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Project-Team RAPSODI

Reliable numerical approximations of dissipative systems.

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

RESEARCH CENTER
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THEME
Numerical schemes and simulations

Table of contents

Project-Team RAPSODI

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Keywords:

Computer Science and Digital Science:

A6. - Modeling, simulation and control
A6.1. - Mathematical Modeling
A6.1.1. - Continuous Modeling (PDE, ODE)
A6.1.4. - Multiscale modeling
A6.1.5. - Multiphysics modeling
A6.2. - Scientific Computing, Numerical Analysis & Optimization
A6.2.1. - Numerical analysis of PDE and ODE

Other Research Topics and Application Domains:

B3. - Environment and planet
B3.3. - Geosciences
B3.3.1. - Earth and subsoil
B3.4. - Risks
B3.4.2. - Industrial risks and waste
B4. - Energy
B4.2. - Nuclear Energy Production
B4.2.1. - Fission

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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 [61].

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 [75], 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 [75]. 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 [7]. The idea and the techniques introduced in [7] 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 [85], 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 [72], 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 [71], the dead-oil model for porous media flows [67] or the Maxwell equations in their quasi-static approximation for some eddy current problems [10] and [70]. 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 [7], [21] 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 [75] 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 [68], [90]).

Recently, C. Chainais-Hillairet and co-authors [3], [8] and [69] 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 [69]. The schemes proposed in [7] and [21] 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* [7] with the methodology of [3], [8], [69] 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 [87]. 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 [83], [88].

3.2. Optimizing the computational efficiency

3.2.1. High order nonlinear numerical methods

The numerical experiments carried out in [7] 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) [78].

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 [91], [84], with high-order accuracy [54], [53], or for parabolic problems [51], [52] 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 [59], *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 [70]) 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 [63], [96]. In the finite volume context, recent references deal with unsteady convection-diffusion equations [95], [57], [73] and [67]. 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 [82]. 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 [61], [60] 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 [56]) 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 [87]. 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

5.1.1. Organization of the FVCA8 conference

The team RAPSODI was deeply involved in the organization of the eighth edition of the conference *Finite Volumes for Complex Application* (FVCA8). The conference was held in Lille on June 2017. The conference was a great success. It gathered about 150 specialists —mostly academics and research engineers from the industry— of the finite volume methods and of their application to real world problems. Claire Chainais-Hillairet headed the organization committee, Clément Cancès was in charge of the publication of the proceedings, Caterina Calgaro and Emmanuel Creusé organized the social events, and all the members of the team were in charge of the reception of the participants.

5.1.2. From a team to a project team

The research team RAPSODI was created on August 2015, but its evolution to the project team level was effective on Nov. 1, 2017. This evolution was based on the positive evaluation by several internationally recognized experts of an extended version of our research program.

6. New Results

6.1. Variational approach for multiphase flows

In [66], 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 [20] is then twofold. First, it extends the variational interpretation of [66] 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 [86] is shown in [20], providing by the way a new existence result for multiphase flows in porous media. The result relies on advances tools related to optimal transportation [94], [93].

Based on the previous work, Clément Cancès, Daniel Matthes, and Flore Nabet derived in [46] a model of degenerate Cahn-Hilliard type for the phase segregation in incompressible multiphase flows. The model is obtained as the Wasserstein gradient flow of a Ginzburg-Landau energy with the constraint that the sum of the volume fractions must stay equal to 1. The resulting model differs from the classical degenerate Cahn-Hilliard model (see [97], [77]) and is closely related to a model proposed by Weinan E and collaborators [76], [89]. Besides the derivation of the model, the convergence of a minimizing movement scheme is proven in [46].

6.2. Calculus of variations applied to Image processing, physics and biology

In [23], Benoît Merlet *et al.* consider the branched transportation problem in dimension two with a cost of transport per unit length of path of the form $f_a(m) = a + m$ where $a > 0$ is fixed and m is the flux along the path. As usual in branched transportation, an admissible transport is represented as a vector measure with prescribed divergence $\sum m_j \delta_{x_j} - \sum m'_l \delta_{y_l}$ (the x_j representing the sources and the y_k the sinks). The paper introduces a family of functionals $\{F^a_\varepsilon\}_{\varepsilon>0}$ and the authors establish that this family of functionals approximate the branched transportation energy in the sense of Γ-convergence. The energy F^a_ε is modeled on the Ambrosio-Tortorelli functional and is easy to optimize in practice (using dual formulation for the

constraints and alternate direction optimization). In [48], the same authors extend their previous work to functionals defined on k-currents: the objects are no more lines that transport masses but k-dimensional surfaces transporting a given quantity of $(k-1)$-dimensional objects. The ambient space is now of any dimension n. A new family of approximate energies $\{F^a_\varepsilon\}_{\varepsilon>0}$ is introduced and a Γ-convergence analysis is performed in the limit $\varepsilon \downarrow 0$. The limit objects are now k-currents with prescribed boundary, the limit functional controls both their masses (the total flux) and sizes (k-dimensional volume of the object). In the limit $a \downarrow 0$, the limit energy is the k-volume of the object so that these energies can be used for the numerical optimization of the size of k-currents with prescribed boundary. Although rather theoretical, the works [23], [48] are motivated by an image reconstruction issue: how to recover the contours of partially masked objects in an image.

In [26], Michael Goldman and Benoît Merlet study the strong segregation limit for mixtures of Bose-Einstein condensates modelled by a Gross-Pitaievskii functional. They study the behavior of minimizers of the Hamiltonian. First, they show that in the presence of a trapping potential, for different intracomponent strengths, the Thomas-Fermi limit is sufficient to determine the shape of the minimizers. Then they study the case of asymptotically equal intracomponent strengths: at leading order the two phases are then undistinguishable, the authors extract the next order and show that the relevant limit optimization problem is a weighted isoperimetric problem. Then, they study the minimizers, proving radial symmetry or symmetry breaking for different values of the parameters. Eventually, they show that in the absence of a confining potential, even for non-equal intracomponent strengths, one needs to study a related isoperimetric problem to gain information about the shape of the minimizers.

In [49], Michael Goldman, Benoît Merlet and Vincent Millot study a variational problem which models the behavior of topological singularities on the surface of a biological membrane in P_β-phase (see [92]). The problem combines features of the Ginzburg-Landau model in 2D and of the Mumford-Shah functional. As in the classical Ginzburg-Landau theory, a prescribed number of point vortices appear in the moderate energy regime; the model allows for discontinuities, and the energy penalizes their length. The novel phenomenon here is that the vortices have a fractional degree $1/m$ with m prescribed. Those vortices must be connected by line discontinuities to form clusters of total integer degrees. The vortices and line discontinuities are therefore coupled through a topological constraint. As in the Ginzburg-Landau model, the energy is parameterized by a small length scale $\varepsilon > 0$. The authors perform a complete Γ-convergence analysis of the model as $\varepsilon \downarrow 0$ in the moderate energy regime. Then, they study the structure of minimizers of the limit problem. In particular, the line discontinuities of a minimizer solve a variant of the Steiner problem.

6.3. Asymptotic analysis for fluid mechanics

In [28], Ingrid Lacroix-Violet and Alexis 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.

In [44], the main objective is to generalize to the Navier-Stokes-Korteweg (with density dependent viscosities satisfying the BD relation) and Euler-Korteweg systems a recent relative entropy proposed in [65]. As a concrete application, this helps to justify mathematically the convergence between global weak solutions of the quantum Navier-Stokes system and dissipative solutions of the quantum Euler system when the viscosity coefficient tends to zero. Our results are based on the fact that Euler-Korteweg systems and corresponding Navier–Stokes-Korteweg systems can be reformulated through an augmented system. As a by-product of our analysis, we show that this augmented formulation helps to define relative entropy estimates for the Euler-Korteweg systems in a simplest way and with less hypothesis compared to recent works [74], [80].

In [27], Pierre-Emmanuel Jabin and Thomas Rey investigate the behavior of granular gases in the limit of small Knudsen number, that is, very frequent collisions. They deal with the strongly inelastic case in one dimension of space and velocity. They are able to prove the convergence toward 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. A more general result is also presented, which can apply to a large class of energy-dissipative kinetic equations.

6.4. Advanced discrete functional analysis results and applications

In [38], Claire Chainais-Hillairet, Benoît Merlet and Alexis Vasseur establish a positive lower bound for the numerical solutions of a stationary convection-diffusion equation on a bounded domain. The proof (which is fully detailed) is based on a celebrated method due to Ennio De Giorgi for showing regularity of the solutions of parabolic and elliptic equations. The robustness of the method allows the authors to adapt it to the discrete solutions obtained by standard finite volume discretizations. Further refinements of this work could lead to improve known error estimates for FV discretizations in L^p-norms to L^∞-norm.

In [14], Marianne Bessemoulin-Chatard and Claire 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 established in [35].

In [43], Marianne Bessemoulin-Chatard and Claire Chainais-Hillairet propose a new proof of existence of a solution to the scheme already introduced in [14] which does not require any assumption on the time step. The result relies on the application of a topological degree argument which is based on the positivity and on uniform-in-time upper bounds of the approximate densities. They also establish uniform-in-time lower bounds satisfied by the approximate densities. These uniform-in-time upper and lower bounds ensure the exponential decay of the scheme towards the thermal equilibrium as shown in [14].

In [12], Boris Andreianov, Clément Cancès, and Ayman Moussa developed a black box to obtain some compactness on the sequence produced by a finite volume discretization for degenerate parabolic problems. Such problems typically appear in the framework of porous media flows or in semi-conductor devices.

6.5. Structure preserving numerical methods

In [7], Clément Cancès and Cindy Guichard proposed in the case of a simple degenerate parabolic equation a nonlinear Control Volume Finite Element (CFVE) scheme that was able to preserve at the discrete level some important features of the continuous problem, namely the positivity of the solution, the decay of the physical energy. The scheme is based on a suitable upwinding procedure and inherits key properties from the Two-Point Flux Approximation (TPFA) finite volume scheme even though the method is not monotone. The convergence of the scheme towards the solution of the continuous problem was also established. In [22], Clément Cancès, Moustafa Ibrahim, and Mazen Saad extend the approach of [7] to the case of the Keller-Segel system with volume filling effect. In [11], Ahmed Ait Hammou Oulhaj, Clément Cancès, and Claire Chainais-Hillairet extend this approach to the Richards equation modeling unsaturated flow in porous media.

In presence of strong anisotropy, the methodology described above may lack robustness: the method is first order accurate, but the error constant may become large in some particularly unfavorable situations. This motivated the development of a new family of schemes with locally positive metric tensor (this denomination was chosen in reference Otto's contribution [90]). The methodology is first developed by Clément Cancès and Cindy Guichard for the so-called Vertex Approximate Gradient (VAG) scheme [79] in [21]. The newly developed method is second order accurate in space and much more robust with respect to the anisotropy than the one of [7] based on upwinding. Then Clément Cancès, Claire Chainais-Hillairet, and Stella Krell extend the methodology to Discrete Duality Finite Volume (DDFV) schemes in [32] and [19].

In [11] (see also the short version [31]), Ahmed Ait Hammou Oulhaj propose an upstream mobility TPFA finite volume scheme for solving a degenerate cross-diffusion problem modeling the flow of two fluids in a porous medium. The scheme has the remarkable property to preserve at the discrete level the local conservation of mass, the positivity of the solution, the decay of the energy. Moreover, the scheme provides a control on the entropy dissipation rate. Thanks to these properties, the convergence of the scheme is established. Numerical simulation show the great robustness of the scheme.

In [37], Clément Cancès and Flore Nabet propose an upstream mobility TPFA finite volume scheme for solving the degenerate Cahn-Hilliard problem. The scheme is designed in order to maintain the positivity of the phase volume fractions, the local conservation of mass and the decay of the energy.

Many applications involve partial differential equations which admits nontrivial steady state solutions. The design of schemes which are able to describe correctly these equilibrium states may be challenging for numerical methods, in particular for high order ones. In [29], inspired by micro-macro decomposition methods for kinetic equations, Lorenzo Pareschi and Thomas Rey 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.

6.6. Numerical approximation of a model for concrete carbonation

In [47], Claire Chainais-Hillairet, Benoît Merlet and Antoine Zurek introduce and study a finite volume scheme for a concrete carbonation model proposed by Aiki and Muntean in [55]. This model consists in a system of two weakly coupled parabolic equations in a varying domain whose length is governed by an ordinary differential equation. The numerical scheme is obtained by a Euler discretization in time and a Scharfetter-Gummel discretization in space. The convergence of the scheme is established and the existence of a solution to the model is obtained as a by product. Finally, some numerical experiments are performed to show the efficiency of the scheme. The main results of this study are also concisely exposed in [34].

6.7. Numerical methods for stratigraphy problems

In the framework of the PhD thesis of Nicolas Peton, numerical methods are developed for nonlinear diffusion equations arising in stratigraphic modeling. In [33], the special case of a p-Laplacian equation with a constraint on the divergence of the flux is considered. Such a model is used to model erosion and sedimentation processes. The constraint is incorporated to take into account a maximal erosion rate.

6.8. Modeling and numerical simulation of complex fluids

In [25], Giacomo Dimarco, Raphaël Loub ere, Jacek Narski, and Thomas Rey extend the Fast Kinetic Scheme (FKS) 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 conservative 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.

In the context of the PhD of Claire Colin-Lecerf, C. Calgaro and co-authors derive in [45] a combined Finite Volumes - Finite Elements (CFVFE) scheme. This work can be seen as a generalization of some previous contributions on incompressible flows [5], [4], [6], in the context of a low-Mach model. Here, the temperature obeying an energy law has been taken into account. The authors chose to solve the continuity equation and the state equation linking temperature, density and thermodynamic pressure is imposed implicitly. Now the velocity field is no more divergence-free, so that the projection method solving the momentum equation has to be adapted. This combined scheme preserve the constant state and ensure the discrete maximum principle on the density. Their numerical results have been compared to some others which use purely finite elements schemes (see [62], [58], [81]) and in particular on a benchmark consisting in a transient hot jet entering in a cavity.

Diffuse interface models, such as the Kazhikhov-Smagulov model, allow to describe some phase transition phenomena. The theoretical analysis of this model was given by Bresch at al. [64] (see also reference therein). In the previous work [6], C. Calgaro et al. have implemented the CFVFE scheme and studied numerically the progression of the front of a powder-snow avalanche with respect to some characteristics parameters of the flow, such as the Froude, Schmidt and Reynolds numbers. In [18], C. Calgaro and co-authors investigate theoretically the CFVFE scheme. They construct a fully discrete numerical scheme for approximating the two-dimensional Kazhikhov-Smagulov model, using a first-order time discretization and a splitting in time to allow the construction of the combined scheme. Consequently, at each time step, one only needs to solve two decoupled problems, the first one for the density (using the Finite Volume method) and the second one for the velocity and pressure (using the Finite Element method). The authors prove the stability of the combined scheme and the convergence towards the global in time weak solution of the model. In this model, the convection-diffusion equation for the density can also be discretized by a implicit-explicit (IMEX) second order method in the Finite Volume scheme. In the framework of MUSCL methods, C. Calgaro and M. Ezzoug prove in [36] that the local maximum property is guaranteed under an explicit Courant-Friedrichs-Levy condition and the classical hypothesis for the triangulation of the domain.

6.9. Cost reduction of numerical methods

This section gathers contributions for which the main motivation was to increase the efficiency of numerical methods, either by localizing the computational effort thanks to mesh refinement

In [24], E. Creusé and his collaborators generalize the equilibrated error estimators developed in the low-frequency magnetostatic case to the case of the harmonic time-dependent one. This contribution allows to obtain a bound of the numerical error equal to one, so that the accuracy of the obtained solution can be explicitly controlled.

The contribution [16] 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 [16], 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 [16] 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 a strong robustness of the method w.r.t. the nonlinearities appearing in the continuous model.

In [39], Ward Melis, Thomas Rey, and Giovanni Samaey present a high-order, fully explicit, asymptotic-preserving projective integration scheme for the nonlinear BGK equation. The method first takes a few small (inner) steps with a simple, explicit method (such as direct forward Euler) to damp out the stiff components of the solution. Then, the time derivative is estimated and used in an (outer) Runge-Kutta method of arbitrary order. Based on the spectrum of the linearized BGK operator, they deduce that, with an appropriate choice of inner step size, the time step restriction on the outer time step as well as the number of inner time steps is independent of the stiffness of the BGK source term. They illustrate the method with numerical results in one and two spatial dimensions.

In [13], Christophe Besse, Guillaume Dujardin, and Ingrid Lacroix-Violet present the numerical integration in time of nonlinear Schrödinger equations with rotating term. After performing a change of unknown so that the rotation term disappears they consider exponential integrators such as exponential Runge-Kutta methods and Lawson methods. They provide an analysis of the order of convergence and some preservation properties of these methods and they present numerical experiments.

7. Bilateral Contracts and Grants with Industry

7.1. 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.

8. Partnerships and Cooperations

8.1. Regional Initiatives

- The region Haut-de-France supported financially the organization of the FVCA8 conference.
- The PhD program of Ahmed Ait Hammou Oulhaj is partially supported (50%) by the region Haut-de-France (formerly Nord–Pas-de-Calais).

8.2. National Initiatives

8.2.1. ANR

C. Cancès is the coordinator of the ANR GEOPOR project (http://www.agence-nationale-recherche.fr/Project-ANR-13-JS01-0007). 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

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 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 - 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.

8.2.2. 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.

8.2.3. Microturbu Project

B. Merlet and T. Rey were both members of the Microturbu project. This project, headed by Stephan De Bièvre, was supported by the interdisciplinarity mission of the CNRS in 2017. Its purpose was to strengthen the collaborations between applied mathematicians from the Paul Painlevé laboratory and physicists from the PhLAM laboratory.

8.3. International Research Visitors

8.3.1. Visits of International Scientists

We have a long time collaboration with Ansgar Jüngel team from TU Wien. He visited Lille on January 9–13, 2017. His PhD Student, Anita Gerstenmayer came for the third time in Lille on July 3–7, 2017.

Ezzeddine Zahrouni (Univ. Carthage, Tunisia) was invited in Lille in May 2017 thanks to a support of the Labex CEMPI.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

Claire Chainais-Hillairet was general chair of the organisation committee of FVCA8 held in Lille on June 12-16, 2017. Clément Cancès was general chair for the Journée de la Fédération de Recherche Mathématique du Nord–Pas-de-Calais on October, 4. He also organized the closing day of the ANR Geopor on Nov. 7, 2017.

Emmanuel Creusé is a member of the organizing committee of the Study Week Mathematics-Enterprises, which will take place in Lille from January 2018, 29 to February 2018, 02. (see https://indico.math.cnrs.fr/event/2413/).

Thomas Rey was a main organizer of the Microturbu workshop held in Lille on Oct. 19–20, 2017.

9.1.1.2. Member of the Organizing Committees

The whole team RAPSODI was involved in the organization of the FVCA8 conference.

9.1.2. Scientific Events Selection

9.1.2.1. Chair of Conference Program Committees

Clément Cancès edited the proceedings of FVCA8 together with Pascal Omnes (CEA Saclay & Univ. Paris Nord).

9.1.2.2. Reviewer

Several member of the team RAPSODI were deeply involved in the reviewing process for the FVCA8 proceedings.

9.1.3. Journal

9.1.3.1. 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/).

9.1.3.2. Reviewer - Reviewing Activities

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

9.1.4. Invited Talks

- C. Cancès was an invited speaker at the MAMERN'11 conference organized at Oujda (Morocco) on May 17-20, 2017: http://mamern11.ump.ma/. He was invited to give talks in several workshops (Oberwolfach $\times 2$, workshop on Finite Volumes in Nice, minisymposium on porous media flows in ENUMATH). He was also invited to give several seminars in France (Inria Paris-LJLL, ENS Rennes, IFPEN Rueil-Malmaison) or abroad (Bonn).
- C. Chainais-Hillairet was an invited plenary speaker at the SMAI Conference held in Ronce les Bains in June 2017. She gave talks in workshops: workshop on Finite Volumes in Nice and Journées multiphasiques et incertitudes in Nantes in October 2017. She was invited to give lectures in two CIMPA Summer Schools: 10 hours lectures in Ifrane (Summer school on numerical analysis and partial differential equations, May 2017) and 8 hours lectures in Kanpur (Summer school on multiscale computational methods and error control, July 2017).
- E. Creusé was invited to give a seminar at LAMFA in Amiens. He also gave talks in International conferences (NUMELEC, Paris and ACOMEN, Ghent) and workshops (GATIPOR, Paris).
- I. Lacroix-Violet was invited to give a seminar at LAMFA in Amiens.
- T. Rey was invited to give plenary talks in several workshops: Mafran Days in Cambridge, Computational Methods in Kinetic Theory and Related Models in Toulouse, and Mathematical Aspects of Fluids: Kinetic and Dynamics at ENS Paris

9.1.5. Scientific Expertise

C. Cancès reported on scientific proposals for the Croatian Science Foundation (HRZZ).

9.1.6. Research Administration

C. 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).

During the training year 2016-2017, E. Creué got an Inria partial delegation (50%). He had in charge to develop some actions promoted by AMIES (Agency for Mathematics in Interaction with Business and Society). More particularly, his action was devoted to several characteristic points:

Management of some PEPS (First support for exploratory projects). Discussions to initiate collaborations between academic researchers in Mathematics and industrial partners,

Talks and meeting animations to promote mathematical studies to high school pupils and their teachers, as well as to bachelor students (in Lens, Lille, Douai).

Presentation of AMIES to the Mathematical Laboratories of the region Hauts-de-France (Lille, Calais, Lens, Amiens, Valenciennes).

Creation of CIME, a node of the network "MSO" (Modelisation - Simulation - Optimisation) developped by AMIES (http://cime.math.cnrs.fr/). CIME is a structure which allows enterprises to find easier mathematician collaborators in the Hauts-de-France, either in the mathematical teams of Inria Lille Nord Europe, or in the mathematical laboratories of the region.

Participation to some national events (RUE (Paris, March 2017) - TERATEC (Palaiseau, June 2017), FEM (Paris, December 2017)).

Participation to the monthly AMIES meeting.

Organisation of the Mathematical Study Week in Mathematics, which will take place in Lille in January 2018.

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

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

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

C. Cancès and B. Merlet are members of the commission des thèses of the Ecole doctorale.

I. Lacroix-Violet was organizing the weekly seminar of the ANEDP team of the Paul Painlevé laboratory until last July. She was substituted by T. Rey in September 2017.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

The group is strongly involved in teaching at the Université Lille 1. C. Calgaro is in charge respectively of the Master of Mathematical Engineering. C. Chainais-Hillairet was in charge of the Master 2 of Scientific Computing until July 2017. She was substituted by B. Merlet for this task. E. Creusé is responsible of the "Cursus Master Ingénierie" in Mathematics, Lille 1 University. C. Cancès gave lectures at Polytech' UPMC.

9.2.2. Supervision

HdR: Ingrid Lacroix-Violet defended her habilitation thesis on Nov. 24, 2017. *Comportements asymptotiques, conditions aux limites et analyse numérique pour des modèles fluides*, Univ. Lille 1.

PhD: Ahmed Ait Hammou Oulhaj defended his PhD thesis on Dec. 11, 2017. *Design and analysis of nonlinear numerical schemes for solving parabolic problems: application to porous media flows*, Univ. Lille 1, advisors: C. Cancès & C. Chainais-Hillairet. *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 reconstruction 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.

Master internship: Aymeric Nayet, *Development and parallelization on GPU of a C++ code for the resolution of a 2D×2D kinetic equation with BGK relaxation*, supervisor: T. Rey.

Master internship: Anissa El Keurti, *Study of an upwind finite volume scheme for non-local transport equation*, supervisor: T. Rey.

9.2.3. Juries

C. Cancès reported on Laurent Quaglia's PhD thesis, defended on Dec. 13, 2017 at Aix-Marseille Univ. Title: *Contribution à l'étude des écoulements diphasiques avec capillarité*.

C. Chainais-Hillairet reported on:

- Clémentine Courtès' PhD thesis, defended on Nov. 23, 2017 at Univ. Paris-Sud (Orsay). Title: *Analyse numérique de systèmes hyperboliques-dispersifs*.
- Laurent Quaglia's PhD thesis, defended on Dec. 13, 2017 at Aix-Marseille Univ. Title: *Contribution à l'étude des écoulements diphasiques avec capillarité*.
- Christophe Le Potier's HdR, defended on Nov. 15,2017 at Univ. Paris-Est (Marne-la-Vallée). Title: *Construction et développement de nouveaux schémas pour des problèmes elliptiques ou paraboliques*.

E. Creusé reported on:

- Sarah Ali Hassan's PhD thesis, defended on June 26, 2017 at UPMC Paris 6. Title: *Estimations d'erreur a posteriori et critères d'arrêt pour des solveurs par décomposition de domain et avec des pas de temps locaux.*
- Rita Riedlbeck' s PhD thesis, defended on November 27, 2017 at Montpellier University. Title: Algorithmes adaptatifs pour la poro-mécanique et la poro-plasticité.

B. Merlet reported Sylvain Dotti's PhD thesis, defended on Dec. 4, 2017 at Aix-Marseille Univ. Title: *Numerical approximation of hyperbolic stochastic scalar conservation laws*.

C. Calgaro and E. Creusé were members of the PhD's jury of Abdullatif Ellawy, defended on Dec. 14, 2017, at Lille 1 University. Title : *Propriétés qualitatives de quelques systèmes de la mécanique des fluides incompressibles*.

C. Cancès was a member of the jury of the PhD thesis of Van Thanh Nguyen, defended on Oct. 3, 2017 at the University of Limoges. Title: *Problèmes de transport partiel optimal et d'appariement avec contrainte*.

C. Chainais-Hillairet was a member of the following juries:

- PhD's jury of Maxime Herda defended on September 20, 2017 at the University of Lyon 1. Title: *Analyse asymptotique et numérique de quelques modèles pour le transport de particules chargées*.
- PhD's jury of Sarah Leclavier defended on December 12, 2017 at the University of Rouen. Title: *Volumes finis et solutions renormalisées, application à des systèmes couplés*.
- HdR's jury of Ingrid Lacroix-Violet defended on November 24, 2017 at Lille 1 University. Title: *Comportements asymptotiques, conditions limites et analyse numérique pour des modèles fluides*.

T. Rey was a member of the PhD's jury of Ward Melis, defended in March 2017 at KU Leuven. Title: *Projective integration for hyperbolic conservation laws and multiscale kinetic equations*.

C. Calgaro and C. Cancès are members of the Jury de l'Agrégation de Mathématiques, which is a national hiring committee for the highest level of high-school teachers.

9.3. 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.

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Major publications by the team in recent years

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