean-Claude Magnier (Mathématiques et Applications parcours Calcul Scientifique, Université de Reims Champagne-Ardenne) supervised by E. Creusé and C. Calgaro: *Numerical methods for the resolution of the quantum Euler and Navier-Stokes equations.* March-August 2022.
- M1 internship of Thomas Gaviard (École Centrale Lille) supervised by C. Chainais-Hillairet and A. Natale: *Numerical study of dynamical models of interacting Voronoi cells and their continuous limits.* October 2022-April 2023.
- M1 internship of Clément Vincent (Université de Lille) supervised by C. Chainais-Hillairet: *Implementation of a numerical scheme for a corrosion model on a moving domain.* June-July 2022.
- M1 internship of Brice Gonel (M1 Université de Lille, CS) supervised by T. Rey: *Particle and fluid models for species competition.* June-July 2022.

9.2.3 Juries

Habilitation à Diriger des Recherches (HDR)

- B. Merlet reported on the HDR manuscript and took part to the HDR defense committee of Matthieu Bonnivard (Université Paris Cité) on January 7. Title: *On the asymptotic analysis and simulation of models from calculus of variations and fluid mechanics.*

PhD defense

- E. Creusé reported on the PhD thesis and took part to the PhD defense committee of Aubin Brunel (Univ. Aix Marseille) on December 12. Title: *Staggered mesh schemes on general meshes for incompressible and compressible flows.*
- C. Chainais-Hillairet reported on the PhD thesis and took part to the PhD defense committee of Mathieu Rigal (Sorbonne Université) which was defended on November 14. Title: *Low Froude regime and implicit kinetic schemes for the Saint-Venant system.*
- B. Merlet reported on the PhD thesis and took part to the PhD defense committee of François L'Official (University of Toulouse) on July 19. Title: *Gamma convergence et singularités vortex au bord dans des films ferromagnétiques minces avec interaction de Dzyaloshinskii-Moriya.*
- C. Cancès reported on the PhD thesis and took part to the PhD defense committee of Félicien Bourdin (Univ. Paris Saclay and ENS Paris) on July 13. Title: *Macroscopic Modeling of the Motion of a Crowd with Two Types, Condensed SIR Models.*

9.3 Popularization

9.3.1 Internal or external Inria responsibilities

C. Calgaro was in charge of the communication of the Laboratoire Paul Painleveé until September 2022.

E. Creusé organized the Troisièmes rencontres mathématiques valenciennoises in Valenciennes on March 24. This meeting is dedicated to undergraduate students as well as secondary school teachers. The goal is to present some aspects of research in mathematics. This event is part of the semaine des mathématiques and gathered 350 persons in 2022. The program consisted in four talks

- E. Creusé: *Le calcul scientifique à travers un exemple en dynamique des populations*
- Florent Dewez (Diagrams Technologies) : *Un peu d'optimisation et d'intelligence artificielle pour un trafic aérien plus écologique ?*
- J. Venel: *Sauve-qui-peut ! Un voyage en grandes dimensions pour prévoir les mouvements de foule*
- Séverine Biard (Univ. Polytech. Hauts-de-France) : *Un aperçu de théorèmes d'approximation en Analyse Complexe.*

9.3.2 Articles and contents

J. Venel participated to the radio programme La Terre au carré on the national radio France Inter on October 26. The programme was dedicated to the mechanics of crowds.

9.3.3 Interventions

In the framework of the *Fête de la Science 2022*, C. Cancès gave talks dedicated to audiences made of schoolchildren on how mathematics can help to store CO2 in the underground.

A. Natale gave a popularisation talk at the scientific conference of the Graduate Programme "Information and Knowledge Society" of the University of Lille, and also in the seminar “30 minutes de science" at Inria Lille.

C. Calgaro gave a talk to an audience of high school students and organized the welcome in the laboratory of 4 middle and high school students for a week as part of a laboratory discovery internship.

E. Creusé and J. Venel gave a popularization talk during the Troisièmes rencontres mathématiques valenciennoises (see Section 9.3.1 for details).

On December 15, T. Rey spent time with last year high school students visiting the University. He presented what mathematical fluid dynamics modeling is and introduced them to numerical simulation with his research codes.

M. Jonval and J. Moatti welcomed a schoolboy (3ème) for half a day to introduce him to the research world.

J. Venel gave a popularization conference during the event Congrès MATh.en.JEANS organized in Perpignan in April. She also took part in the scientific committee of a temporary exhibition entitled Foules which holds from October 18, 2022 to August 6, 2023 in the *Cité des Sciences et de l'Industrie*. On October 11 2022, J. Venel was the chairwoman of the round table "Mobilité et Transport : défis actuels" during the event "Forum Emploi Maths" in La Villette. The speakers talked about the mobility in a broad sense. The road traffic modeling, the pedestrian flows, the freight transport and the self-driving vehicles were the topics respectively discussed by Paola Goatin (INRIA - Université Côte d'Azur), Sylvain Faure (Signactif), Jean-Pierre Tyberghein (Organisation & Entreprise) and Gérard Yahiaoui (Nexyad).

10 Scientific production

10.1 Major publications

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

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

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

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

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

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

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