Activity Report 2016

Team RAPSODI

Reliable numerical approximations of dissipative systems

Inria teams are typically groups of researchers working on the definition of a common project, and objectives, with the goal to arrive at the creation of a project-team. Such project-teams may include other partners (universities or research institutions).

RESEARCH CENTER
Lille - Nord Europe

THEME
Numerical schemes and simulations

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Team RAPSODI

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2. Overall Objectives

2.1. Overall Objectives

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

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

1. preservation at the discrete level of some crucial features of the solution, such as positivity of solutions, conservation of prescribed quantities (e.g., mass, the decay of physically motivated entropies, etc.);
2. provide accurate numerical approximations at a reasonable computational cost (and ultimately maximize the accuracy at a fixed computational effort);
3. robustness with respect to physical conditions: the computational cost for a given accuracy should be essentially insensitive to change of physical parameters.

We aim to develop methods fulfilling the above quality criteria for physical models which all display a dissipative behavior, and that are motivated by industrial collaborations or multidisciplinary projects. In particular, we have identified a couple of specific situations we plan to investigate: models from corrosion science (in the framework of nuclear waste repository) [1], low-frequency electromagnetism [10], and mechanics of complex inhomogeneous fluids arising in avalanches [6] or in porous media [46].

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

2.2. Scientific Context

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

Let us mention for example the review paper by J. Droniou [58], where it is highlighted that all the linear methods for solving diffusion equations on general meshes suffer from the same lack of monotonicity and preserve neither the positivity of the solutions nor the decay of the entropy. Moreover, there is no complete convergence proof for the nonlinear methods exposed in [58]. The first convergence proof for a positivity preserving and entropy diminishing method designed to approximate transient dissipative equation on general meshes was proposed very recently in [16]. The idea and the techniques introduced in [16] should be extended to practical applications.

In systems of PDEs, the values of physical parameters often change the qualitative behavior of the solution. Then, one challenge in the numerical approximation of such systems is the design of methods which can be applied for a large range of parameters, as in particular in the regime of singular perturbations. Such schemes, called *asymptotic-preserving* (AP) schemes [65], are powerful tools as they permit the use of the same scheme for a given problem and for its limit with fixed discretization parameters. In many cases, the AP property of

numerical schemes is just empirically established, without any rigorous proof. We aim to extend the techniques recently introduced in [3] for the drift-diffusion system, and based on the control of the numerical dissipation of entropy, to other dissipative systems in order prove the AP property of numerical schemes.

The question of the robustness of the numerical methods with respect to the physical parameters is also fundamental for fluid mixtures models. The team already developed such schemes for the variable density Navier-Stokes system [5] or [6]. We aim to propose new ones for more complex models with the same philosophy in mind. On the one hand, we will be interested in high-order schemes, which must be as simple as possible in view of 3D practical implementations. Let us stress that combining high order accuracy and stability is very challenging. On the other hand, the optimization of the computation will have to be considered, in particular with the development of some *a posteriori error* estimators. Impressive progresses have been achieved in this field [54], allowing important computational savings without compromising the accuracy of the results. Recently, we successfully applied this strategy to the Reissner-Mindlin model arising in solid mechanics [53], the dead-oil model for porous media flows [50] or the Maxwell equations in their quasi-static approximation for some eddy current problems [10] and [52]. We aim to develop new *a posteriori* estimators for other dissipative systems, like fluid mixtures models.

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

1. *Design and numerical analysis of structure preserving numerical methods*.
2. *Computational optimization*.

3. Research Program

3.1. Design and analysis of structure preserving schemes

3.1.1. Numerical analysis of nonlinear numerical methods

Up to now, the numerical methods dedicated to degenerate parabolic problems that the mathematicians are able to analyze almost all rely on the use of mathematical transformations (like e.g. the Kirchhoff's transform). It forbids the extension of the analysis to complex realistic models. The methods used in the industrial codes for solving such complex problems rely on the use of what we call NNM, i.e., on methods that preserve all the nonlinearities of the problem without reducing them thanks to artificial mathematical transforms. Our aim is to take advantage on the recent breakthrough proposed by C. Cancès & C. Guichard [16], [30] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness w.r.t. physical parameters, ...).

3.1.2. Design and analysis of asymptotic preserving schemes

There has been an extensive effort in the recent years to develop numerical methods for diffusion equations that are robust with respect to heterogeneities, anisotropy, and the mesh (see for instance [58] for an extensive discussion on such methods). On the other hand, the understanding of the role of nonlinear stability properties in the asymptotic behaviors of dissipative systems increased significantly in the last decades (see for instance [51], [72]).

Recently, C. Chainais-Hillairet and co-authors [3], [8] and [19] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization characteristic parameters, or in the long-time asymptotic. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes...) are required in [3], [8] and [19]. The schemes proposed in [16], [30] allow to handle nonlinear test functions in the analysis

without restrictions on the mesh and on the anisotropy of the problem. Combining the nonlinear schemes *à la* [16] with the methodology of [3], [8], [19] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would be also robust under adaptive mesh refinement.

3.1.3. Design and stability analysis of numerical methods for mixture problems

We aim at extending the range of the `NS2DDV-M` software by introducing new physical models, like for instance the Kazhikov and Smagulov model [68]. This will require a theoretical study for proving the existence of weak solutions to this model. Then, we will need to design numerical schemes to approximate these models and study their stability. We will also study their convergence following the path proposed in [62], [69].

3.2. Optimizing the computational efficiency

3.2.1. High order nonlinear numerical methods

The numerical experiments carried out in [16] show that in case of very strong anisotropy, the convergence of the proposed NNM becomes too slow (less than first order). Indeed, the method appears to strongly overestimate the dissipation. In order to make the method more competitive, it is necessary to estimate the dissipation in a more accurate way. Preliminary numerical results show that second order accuracy in space can be achieved in this way. One also aims to obtain (at least) second order accuracy in time without jeopardizing the stability. For many problems, this can be done by using so-called two-step backward differentiation formulas (BDF2) [59].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider *residual distribution* (RD) schemes, that appear as an alternative to finite volume methods. RD schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D yield reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [73], [64], with high-order accuracy [40], [39], or for parabolic problems [37], [38] make them very competitive. Relying on these breakthroughs, we aim at designing new RD schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2. A posteriori error control

The question of the *a posteriori* error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuska and Rheinboldt more than thirty years ago [44], *a posteriori* error estimators have been widely studied. We will take advantage of the huge corresponding bibliography database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g. [10] and [52]) to the temporal magnetodynamic one, for which space/time *a posteriori* error estimators have to be developed. A space/time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop *a posteriori* estimators for the variable density Navier-Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [5], [6] we developed combines features from finite elements and finite volumes. Fortunately, we do not start from scratch. Some recent references are devoted to the unsteady Navier-Stokes model in the finite element context [47], [77]. In the finite volume context, recent references deal with unsteady convection-diffusion equations [76], [43], [57] and [50]. We want to adapt some of these results to the variable density Navier-Stokes system, and to be able to design an efficient space-time remeshing algorithm.

3.2.3. Efficient computation of pairwise interactions in large systems of particles

Many systems are modeled as a large number of punctual individuals (N) which interact pairwise which means $N(N-1)/2$ interactions. Such systems are ubiquitous, they are found in chemistry (Van der Waals interaction between atoms), in astrophysics (gravitational interactions between stars, galaxies or galaxy clusters), in biology (flocking behavior of birds, swarming of fishes) or in the description of crowd motions. Building on the special structure of convolution type of the interactions, the team develops computation methods based on the Non Uniform Fast Fourier Transform [61]. This reduces the $O(N^2)$ naïve computational cost of the interactions to $O(N \log N)$, allowing numerical simulations involving millions of individuals.

4. Application Domains

4.1. Porous media flows

Porous media flows are of great interest in many contexts, like, e.g., oil engineering, water resource management, nuclear waste repository management, or carbon dioxyde sequestration. We refer to [46], [45] for an extensive discussion on porous media flow models.

From a mathematical point of view, the transport of complex fluids in porous media often leads to possibly degenerate parabolic conservation laws. The porous rocks can be highly heterogeneous and anisotropic. Moreover, the grids on which one intends to solve numerically the problems are prescribed by the geological data, and might be non-conformal with cells of various shapes. Therefore, the schemes used for simulating such complex flows must be particularly robust.

4.2. Corrosion and concrete carbonatation

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

From a mathematical point of view, the modeling of concrete carbonation (see [41]) as the modeling of corrosion in an underground repository (DPCM model developed by Bataillon *et al.* [1]) lead to systems of PDEs posed on moving domains. The coupling between convection-diffusion-reaction equations and moving boundary equations leads to challenging mathematical questions.

4.3. Complex fluid flows

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

Let us first focus on fluid mixture flows. The fluid is described by its density, its velocity and its pressure. These quantities obey mass and momentum conservation. On the one hand, when we deal with the 2D variable density incompressible Navier-Stokes equations, we aim to study the ability of the numerical scheme to reproduce some instabilities phenomena such as the Rayleigh-Taylor instability. On the other hand, diffuse interface models have gained renewed interest for the last few years in fluid mechanics applications. From a physical viewpoint, they allow to describe some phase transition phenomena. If the Fick's law relates the divergence of the velocity field to derivatives of the density, one obtains the so called Kazhikhov-Smagulov model [68]. Here, the density of the mixture is naturally highly non homogeneous, and the constitutive law accounts for diffusion effects between the constituents of the mixture. Models of this type can be used for instance to simulate powder-snow avalanches [6], low-Mach flows, or hydrodynamic models arising in combustion theory or transport of pollutants.

Kinetic theory of molecular gases models a gas as a system of elastically colliding spheres, conserving mechanical energy during impact. Once initialized, it takes a molecular gas not more than few collisions per particle to relax to its equilibrium state, characterized by a Maxwellian velocity distribution and a certain homogeneous density (in the absence of external forces). A granular gas is a system of dissipatively colliding, macroscopic particles (grains). This slight change in the microscopic dynamics (converting energy into heat) cause drastic changes in the behavior of the gas: granular gases are open systems, which exhibits self-organized spatio-temporal cluster formations, and has no equilibrium distribution. They can be used to model silos, avalanches, pollen or planetary rings.

The quantum models can be used to describe superfluids, quantum semiconductors, weakly interacting Bose gases or quantum trajectories of Bohmian mechanics. They have attracted considerable attention in the last decades, due in particular to the development of the nanotechnology applications. To describe quantum phenomena, there exists a large variety of models. In particular there exist three different levels of description: microscopic, mesoscopic and macroscopic. The quantum Navier-Stokes equations deal with a macroscopic description in which the quantum effects are taken into account through a third order term called the quantum Bohm potential. This Bohm potential arises from the fluid dynamical formulation of the single-state Schrödinger equation. The non-locality of quantum mechanics is approximated by the fact that the equations of state do not only depend on the particle density but also on its gradient. These equations were employed to model field emissions from metals and steady-state tunneling in metal- insulator- metal structures and to simulate ultra-small semiconductor devices.

4.4. Stratigraphy

The knowledge of the geology is a prerequisite before simulating flows within the subsoil. Numerical simulations of the geological history thanks to stratigraphy numerical codes allow to complete the knowledge of the geology where experimental data are lacking. Stratigraphic models consist in a description of the erosion and sedimentation phenomena at geological scales.

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

4.5. Low frequency electromagnetism

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

5. Highlights of the Year

5.1. Highlights of the Year

The paper [31], written by Giacomo Dimarco, Raphaël Loubère, Jacek Narski and Thomas Rey presents a new deterministic numerical scheme for the resolution of the full 7d Boltzmann equation. The scheme combines a robust and fast method for treating the transport part based on an innovative Lagrangian technique

supplemented with fast spectral solvers to treat the collision operator. This approach along with several implementation features related to the parallelization of the algorithm permits to construct an efficient simulation tool which is numerically tested against exact and reference solutions on classical problems arising in rarefied gas dynamics.

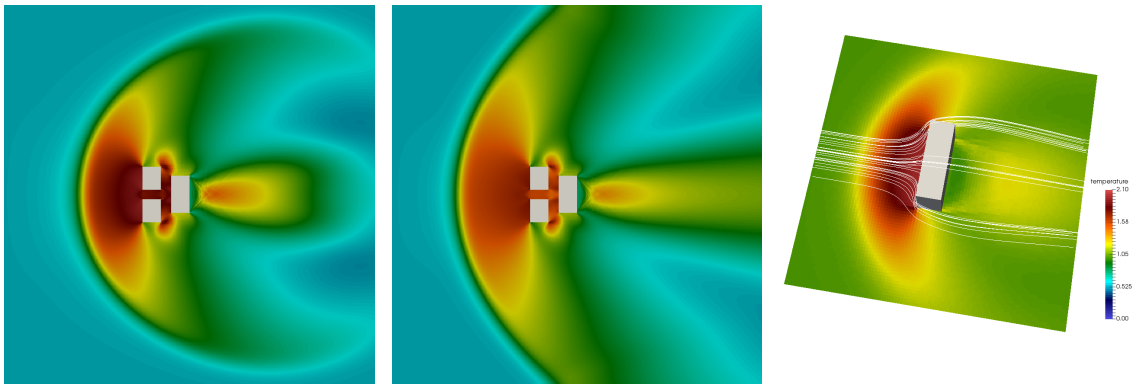

Figure 1. Simulation of a space shuttle atmospheric reentry (pictures from [31])

The paper presents results up to the very challenging 3D×3D case for unsteady flows arising during a space shuttle atmospheric reentry (which was simulated in the deterministic case in the paper for the first time up to our knowledge), which may serve as benchmark for future comparisons between different numerical methods for solving the multidimensional Boltzmann equation. For this reason, the paper also provide for each problem studied details on the implementation, computational cost and memory consumption as well as comparisons with the more standard BGK model or the limit model of compressible Euler equations.

6. New Software and Platforms

6.1. New Software

6.1.1. NS2DDV-M: a code for the simulation of inhomogeneous fluid flow

We develop and freely distribute a new version of the matlab code NS2DDV-M (equipped with a graphic interface and an accurate documentation) to promote new collaborations in the domain, allow some easy comparisons with concurrent codes on the same benchmark cases, and compare alternative numerical solution methods. Contacts: Caterina Calgaro & Emmanuel Creusé.

6.1.2. A scientific computing software for fast simulation of large systems of interacting particles

Benoît Merlet and Thomas Rey have developed a set of numerical codes for the numerical simulation of large systems of interacting particles. For a system of N particles, the number of interactions is a quadratic functions of N, leading to a quadratic cost of a brut force implementation. This fact limits simulations by "naïve" methods to systems with "only" tenth of thousands of particles. In order to treat larger systems (involving millions of particles), the team has implemented a method based on the Non Uniform Fast Fourier Transform which reduces the computation cost of the interactions to $O(N \log N)$. The NUFFT is used to handle the long range smooth interactions. To treat the possibly singular short range interactions (involving only neighboring particles) a quadtree-like method is used. The method is applied to two kind of problems : computations

of the dynamics of interacting particles where a standard ordinary differential equation is used; numerical optimization of the energy of a system of interacting particles thanks to a Nonlinear Conjugate Gradient method.
As an illustration of the efficiency of the code, the team has performed numerical experiments which support the following crystallization conjecture : in 2D, a large number of identical charged particles tend to arrange themselves into a regular triangular lattice.
A user friendly version will be released to the public in 2017.

6.1.3. The Fast Spectral Kinetic Scheme

The Fast Spectral Kinetic Scheme (FSKS), has been jointly developed by researchers from the universities of Ferrara, Toulouse, and Lille, and is the first high-order 7-dimensional deterministic numerical method capable of dealing with the complete physics of rarefied gas dynamics. The FSKM indeed solves the Boltzmann equation in 1 dimension of time, 3 of physical space and 3 of velocity space, and has been used to model accurately aerospace engineering problems such as space shuttle re-entry in the atmosphere or very rarefied gas flow in microscopic devices (Knudsen pump).

7. New Results

7.1. large-time behavior of some numerical schemes

In [19], C. Chainais-Hillairet, A. Jüngel and S. Schuchnigg prove the time decay of fully discrete finite-volume approximations of porous-medium and fast-diffusion equations with Neumann or periodic boundary conditions in the entropy sense. The algebraic or exponential decay rates are computed explicitly. In particular, the numerical scheme dissipates all zeroth-order entropies which are dissipated by the continuous equation. The proofs are based on novel continuous and discrete generalized Beckner inequalities.

In [13], M. Bessemoulin-Chatard and C. Chainais-Hillairet study the large-time behavior of a numerical scheme discretizing drift-diffusion systems for semiconductors. The numerical method is based on a generalization of the classical Scharfetter-Gummel scheme which allows to consider both linear or nonlinear pressure laws.They study the convergence of approximate solutions towards an approximation of the thermal equilibrium state as time tends to infinity, and obtain a decay rate by controlling the discrete relative entropy with the entropy production. This result is proved under assumptions of existence and uniform-in-time L^∞ estimates for numerical solutions, which are then discussed.

The question of uniform-in-time L^∞ estimates for the scheme proposed in [13] has then be tackled by M. Bessemoulin-Chatard, C. Chainais-Hillairet and A. Jüngel. The result is obtained *via* a Moser's iteration technique adapted to the discrete setting. Related to this question, the existence of a positive lower bound for the numerical solution of a convection-diffusion equation has been studied by C. Chainais-Hillairet, B. Merlet and A. Vasseur. They apply a method due to De Giorgi in order to establish a positive lower bound for the numerical solution of a stationary convection-diffusion equation. These results are submitted for publication in the FVCA8 conference (to be held in June 2017).

In [11] B. Merlet *et al.* consider a second-order two-step time discretization of the Cahn-Hilliard equation with an analytic nonlinearity. They study the long time behavior of the discrete solution and show that if the time-step is chosen small enough, the sequence generated by the scheme converges to a steady state as time tends to infinity. Convergence rates are also provided. This parallels the behavior of the solutions of the non-discretized solutions and shows the reliability of the scheme for long time simulations. The method of proof is based on the Lojasiewicz-Simon inequality and on the study of the pseudo-energy associated with the discretization which is shown to be non-increasing.

7.2. Theoretical and numerical analysis of corrosion models

The Diffusion Poisson Coupled Model [1] is a model of iron based alloy in a nuclear waste repository. It describes the growth of an oxide layer in this framework. The system is made of a Poisson equation on the electrostatic potential and convection-diffusion equations on the densities of charge carriers (electrons, ferric cations and oxygen vacancies). The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations. Numerical experiments done for the simulation of this model with moving boundaries show the convergence in time towards a pseudo-steady-state. C. Chainais-Hillairet and T. O. Gallouët prove in [18] the existence of pseudo-stationary solutions for some simplified versions of the DPCM model. They also propose a new scheme in order to compute directly this pseudo-steady-state. Numerical experiments show the efficiency of this method.

The modeling of concrete carbonation also leads to a system of partial differential equations posed on a moving domain. C. Chainais-Hillairet, B. Merlet and A. Zurek propose and analyze a finite volume scheme for the concrete carbonation model. They prove the convergence of the sequence of approximate solutions towards a weak solution. Numerical experiments show the order 2 in space of the scheme and illustrate the $\sqrt{t}$ law of propagation of the size of the carbonated zone. This result is submitted for publication.

7.3. Modeling and numerics for porous media flows

In [16], C. Cancès and C. Guichard propose a nonlinear Control Volume Finite Elements method with upwinding in order to solve possibly nonlinear and degenerate parabolic equations. This method was designed in order to preserve at the discrete level the positivity and the nonlinear stability of the solutions. In [25], A. Ait Hammou Oulhaj, C. Cancès, and C. Chainais-Hillairet extend the approach of [16] to the more complex case of Richards equation modeling saturated/unsaturated flows in anisotropic porous media. The additional complexity comes from the fact that convective terms and elliptic degeneracy are considered in [25]. The scheme preserves at the discrete level the nonnegativity and the nonlinear stability of the solutions. Its convergence is rigorously proved, and numerical results are provided in order to illustrate the behavior of the scheme.

In [49], C. Cancès, T. O. Gallouët, and L. Monsaingeon show that the equations governing two-phase flows in porous media have a formal gradient flow structure. The goal of the longer contribution [29] is then twofold. First, it extends the variational interpretation of [49] to the case where an arbitrary number of phases are in competition to flow within a porous medium. Second, we provide rigorous foundations to our claim. More precisely, the convergence of a minimizing movement scheme *à la* Jordan, Kinderlehrer, and Otto [66] is shown in [29], providing by the way a new existence result for multiphase flows in porous media. The result relies on advances tools related to optimal transportation [75], [74].

7.4. Complex fluid flows: modeling, analysis and numerics

The analysis of the Kazhikhov-Smagulov model was given by Bresch at al. [48] (see also reference therein). These authors prove the global existence of weak solution without assuming small data and without any assumption on the diffusivity coefficient. Following the physical experiment given by Joseph [67], we introduce a Korteweg stress tensor in the previous model. The theory of Korteweg considers the possibility that motions can be driven by additional stresses associated with gradients of density. In process of slow diffusion on miscible incompressible fluids, for example water and glycerin, dynamical effects which mimic surface tension can arise in thin mixing layers where the gradients of density are large. In the context of the PhD thesis of Meriem Ezzoug (July 2016, University of Monastir, Tunisia), C. Calgaro and co-authors study a multiphase incompressible fluid model, called the Kazhikhov-Smagulov-Korteweg model. They prove in [14] that this model is globally well posed in a 3D bounded domain.

In [21], P.-E. Jabin and T. Rey investigate the behavior of granular gases in the limit of small Knudsen number, that is very frequent collisions. They deal with the physically relevant strongly inelastic case, in one dimension of space and velocity. The study of such limit, also known as hydrodynamic limit is to give a reduced description of the kinetic equation, using a fluid approximation. They are able to prove the convergence of

the particle distribution function toward a monokinetic distribution, whose moments verify the pressureless Euler system. The proof relies on dispersive relations at the kinetic level, which leads to the so-called Oleinik property at the limit, and in particular stability of the solution to the fluid problem.

In [34], I. Lacroix-Violet and A. Vasseur present the construction of global weak solutions to the quantum Navier-Stokes equation, for any initial value with bounded energy and entropy. The construction is uniform with respect to the Planck constant. This allows to perform the semi-classical limit to the associated compressible Navier-Stokes equation. One of the difficulty of the problem is to deal with the degenerate viscosity, together with the lack of integrability on the velocity. The method is based on the construction of weak solutions that are renormalized in the velocity variable. The existence, and stability of these solutions do not need the Mellet-Vasseur inequality [71].

In [31], G. Dimarco, R. Loubère, J. Narski and T. Rey deal with the extension of the Fast Kinetic Scheme (FKS) [55], [56] originally constructed for solving the BGK equation, to the more challenging case of the Boltzmann equation. The scheme combines a robust and fast method for treating the transport part based on an innovative Lagrangian technique supplemented with fast spectral schemes to treat the collisional operator by means of an operator splitting approach. This approach along with several implementation features related to the parallelization of the algorithm permits to construct an efficient simulation tool which is numerically tested against exact and reference solutions on classical problems arising in rarefied gas dynamic. They present results up to the 3D×3D case for unsteady flows for the Variable Hard Sphere model which may serve as benchmark. For this reason, they also provide for each problem details on the computational cost and memory consumption as well as comparisons with the BGK model or the limit model of compressible Euler equations.

7.5. Improving the numerical efficiency of numerical methods

In this section, we gather contributions in which a methodology was introduced in order to reduce the computational cost at fixed accuracy or to improve the accuracy for a fixed computational cost.

In [20], E. Creusé and his collaborators generalized some of their previous results on residual a posteriori error estimators for low electromagnetism [10] , [52] to the case where some voltage or current excitation is specified in the model (see e.g. such models in [63], [42]). It consequently led to consider different formulations and to overcome some specific difficulties in order to derive the reliability of the involved estimators.

It is now well accepted that well-balanced schemes are of great interest in order to compute accurate solutions to systems of PDEs (see for instance [60]). In [36], L. Pareschi and T. Rey propose a systematic way to tune classical numerical schemes in order to make them well-balanced and asymptotic preserving. Inspired by micro-macro decomposition methods for kinetic equations, they present a class of schemes which are capable to preserve the steady state solution and achieve high order accuracy for a class of time dependent partial differential equations including nonlinear diffusion equations and kinetic equations. Extension to systems of conservation laws with source terms are also discussed, as well as Total Variation Diminishing preserving properties.

The contribution [26] by K. Brenner and C. Cancès is devoted to the improvement of the behavior of Newton's method when solving degenerate parabolic equations. Such equations are very common for instance in the context of complex porous media flows. In [26], the presentation focuses on Richards equation modeling saturated/unsaturated flows in porous media. The basic idea is the following: Newton's method is not invariant by nonlinear change of variables. The choice of the primary variable then impacts the effective resolution of the nonlinear system provided by the scheme. The idea developed in [26] is then to construct an abstract primary variable to facilitate Newton's method's convergence. This leads to an impressive reduction of the computational cost, a better accuracy in the results and an strong robustness of the method w.r.t. the nonlinearities appearing in the continuous model.

7.6. Variational modeling and analysis

Bose-Einstein condensates are a unique way to observe quantum effects at a (relatively) large scale. The fundamental states of such condensates are obtained as minimizers of a Gross-Pitaievskii functional. In [33],

M. Goldman and B. Merlet consider the case of a two component Bose-Einstein condensate in the strong segregation regime (the energy favors spatial segregation of the two different Boson species). They identify two different regimes in the strong segregation and small healing length limit. In one of these regimes, the relevant limit is an interesting weighted isoperimetric problem which explains some of the numerical simulations of [70].

In [32], B. Merlet *et al.* consider the branched transportation problem in 2D associated with a cost per unit length of the form $1 + \alpha m$ where m denotes the amount of transported mass and $\alpha > 0$ is a fixed parameter (the limit case $\alpha = 0$ corresponds to the classical Steiner problem). Motivated by the numerical approximation of this problem, they introduce a family of functionals $(\{F_\varepsilon\}_{\varepsilon>0})$ which approximate the above branched transport energy. They justify rigorously the approximation by establishing the equicoercivity and the Γ-convergence of F_ε as $\varepsilon \downarrow 0$. These functionals are modeled on the Ambrosio-Tortorelli functional and are easy to optimize in practice (the algorithm amounts to perform repetitively the alternate optimization of two quadratic functionals). Numerical evidences of the efficiency of the method are presented.

7.7. Miscellaneous

This section gathers results from members of the team that are not directly related to the core of the scientific program of the team.

In [12], I. Violet-Lacroix and co-authors consider the derivation of continuous and fully discrete artificial boundary conditions for the linearized Korteweg-de-Vries equation. They are provided for two different numerical schemes. The boundary conditions being nonlocal with respect to time variable, they propose fast evaluations of discrete convolutions. Various numerical tests are presented to show the effectiveness of the constructed artificial boundary conditions.

A semi-discrete in time Crank-Nicolson scheme to discretize a weakly damped forced nonlinear fractional Schrödinger equation in the whole space ($\mathbb{R}$ is considered by C. Calgaro and co-authors in [28]. They prove that such semi-discrete equation provides a discrete infinite dimensional dynamical in $H^\alpha(\mathbb{R})$ that possesses a global attractor. They show also that if the external force is in a suitable weighted Lebesgue space then this global attractor has a finite fractal dimension.

In [35], F. Nabet considers a finite-volume approximation, based on a two point flux approximation, for the Cahn-Hilliard equation with dynamic boundary conditions. An error estimate for the fully-discrete scheme on a possibly smooth non-polygonal domain is proved and numerical simulations which validate the theoretical result are given.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

C. Cancès supervises the PhD Thesis of Nicolas Peton at IFPEN since October 15, 2015. The bilateral contract enters the framework agreement between Inria and IFPEN.

9. Partnerships and Cooperations

9.1. Regional Initiatives

The PhD program of Ahmed Aït Hammou Oulhaj is partially supported (50%) by the Region Nord-Pas-de-Calais.

9.2. National Initiatives

9.2.1. ANR

C. Cancès is the coordinator of the ANR GEOPOR project. (https://www.ljll.math.upmc.fr/cances/ANR-GEOPOR/). This project aims to study realistic models for complex porous media flows from a variational point of view, and to take advantage of this new approach to design and analyze some efficient numerical methods.

Title: Approche géométrique pour les écoulements en milieux poreux : théorie et numérique.

Type: Jeunes Chercheuses Jeunes Chercheurs SIMI 1- 2013

ANR Reference: ANR-13-JS01-0007-01

Coordinator: Clément Cancès, Inria Lille - Nord Europe.

Duration: January 2014 – June 2017

I. Lacroix is the local coordinator at Université Lille 1 of the ANR BECASIM project (http://becasim.math.cnrs.fr/). This ANR project gathers mathematicians with theoretical and numerical backgrounds together with engineers. The objective is to develop numerical methods to accurately simulate the behavior of Bose-Einstein condensates.

Title: Simulation numérique avancée pour les condensats de Bose-Einstein.

Type: Modèles Numériques - 2012

ANR reference: ANR-12-MONU-0007

Coordinator: Ionut DANAILA, Université de Rouen.

Duration: January 2013 - November 2017.

C. Chainais-Hillairet is a member of the ANR MOONRISE project (http://moonrise.math.cnrs.fr/). The MOONRISE project aims at exploring modeling, mathematical and numerical issues originating from the presence of high oscillations in nonlinear PDEs mainly from the physics of nanotechnologies and from the physics of plasmas.

Title: Modèles, Oscillations et schémas numériques.

Type: Fondements du numérique (DS0705) - 2014

ANR reference: ANR-14-CE23-0007

Coordinator: Florian MEHATS, Université de Rennes 1.

Duration: October 2014 - September 2019.

B. Merlet is a member of the ANR GEOMETRYA project (https://www.ljll.math.upmc.fr/lemenant/GEOMETRYA/) The GEOMETRYA project addresses several problems within the framework of geometric measure theory, from both theoretical and numerical viewpoints. Most of these problems are derived from the modeling of physical phenomenons. The main topics are: the Geometric Measure Theory in singular metric spaces, the Plateau problem, the Mumford-Shah functional, irrigation and branched transport problems, the Willmore energy.

Title: Théorie gémométrique de la mesure et applications

Type: Blanc SIMI 1 - 2012

ANR reference: ANR-12-BS01-0014

Coordinator: Hervé Pajot, Université Joseph Fourier (Grenoble).

Duration: january 2013 - december 2016.

9.2.2. Labex CEMPI

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

Coordinator: Stephan De Bièvre.

Duration: January 2012 - December 2019.

Partners: Laboratoire Paul Painlevé and Laser physics department (PhLAM), Université Lille 1.

The “Laboratoire d’Excellence” Centre Européen pour les Mathématiques, la Physique et leurs interactions (CEMPI), a project of the Laboratoire de Mathématiques Paul Painlevé and the Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), was created in the context of the "Programme d’Investissements d’Avenir" in February 2012.

The association Painlevé-PhLAM creates in Lille a research unit for fundamental and applied research and for training and technological development that covers a wide spectrum of knowledge stretching from pure and applied mathematics to experimental and applied physics.

One of the three focus areas of CEMPI research is the interface between mathematics and physics. This focus area encompasses three themes. The first is concerned with key problems of a mathematical, physical and technological nature coming from the study of complex behavior in cold atoms physics and non-linear optics, in particular fibre optics. The two other themes deal with fields of mathematics such as algebraic geometry, modular forms, operator algebras, harmonic analysis and quantum groups that have promising interactions with several branches of theoretical physics.

9.3. International Research Visitors

9.3.1. Visits of International Scientists

Alexis Vasseur (UT Austin, Texas) was invited in Lille in June 2016 thanks to a support of the Labex CEMPI.

We have a long time collaboration with Ansgar Jüngel’s team from TU Wien. In 2016, we hosted 2 PhD students advised by A. Jüngel : Anita Gerstenmayer for a first one month and a second one week research stays, Polina Shpartko for a one week research stay.

Kyle Talbot, a PhD student advised by Jérôme Droniou at Monash University (Melbourne, Australia), and Ward Melis, a PhD student supervised by Giovanni Samaey (KU Leuven, Belgium), spent both one week in our team.

9.3.2. Visits to International Teams

Claire Chainais-Hillairet and Ingrid Lacroix-Violet visited Ansgar Jüngel in Vienna (May 17-20, 2016). Claire Chainais-Hillairet visited Jürgen Fuhrmann, Patricio Farrell and Nella Rotundo at WIAS (Berlin) to work on numerical schemes for semiconductor devices models. Clément Cancès visited Léonard Monsaingeon in Lisbon (Feb. 29 to March 4, 2016) Clément Cancès and Flore Nabet visited Daniel Matthes in Munich (June 6-8).

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

The team organized the second edition of the conference ABPDE *Asymptotic Behavior of systems of PDE arising in physics and biology: theoretical and numerical points of view* in Lille (June 15-17, 2016). See https://indico.math.cnrs.fr/event/939/.

The kick-off meeting of the GdR MaNu was organized by Clément Cancès, Corinne Jamroz, and Nicolas Seguin (Univ. Rennes) in Saint-Valery-sur-Somme in October 2016. See https://indico.math.cnrs.fr/event/1575/.

Claire Chainais-Hillairet and Clément Cancès are members of the organizing committee of the eighth symposium on Finite Volumes for Complex Applications (FVCA8) to be held in Lille next June 2017. See https://indico.math.cnrs.fr/event/1299/.

I. Lacroix-Violet is in charge of the organization of the weekly seminary of the Numerical Analysis and Partial Differential Equations (ANEDP) research team at the Laboratoire Paul Painlevé, Université de Lille 1.

10.1.2. Journal

10.1.2.1. Member of the editorial boards

C. Chainais-Hillairet is a member of the editorial board of the North-Western European Journal of Mathematics (`http://math.univ-lille1.fr/ nwejm/`) and of the International Journal on Finite Volumes (`http://www.i2m.univ-amu.fr/IJFV/`).

10.1.2.2. Reviewer - Reviewing activities

The members of the team RAPSODI reviewed numerous papers for numerous international journals.

10.1.3. Invited Talks

C. Cancès was an invited speaker at the international conference *Advanced numerical methods: recent developments, analysis, and applications* held in the framework of the IHP quarter on *Numerical Methods for PDEs*.

10.1.4. Scientific Expertise

C. Chainais-Hillairet and E. Creusé were experts for the HCERES.

10.1.5. Research Administration

Clément Cancès is the head of the MaNu Research Group (GdR MaNu, http://gdr-manu.math.cnrs.fr/) funded by the Institute for Mathematical Sciences and Interaction (INSMI) of the French National Center for Research (CNRS).

E. Creusé is AMIES Facilitator (Agency for the Interaction of Mathematics with Enterprise and Society) for the Northern France area. He is also the industrial representative of the Paul Painlevé Laboratory.

C. Chainais-Hillairet is head of the Commission Emplois de Recherche of the Lille - Nord Europe Inria research center.

Caterina Calgaro is a member of the Commission de la Formation et de la Vie Universitaire of the Academic Council of Université Lille 1.

Ingrid Lacroix-Violet, Benoît Merlet and Thomas Rey are members of the Conseil du Laboratoire Paul Painlevé.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

The group is strongly involved in teaching at the Université Lille 1. C. Calgaro and C. Chainais-Hillairet are in charge respectively of the Master of Mathematical Engineering and of the Master 2 of Scientific Computing, whereas E. Creusé is responsible of the "Cursus Master Ingénierie" in Mathematics, Lille 1 University. C. Cancès gives lectures at Polytech' UPMC.

10.2.2. Supervision

PhD : Pierre-Louis Colin has defended his PhD thesis on June 27, 2016. *Analyse numérique de modèles de dérive-diffusion : convergence et comportements asymptotiques*, Univ. Lille 1. advisors: C. Chainais-Hillairet and I. Lacroix-Violet.

PhD : Roberta Tittarelli, *A posteriori error estimators for Maxwell equations in potential and temporal formulations*, Univ. Lille 1, defended on September 27, 2016, advisors: E. Creusé & F. Piriou.

PhD in progress: Ahmed Aït Hammou Oulhaj, *Design and analysis of nonlinear numerical schemes for solving parabolic problems: application to porous media flows*, since 01/10/2014, advisors: C. Cancès & C. Chainais-Hillairet.

PhD in progress: Claire Colin, *Analyse numérique et simulations de modèles multifluides*, since 01/10/2015, advisors: C. Calgaro & E. Creusé.

PhD in progress: Luca Ferrari, *Line energies and applications to image reconstruc- tion of partially masked objects*, since 01/09/2015, advisors: A. Chambolle (CNRS & CMAP, École Polytechnique) & B. Merlet.

PhD in progress: Nicolas Peton, *Numerical methods for a stratigraphic model with nonlinear diffusion and moving frontier areas*, 15/10/2015, C. Cancès, Q. H. Tran (IFPEN) & S. Wolf (IFPEN).

PhD in progress: Antoine Zurek, *Numerical and theoretical analysis of models describing the corrosion of materials*, since 01/10/2016, advisors: C. Chainais-Hillairet & B. Merlet.

10.2.3. Juries

C. Cancès reported on Mayya Groza's PhD thesis, defended on November 10, 2016 at Univ. Nice - Sophia Antipolis. Title: *Modélisation et discrétisation des écoulements diphasiques en milieux poreux avec réseaux de fractures discrètes*

C. Chainais-Hillairet reported on Polina Shpartko's PhD thesis, defended on June 6, 2016 at TU Wien. Title: *Analytical and numerical study of drift-diffusion models for spin-transport in semiconductors*. She was also a member of the jury of Toko Kamtchueng's PhD thesis, defended on December 7, 2016 at Université d'Orléans. Title: *Formulation généralisée du transport réactif pour les modèles de réseaux de pores saturés en eau*.

E. Creusé reported on Azba Riaz' PhD thesis, defended on April 4, 2016 at Univ. Cergy-Pontoise. Title: *A new discontinuous Galerkin formulation for time dependant Maxwell's equation : a priori and a posteriori error estimation*. He was also a member of the jury of Florent Dewez' PhD thesis defended on November 3, 2016 at Univ. Lille 1. Title: *Estimations sans pertes pour des méthodes asymptotiques et notion de propagation pour des équations dispersives.*

B. Merlet reported François Dayrens' PhD thesis, defended in july 1st, 2016 at University Lyon 1. Title: *Minimizing movement and gradient flows for second order geometric functionals*.

10.3. Popularization

C. Calgaro is in charge of the communication of "Laboratoire Paul Painlevé" and she is in charge of the relation between the University of Lille 1 and high schools. Accordingly, she organizes various events which promote mathematics among young peoples like

Les Mathématiques itinérantes (http://mathematiques.univ-lille1.fr/Ouvertures/Mathematiques-itinerantes/)

La semaine des Mathématiques (http://mathematiques.univ-lille1.fr/Ouvertures/Mathematiques-itinerantes/)

Stage en sciences pour les élèves de seconde (http://www.univ-lille1.fr/etudes/stageseconde)

Members of the team participate regularly in theses actions.

Thomas Rey animates a Mathematics workshop (Math en Jeans) in the Adolphe Delégorgue middle school at Courcelles-lès-Lens.

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Major publications by the team in recent years

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