



Activity Report 2015

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

Creation of the Team: 2015 August 01

Keywords:

Computer Science and Digital Science:

- 6.1. - Mathematical Modeling
- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.1.4. - Multiscale modeling
- 6.2. - Scientific Computing, Numerical Analysis & Optimization
- 6.2.1. - Numerical analysis of PDE and ODE

Other Research Topics and Application Domains:

- 3.3.1. - Earth and subsoil
- 3.4.2. - Industrial risks and waste
- 4.1.1. - Oil, gas
- 4.1.2. - Nuclear energy

The research team RAPSODI was created on August 1, 2015. It is therefore only 5 month old.

1. Members

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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 the 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 [9], and mechanics of complex inhomogeneous fluids arising in avalanches [12] or in porous media [47].

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

2.2. Scientific Context

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

Let us mention for example the review paper by J. Droniou [55], 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 [55]. 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 [15]. The idea and the techniques introduced in [15] 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 [60], 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 [12]. 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 [53], 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 [52], the dead-oil model for porous media flows [49] or the Maxwell equations in their quasi-static approximation for some eddy current problems [9] and [51]. 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 [15], [35] 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 [55] 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 [50], [65]).

Recently, C. Chainais-Hillairet and co-authors [3], [7] and [17] 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], [7] and [17]. The schemes proposed in [15], [35] 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* [15] with the methodology of [3], [7], [17] 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 [61]. 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 [58], [62].

3.2. Optimizing the computational efficiency

3.2.1. High order nonlinear numerical methods

The numerical experiments carried out in [15] 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) [56].

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 [66], [59], with high-order accuracy [43], [42], or for parabolic problems [40], [41] 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 [45], *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. [9] and [51]) 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], [12] 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 [48], [68]. In the finite volume context, recent references deal with unsteady convection-diffusion equations [67], [44], [54] and [49]. 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.

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 dioxide sequestration. We refer to [47], [46] 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

The concept for long term storage of high-level radioactive waste in France under study is based on an underground repository. The waste shall be confined in a glass matrix and then placed into cylindrical steel canisters. These containers shall be placed into micro-tunnels in the highly impermeable Callovo-Oxfordian claystone layer at a depth of several hundred meters. At the request of the French nuclear waste management agency ANDRA, investigations are conducted to optimize and finalize this repository concept with the aim to ensure its long-term safety and its reversibility. The long-term safety assessment of the geological repository has to take into account the degradation of the carbon steel used for the waste overpacks and the cell disposal liners, which are in contact with the claystone formation. This degradation is mainly caused by generalized corrosion processes which form a passive layer on the metal surface consisting of a dense oxide inner layer and a porous hydroxide outer layer in contact with the groundwater in the pore space of the claystones. The processes take place under anaerobic conditions, since the groundwater is anoxic.

As a tool to investigate the corrosion processes at the surface of the carbon steel canisters, the Diffusion Poisson Coupled Model (DPCM) for corrosion has been developed by Bataillon *et al.* [1]. The numerical approximation of this corrosion model and some associated models by accurate and efficient methods is challenging. Theoretical study of the models (existence of solutions, long time behavior) is also worth of interest.

4.3. Complex fluid flow simulations

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

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 [61]. 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. The first phenomena that we want to reproduce are the powder-snow avalanches. We investigate the influence of the characteristics parameters (Froude, Schmidt and Reynolds numbers) on the progression of the front. Other similar hydrodynamic models arise 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.

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 research team RAPSODI was created on August 1, 2015.

A new nonlinear numerical method for solving possibly degenerate parabolic problems with gradient flow structure was proposed and analyzed by C. Cancès & C. Guichard in [35]. This method is second order accurate in space and preserves the variational structure of the continuous problem, ensuring by the way the decay of the physical entropy. Moreover, it is more robust with respect to strong anisotropy ratios than the method proposed in [15] that was only first order accurate in space.

6. New Software and Platforms

6.1. New Software and Platforms

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.

7. New Results

7.1. Design and analysis of advanced finite volumes schemes

The fact that a numerical method is able to handle nonlinear test functions in its numerical analysis is crucial in order to ensure its physical relevance, and consequently its good behavior.

In [15], C. Cancès and C. Guichard proposed a first nonlinear numerical method to solve possibly degenerate parabolic equations with anisotropy on general simplicial meshes. The nonlinear control volume finite element (CVFE) scheme is based on P1 finite elements with mass-lumping combined with a tricky upwinding of the mobilities. The method has the remarkable property of preserving the positivity of the solutions. Moreover, it ensures the decay of the physical entropy. Its convergence is proved in [15] and numerical results are exhibited. In particular, they show that the method is first order accurate in space in standard situations, but can lack robustness w.r.t. the anisotropy in some particularly unfavorable situations.

This drawback was corrected by C. Cancès and C. Guichard in [35], where a second order in space method based on the so-called VAG scheme [57] was proposed. This method is able to handle very general grids, heterogeneous data and strong anisotropy ratios. Moreover, it preserves at the discrete level the variational structure of the continuous problem, yielding the nonlinear stability of the scheme. A complete convergence analysis was performed in [35]. The numerical results presented in [35] show that the robustness default of the first nonlinear method [15] has been corrected.

In [36], C. Cancès *et al.* proposed and analyzed a nonlinear CVFE scheme for a degenerate Keller-Segel model with anisotropic and heterogeneous diffusion tensors. The scheme is based on the one proposed in [15]. The convergence of the scheme is proved under very general assumptions. Finally, some numerical experiments are carried out to prove the ability of the scheme to tackle degenerate anisotropic and heterogeneous diffusion problems over general meshes without jeopardizing the positivity of the solutions.

In [17], 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 [18], C. Chainais-Hillairet, A. Jüngel and P. Shpartko propose and analyze a numerical scheme for a spinorial matrix-diffusion model for semiconductors. The model consists of strongly coupled parabolic equations for the electron density matrix or, alternatively, of weakly coupled equations for the charge and spin-vector densities, coupled to the Poisson equation for the electric potential. The main features of the numerical scheme are the preservation of nonnegativity and L^∞ bounds of the densities and the dissipation of the discrete free energy. The existence of a bounded discrete solution and the monotonicity of the discrete free energy are proved. The fundamental ideas are reformulations using spin-up and spin-down densities and certain projections of the spin-vector density, free energy estimates, and a discrete Moser iteration. Furthermore, numerical simulations of a simple ferromagnetic-layer field-effect transistor in two space dimensions are presented.

In [32], 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 finite volume in space, implicit in time, and the numerical fluxes are 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.

7.2. A posteriori analysis and computational optimization

In 2015, E. Creusé *et al.* have developed a posteriori error estimators for the harmonic potential formulations of the Maxwell system, in order to simulate eddy-current problems arising in the context of quasi-static approximations. The originality of our contribution is to provide estimators with sharp bounds and explicit constants. It was achieved by solving in the same time the so-called " \mathbf{A}/φ " and " \mathbf{T}/Ω " potential formulations [38]. If this way to proceed was already known and usually used for stationary problems, the extension to harmonic ones constitutes the novelty of our contribution. It was in particular necessary to prove some superconvergence properties of additional terms. The reliability as well as the local efficiency of the derived estimator have been established without any generic constant, and numerical tests clearly illustrate their optimal behavior, from academic benchmarks to more industrial ones.

Another track to optimize the computational effort consists in refining and coarsening the model. This approach is based on the following ansatz : the more the model is complex, the more expensive are the computations. This approach was used by F. Filbet and T. Rey in [23] to simulate kinetic equations, the kinetic equations being replaced by cheaper hydrodynamic limits when it is relevant. The same idea was used

in H. Mathis *et al.* [27] in order to simulate complex flows modeled by hyperbolic systems with relaxation. A rigorous error analysis of such a model adaptation procedure was performed on a simplified model by C. Cancès *et al.* in [13].

7.3. Modeling and numerical simulation of complex fluids

Recently, C. Calgaro *et al.* compared some very recent numerical schemes for the resolution of incompressible variable density flows; namely an Hybrid Finite Volume/Finite Element scheme, and a Discrete Duality Finite Volume one [34]. This work was performed in collaboration with the Inria team COFFEE (Inria Nice Sophia-Antipolis). In addition to this original and attentive comparison, our main contribution has been to improve the way to implement the Neumann boundary condition on the density, when a second-order accurate scheme is considered in space. Indeed, for some critical situations such as the simulation of Rayleigh-Taylor instabilities using unstructured meshes, this point is crucial to avoid unphysical numerical instabilities in the vicinity of the boundaries corresponding to symmetric axis. The obtained results are very promising, and constitute an important step towards the simulation of more complex models on which we are working at the moment.

In [25], M. Gisclon and I. Lacroix-Violet consider the barotropic compressible quantum Navier-Stokes equations with a linear density dependent viscosity and its limit when the scaled Planck constant vanish. Following recent works on degenerate compressible Navier-Stokes equations, we prove the global existence of weak solutions by the use of a singular pressure close to vacuum. With such singular pressure, we can use the standard definition of global weak solutions which also allows to justify the limit when the scaled Planck constant denoted by ε tends to 0.

The H-theorem, originally derived at the level of the Boltzmann nonlinear kinetic equation for a dilute gas undergoing elastic collisions, strongly constrains the velocity distribution of the gas to evolve irreversibly towards equilibrium. As such, the theorem could not be generalized to account for dissipative systems: the conservative nature of collisions is an essential ingredient in the standard derivation. The work [24] gives the first strong numerical evidences, along with a proof for a simplified model, of dissipation of the Boltzmann entropy (the so-called H-theorem) for solutions to the granular gases equation. This dissipative kinetic equation describes the non-equilibrium behavior of a gas composed of macroscopic particles, namely complex fluids such as avalanches, pollens flows or planetary rings.

7.4. 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), supplemented with coupled Robin boundary conditions. The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations.

In [19], C. Chainais-Hillairet and I. Lacroix-Violet consider a simplified version of this model, where only two charge carriers are taken into account and where there is no evolution of the layer thickness. They prove the existence of a solution for the time-dependent simplified model.

P.-L. Colin, C.Chainais-Hillairet and I. Lacroix-Violet have performed in [16] the numerical analysis of the numerical scheme presented in [2] for the same model. The scheme is a Euler implicit in time scheme with Scharfetter-Gummel approximation of the convection-diffusion fluxes. They prove existence of a solution to the scheme, a priori estimates satisfied by the solution and convergence of the numerical scheme to a weak solution of the corrosion model.

Numerical experiments done for the simulation of the full DPCM model with moving boundaries shows the convergence in time towards a pseudo-steady-state. C. Chainais-Hillairet and T. O. Gallouët show in [37] 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.

7.5. 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 [39], 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 [63].

In [14], C. Cancès *et al.* show that the equations that are classically used for modeling the motion of two incompressible immiscible phases in a porous medium can be formally reinterpreted as the gradient flow of the free energy in a degenerated geometry closely related to the Wasserstein metric. This extends to realistic models the seminal approach [65] and the more recent one [64].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Roberta Tittarelli was in PhD under the co-direction of Emmanuel Creusé (with S. Nicaise, LAMAV Valenciennes and F. Piriou, L2EP Lille 1) on an EDF R&D Support (CIFRE) from October 2012 to October 2015. She worked on a posteriori error estimators for problems arising in low-frequency electromagnetics. She developed residual estimators for unsteady problems, as well as equilibrated ones for harmonic formulations (see section 6.2 for new results about this last point). Its contributions have been implemented in the EDF R&D code "Carmel-3D", and allow to improve the simulations by providing an efficient tool driving the mesh refinement algorithms. She is now on an ATER support at Lille 1 University and and the PhD's defense should occur before the middle of 2016.

C. Cancès supervises the PhD Thesis of Nicolas Peton at IFPEN since October 15, 2015. The bilateral contract should be signed in the forthcoming weeks.

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 - December 2016.

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 phenomena. 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 géométrique 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 behaviour 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.

9.2.3. PEPS égalité

I. Lacroix-Violet was the coordinator of the project *Theoretical and numerical study of the quantum Navier-Stokes system* supported by the Institute for Mathematical Sciences and Interaction (INSMI) of the French National Center for Research (CNRS) in the framework of the PEPS égalité call for proposal. In this project, the members have considered the quantum Navier-Stokes equations with a linear density dependent viscosity from a numerical and a theoretical point of view. From a theoretical point of view, I. Lacroix-Violet, M. Gisclon and D. Bresch studied the limit of the system when the viscosity parameter tends to zero. This work is still in progress. From a numerical point of view, following the recent work of D. Bresch, F. Couderc, P. Noble et J.-P. Vila, I. Lacroix-Violet and A. Jüngel have tried to design some numerical methods for the simulation of the complete model.

Title: Theoretical and numerical study of the quantum Navier-Stokes system

Coordinator: I. Lacroix-Violet

Members-: M. Gisclon (Université Savoie Mont-Blanc) & A. Jüngel (Technische Universität Wien)

Duration: January 2015 June 2015

9.3. International Research Visitors

9.3.1. Visits of International Scientists

We have a long-time collaboration with Ansgar Jüngel's research group from TU Wien. We hosted several PhD students during the last years and Ansgar Jüngel came for a one week research stay in 2015.

Patrick Dular from Liège University (Belgium) was invited in Lille from May, 15 to June, 15 on a Labex CEMPI support.

Ezzeddine Zahrouni from Nabeul University (Tunisia) was invited in Lille from Mai, 27 to Juin, 10 on a Lille University support.

9.3.2. Visits to International Teams

Thomas Rey visited Lorenzo Pareschi (March 9-14, 2015) and Giacomo Dimarco (June 23-27, 2015) in the Department of Mathematics and Computer Science of the University of Ferrara (Italy) to work on hyperbolic balance laws and on semi-lagrangian methods for the Boltzmann equation respectively.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific events organisation

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.

In the framework of the ANR GEOPOR project, C. Cancès organized a two-days workshop on gradient flows in metric spaces in Paris last June 22-23 (<https://www.ljll.math.upmc.fr/cances/GFIP/>).

B. Merlet organized of a one day conference on *Calculus of Variations* at Université Lille 1, October 15, 2015.

E. Creusé organized a one-day workshop on Mathematics and Entrepreneurship on November 17, 2015.

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. Research administration

C. Cancès was vice-head of the MoMaS research group (<http://www.gdrmmas.org>) funded by the Institute for Mathematical Sciences and Interaction (INSMI) of the French National Center for Research (CNRS)

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. C. Calgaro has contacts with the University of Padua (Italy). Each year, the reception of an Erasmus student (with a strong mathematical background) at the master's level is possible.

10.2.2. Supervision

HDR : C. Cancès, *Analyse mathématique et numérique d'équations aux dérivées partielles issues de la mécanique des fluides : applications aux écoulements en milieux poreux*, defended at Université Pierre et Marie Curie on December 7, 2015.

PhD in progress: P.-L. Colin, *Theoretical and numerical study of some corrosion models*, since 01/10/2012, advisors: C. Chainais-Hillairet & I. Lacroix-Violet.

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

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

10.2.3. Juries

- B. Merlet was a member of Pierre Bochard's PhD Thesis jury on June 24, 2015 at Université Paris-Sud. Title: "Vortex, entropies et énergies de ligne en micromagnétisme".
- E. Creusé was a member of Matthieu Merle's PhD Thesis jury on September 25, 2015 at École Nationale des Arts et Métiers, Paris. Title: "Approches numériques pour l'analyse de stabilité globale d'écoulements pariétaux en régime subsonique".
- Claire Chainais-Hillairet was a member of different juries:
 - Pierre Feron's PhD thesis on November 16, 2015 at Université Paris-Est (Marne-la-Vallée). Title: "Schémas gradients appliqués aux équations elliptiques et paraboliques, linéaires et non-linéaires."

- Yumeng Zhang’s PhD thesis on December 17, 2015 at Université de Nice. Title: "Modélisation et simulation des dispositifs de ventilation dans les stockages de déchets radioactifs."
- Ulrich Razafison’s HDR on December 3, 2015 at Université de Franche-Comté. Title: "Contribution à l’analyse théorique de problèmes elliptiques en domaine non borné, à la simulation numérique d’équations hyperboliques et aux méthodes de bases réduites."
- C. Cancès and C. Chainais-Hillairet were members of the hiring jury of french Agrégation de mathématiques.

10.3. Popularization

C. Calgario is the organizer of the action "Mathématiques itinérantes" (<http://mathematiques.univ-lille1.fr/Ouvertures/Mathematiques-itinerantes/>), which promotes mathematics among young people (conferences in highschoools, "journées de la science", etc.). Members of the team regularly participate in these actions.

11. Bibliography

Major publications by the team in recent years

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Doctoral Dissertations and Habilitation Theses

- [10] C. CANCÈS. *Analyse mathématique et numérique d'équations aux dérivées partielles issues de la mécanique des fluides : applications aux écoulements en milieux poreux*, Université Pierre et Marie Curie , December 2015, Habilitation à diriger des recherches, <https://hal.archives-ouvertes.fr/tel-01239700>

Articles in International Peer-Reviewed Journals

- [11] B. ANDREIANOV, C. CANCÈS. *On interface transmission conditions for conservation laws with discontinuous flux of general shape*, in "Journal of Hyperbolic Differential Equations", July 2015, vol. 12, n° 2, pp. 343-384 [DOI : 10.1142/S0219891615500101], <https://hal.archives-ouvertes.fr/hal-00940756>
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