



Activity Report 2013

## **Project-Team SIMPAF**

Simulations and Modeling for PArticles and Fluids

RESEARCH CENTER  
Lille - Nord Europe

THEME  
Computational models and simulation



## Table of contents

<b>1. Members</b> .....	<b>1</b>
<b>2. Overall Objectives</b> .....	<b>1</b>
2.1. Overall Objectives	1
2.2. Highlights of the Year	2
<b>3. Research Program</b> .....	<b>2</b>
3.1. General framework	2
3.2. Interactions of Micro- and Macroscopic Scales and Simulations	3
3.2.1. Homogenization methods	3
3.2.2. Statistical physics: dynamical friction, fluctuations and approach to equilibrium	3
3.2.3. Cold Atoms	3
3.3. Finite element and finite volume methods	3
3.3.1. Control in Fluid Mechanics	3
3.3.2. Numerical Methods for Viscous Flows	4
3.3.3. A posteriori error estimators for finite element methods	4
3.4. Numerical analysis of Schrödinger equations	4
3.4.1. Modelling of quantum dot-helium	4
3.4.2. Dispersive Schrödinger-like equations	4
3.4.3. Absorbing boundary conditions for Korteweg de Vries equation	5
<b>4. Application Domains</b> .....	<b>5</b>
4.1. Physics	5
4.1.1. Non-equilibrium statistical physics	5
4.1.2. Cold atoms	5
4.1.3. Laser propagation	5
4.1.4. Maxwell equations	5
4.2. Continuum mechanics	5
4.2.1. Numerical simulation of viscous flows	6
4.2.2. From polymer physics to rubber elasticity	6
4.3. Corrosion models	6
4.3.1. Corrosion modelling of iron based alloy in nuclear waste repository	6
4.3.2. Corrosion modeling of Ni-base alloys in Pressurized Water Reactor primary water	6
<b>5. Software and Platforms</b> .....	<b>7</b>
5.1. ns2ddv-M	7
5.2. ns2ddv-C++	7
5.3. RTcodes	7
5.4. FPcodes	8
5.5. CLAToolBox	8
5.6. SPARCS	8
5.7. Code-Carmel3D	8
<b>6. New Results</b> .....	<b>9</b>
6.1. Quantitative homogenization theory	9
6.2. Corrosion	9
6.3. New results on finite volume schemes	9
6.4. New results in numerical fluid dynamics	10
6.5. New results on a posteriori estimates	10
6.6. New results in control in fluid mechanics	10
<b>7. Bilateral Contracts and Grants with Industry</b> .....	<b>10</b>
7.1. Study of the EKINOX model of corrosion (CNRS Contract with CEA, Univ Lille1, Univ B. Pascal)	10
7.2. Numerical methods for the DPCM model (Inria/ANDRA Contract)	11

---

<b>8. Partnerships and Cooperations</b> .....	<b>11</b>
8.1. Regional Initiatives	11
8.2. National Initiatives	11
8.2.1. Collaborations within Inria	11
8.2.2. ANR	11
8.2.2.1. ANR IODISSEE (2009-2013)	11
8.2.2.2. ANR AMAM (2011-2014)	12
8.2.2.3. ANR STAB (2013-2017)	12
8.2.2.4. ANR BECASIM(2013-2017)	12
8.2.3. Competitivity Clusters	12
8.3. European Initiatives	13
8.3.1. FP7 Projects	13
8.3.2. Collaborations with Major European Organizations	13
8.4. International Research Visitors	13
8.4.1. Visits of International Scientists	13
8.4.2. Visits to International Teams	13
<b>9. Dissemination</b> .....	<b>13</b>
9.1. Scientific Animation	13
9.2. Teaching - Supervision - Juries	13
9.2.1. Supervision	13
9.2.2. Juries	13
9.3. Popularization	13
<b>10. Bibliography</b> .....	<b>14</b>

## Project-Team SIMPAF

**Keywords:** Scientific Computation, Fluid Dynamics, Particles, Homogenization

*Creation of the Project-Team: 2007 July 01, updated into Team: 2013 January 01, end of the Project-Team: 2013 December 31.*

## 1. Members

### Research Scientists

Antoine Gloria [Team leader, Université Libre de Bruxelles and Inria]  
Guillaume Dujardin [Inria, Researcher]

### Faculty Members

Christophe Besse [Université Lille 1, Professor, HdR]  
Caterina Calgaro-Zotto [Université Lille 1, Associate Professor]  
Claire Chainais-Hillairet [Université Lille 1, Professor]  
Emmanuel Creusé [Université Lille 1, Professor, HdR]  
Stephan de Bièvre [Université Lille 1, Professor, HdR]  
Ingrid Lacroix-Violet [Université Lille 1, Associate Professor]

### External Collaborators

Clément Cancès [Université Paris 6, Associate Professor]  
Pauline Lafitte [École Centrale de Paris, Professor, HdR]

### Engineer

Ralitsa Ivanova [Inria, granted by ANR IODISSEE project, from Apr 2013 until Sep 2013]

### PhD Students

Pierre-Louis Colin [Université Lille 1]  
Émilie Soret [Inria]

### Post-Doctoral Fellows

Thomas Gallouët [Inria, granted by ANDRA]  
Maxime Gazeau [Inria, from Jan 2013]

### Administrative Assistant

Karine Lewandowski [Inria]

### Others

Gonzalo Jose Carracedo Carballal [Inria, from Apr 2013 until Jun 2013]  
Adrien Corenflos [ENS Lyon, from Jun 2013 until Aug 2013]  
Francesca Miscioscia [Erasmus student, in Master 2 in Padua (Italy), from Mar 2013 until Jun 2013]  
Alessandro Mozzato [Erasmus student, in Master 2 in Padua (Italy), from Mar 2013 until Jun 2013]  
Mohamed Riad Sanchez [In Master 2 in Nice, from Feb 2013 until Jul 2013]

## 2. Overall Objectives

### 2.1. Overall Objectives

The project aims at

- Studying models that describe the evolution of a fluid and/or of a large number of particles;
- Discussing the relevance and the range of validity of these models;
- Analyzing connections between different levels of modelling;
- Developing efficient numerical methods to compute the solutions of such models.

## 2.2. Highlights of the Year

A. Gloria was awarded an ERC Starting Grant.

# 3. Research Program

## 3.1. General framework

Partial Differential Equations, Kinetic Equations, Conservation Laws, Hyperbolic Systems, Fluid Mechanics, Parabolic Systems, Computational Fluid Dynamics, Plasma Physics, Asymptotic analysis

The scientific activity of the project is concerned with Partial Differential Equations (PDE) arising from the physical description of particles and fluids. It covers various viewpoints:

- At first, the words “particles and fluids” could simply mean that we are interested independently in models for particles, which can either be considered as individuals (which leads to “ $N$ -particle models”,  $N$  ranging from 1 to many) or through a statistical description (which leads to kinetic equations) as well as in models for fluids like Euler and Navier-Stokes equations or plasma physics.
- However, many particle systems can also be viewed as a fluid, via a passage from microscopic to macroscopic viewpoint, that is, a hydrodynamic limit.
- Conversely, a fruitful idea to build numerical solvers for hyperbolic conservation laws consists in coming back to a kinetic formulation. This approach has motivated the introduction of the so-called kinetic schemes.

By nature these problems describe multiscale phenomena and one of the major difficulties when studying them lies in the interactions between the various scales: number of particles, size, different time and length scales, coupling...

The originality of the project is to consider a wide spectrum of potential applications. In particular, the word “particles” covers various and very different physical situations and it has evolved with the composition of the team. One may think of:

- charged particles: description of semi-conductor devices or plasmas;
- bacteria, individuals or genes as in models motivated by biology or population dynamics;
- droplets and bubbles, as in Fluid/Particles Interaction models which arise in the description of sprays and aerosols, smoke and dust, combustion phenomena (aeronautics or engine design), industrial process in metallurgy...
- cross-links in polymer chains to describe rubber elasticity;
- oxide molecules to model corrosion phenomena at the microscopic scale and derive effective macroscopic equations;
- cold atoms...

We aim at focusing on all the aspects of the problem:

- Modelling mathematically complex physics requires a deep discussion of the leading phenomena and the role of the physical parameters. With this respect, the asymptotic analysis is a crucial issue, the goal being to derive reduced models which can be solved with a reduced numerical cost but still provide accurate results in the physical situations that are considered.
- The mathematical analysis of the equations provides important qualitative properties of the solutions: well-posedness, stability, smoothness of the solutions, large time behavior... which in turn can motivate the design of numerical methods.
- Eventually, we aim at developing specific numerical methods and performing numerical simulations for these models, in order to validate the theoretical results and shed some light on the physics.

The team has been composed in order to study these various aspects simultaneously. In particular, we wish to keep a balance between modelling, analysis, development of original codes and simulations.

## 3.2. Interactions of Micro- and Macroscopic Scales and Simulations

Statistical Physics, Homogenization, Asymptotic Preserving Schemes

### 3.2.1. Homogenization methods

Homogenization methods aim at replacing a PDE with highly oscillatory coefficients by an effective PDE with smoother coefficients, whose solution captures the averaged behavior of the true oscillatory solution. The effective determination of the homogenized PDE is however not trivial (especially in the nonlinear or/and stochastic cases). Numerical approximations of the solution of the homogenized PDE is the heart of numerical homogenization.

Homogenization methods are used in many application fields. The two applications we are specifically interested in are material sciences (in particular the determination of macroscopic constitutive laws for rubber starting from polymer-chain networks) and nuclear waste storage (in particular the evolution of nuclear wastes in complex storage devices).

The team is interested in qualitative as well as quantitative results, and theoretical as well as numerical results. Challenging questions are mainly related to nonlinear problems (nonlinear elasticity for instance) and stochastic problems (especially regarding quantitative results).

### 3.2.2. Statistical physics: dynamical friction, fluctuations and approach to equilibrium

In models of charge transport, say transport of electrons, a phenomenological friction force is generally introduced, which is proportional to the velocity  $v$ . The dissipation induced by such a term is essential for the description of phenomena such as Ohm's law and approach to equilibrium. Our idea is to go back to a microscopic framework, with a description of the energy exchanges between the electrons and the surrounding medium which is the ultimate source of the dissipation of energy by the medium and of an effective friction force. We have shown numerically and argued theoretically that the balance between the fluctuations and the dissipation by the medium drives the particle to thermal equilibrium. The goal is now to provide rigorous proof of this statement. As a first step in this program, results will be obtained in an appropriate weak coupling limit. This program requires efforts in modelling, probability and analysis, but the questions are also really challenging for numerics, due, notably, to the large number of degrees of freedom involved in the equation. The subject is at the heart of the PhD work of É. Soret, now in her third year as a PhD student.

### 3.2.3. Cold Atoms

In the framework of the Labex CEMPI, C. Besse, S. De Bièvre and G. Dujardin are working, in collaboration with J.-C. Garreau and the cold-atom team at PhLAM, on the mathematical analysis and the numerical simulation of kicked rotor systems. Such systems are experimentally realized at PhLAM. A triple goal is being pursued: understand the effect of non-linearities on dynamical localization, understand dynamical localization in systems other than kicked rotors, and exploring the limits of the analogy between kicked systems and the Anderson model.

## 3.3. Finite element and finite volume methods

Conservation Laws, Anti-Diffusive Schemes, Viscous Flows, Control, Turbulence, Finite element methods, Finite volume methods

### 3.3.1. Control in Fluid Mechanics

Flow control techniques are widely used to improve the performances of planes or vehicles, or to drive some internal flows arising for example in combustion chambers. Indeed, they can sensibly reduce energy consumption, noise disturbances, or prevent the flow from undesirable behaviors. Passive as well as active control were performed on the "Ahmed body geometry", which can be considered as a first approximation of a vehicle profile. This work was carried out in collaboration with the EPI Inria MC2 team in Bordeaux (C.H. Bruneau, I. Mortazavi and D. Depeyras), as well as with Renault car industry (P. Gillieron). We combined active and passive control strategies in order to reach efficient results, especially concerning the drag coefficient, for two and three dimensional simulations [36], [37].

### 3.3.2. Numerical Methods for Viscous Flows

Numerical investigations are very useful to check the behavior of systems of equations modelling very complicate dynamics. In order to simulate the motion of mixtures of immiscible fluids having different densities, a recent contribution of the team was to develop an hybrid Finite Element / Finite Volume scheme for the resolution of the variable density 2D incompressible Navier-Stokes equations. The main points of this work were to ensure the consistency of the new method [41] as well as its stability for high density ratios [38]. Now, C. Calgario and E. Creusé, in collaboration with T. Goudon (Inria-COFFEE), have in mind the following objectives :

- Develop and freely distribute a new version of the matlab code (<http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV/> 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 (for instance to compare updating LU factorizations, see [40]);
- To generalize the stability results obtained in [39] for the scalar transport equation to the full 2D Euler system, in particular very low density values (near vacuum);
- Complete the C++ code to treat more general hydrodynamic models (combustion theory, transport of pollutants). We plan to check the behavior of the equations (typically the Kazhikhov-Smagulov model of powder-snow avalanches) in the regime when the current existence theory does not apply, and extend our kinetic asymptotic-based schemes to such problems.

### 3.3.3. A posteriori error estimators for finite element methods

A posteriori estimates, finite element methods

We are interested in a posteriori error estimators for finite element methods, applied to the resolution of several partial differential equations. The objective is to obtain useful tools in order to control the global error between the exact solution and the approximated one (reliability of the estimator), and to control the local error leading to adaptive mesh refinement strategies (efficiency of the estimator). There is a large bibliography database devoted to this topic, but a lot of problems remain to address. For example how to obtain explicit, sharp and robust bounds of the error ?

## 3.4. Numerical analysis of Schrödinger equations

Dispersive equations, Schrödinger equations

### 3.4.1. Modelling of quantum dot-helium

In collaboration with G. Reinish (Nice Observatory) and V. Guðmundsson (University of Reykjavik), C. Besse and G. Dujardin are working on the numerical computation of the ground state and the first bound states of the non linear Schrödinger-Poisson system with confining quadratic potential in 2 space dimensions. This models quatum dot helium (*i.e.* the behavior of a pair of quantum electrons in a strong confining potential). The goal is to perform after that numerical time stepping methods to simulate the dynamics of the NLSP system and compute accurately some quantities of physical interest as functions of time, in order to be able to compare the competition between the Coulomb (repulsive) interaction and the binding (attractive) forces due to the confinement in this model as well as in other quantum mechanics models.

### 3.4.2. Dispersive Schrödinger-like equations

In collaboration with M. Taki (PhLAM laboratory, Lille), C. Besse and G. Dujardin are considering dispersive equations modelling the propagation of a laser beam in an optical fiber. They are trying to explain the possible ways of creating rogue waves in the propagation of laser beams. More generally, they are trying to explain which terms in the dispersive Schrödinger-like equations obtained by the physicists allow which physical behaviour of the solutions (e.g. the creation of rogue waves).



### 3.4.3. Absorbing boundary conditions for Korteweg de Vries equation

The solution of the Korteweg de Vries equation is defined on an unbounded domain. If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational domain by introducing artificial boundary conditions. So, the objective is to approximate the exact solution of the whole-space problem, restricted to a finite computational domain. This equation is difficult to study due to its third order space derivative. C. Besse and I. Lacroix-Violet, in collaboration with M. Ehrhardt, work on new developments.

## 4. Application Domains

### 4.1. Physics

Our applications to physics concern:

- non-equilibrium statistical physics
- cold atoms
- laser propagation
- Maxwell equations

#### 4.1.1. Non-equilibrium statistical physics

Describing, understanding, predicting and controlling the complex physical phenomena occurring in classical or quantum dynamical systems with a large or infinite number of degrees of freedom are important issues for equilibrium and non-equilibrium statistical mechanics and remain an important challenge for mathematical physics. Some of the typical questions are the following. How does a collective dynamics emerge from the interactions of individual entities? How to compute transport coefficients in terms of microscopic quantities and more generally, what is the role of the local (microscopic) dynamics on global transport properties? What are the system ergodic properties and how are asymptotic states, if they exist, approached? What are the dynamical mechanisms for approach to equilibrium in such systems?

#### 4.1.2. Cold atoms

A typical problem we are concerned with is the effect of interactions (modeled by a nonlinearity in the evolution equation) on the localization properties of quantum kicked rotors, experimentally realized in cold-atom experiments.

#### 4.1.3. Laser propagation

We are interested in variants of the NonLinear Schrödinger Equation (NLSE), which govern the evolution of optical fibers, and in particular photonic crystal fibers (PCF). These are key to information and communication technology, and form an unmatched platform to explore complex nonlinear phenomena.

#### 4.1.4. Maxwell equations

A posteriori error estimators developed for the Maxwell equations are very useful tools for practical computations. They are implemented in the software "Carmel-3D" (see the softwares section). This numerical code is used in order to study some original applications, like electrical machines or specific actuators. It is also devoted to nondestructive control by the use of Foucault currents, to the simulation of devices using magnetic fluids or of induced currents in human bodies.

### 4.2. Continuum mechanics

Our applications to continuum mechanics concern:

- the numerical simulation of viscous flows
- the mathematical and numerical derivation of rubber elasticity from polymer physics

#### **4.2.1. Numerical simulation of viscous flows**

We are concerned with systems of PDEs describing the evolution of mixture flows. The fluid is described by the density, the velocity and the 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 some instabilities phenomena such as the Raileigh-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 obtain the so called Kazhikhov-Smagulov model. 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. Furthermore, a surface tension force can be added to the momentum equation introducing a specific stress tensor, proposed for the first time by Korteweg. The first phenomena that we try to reproduce are the powder-snow avalanches, but we can also model flows where species (like salt or pollutant) are dissolved in a compressible or incompressible fluid. Other similar hydrodynamic models arise in combustion theory.

Flow control strategies using passive or active devices are crucial tools in order to save energy in transports (especially for cars, trucks or planes), or to avoid the fatigue of some materials arising in a vast amount of applications. Nowadays, shape optimization needs to be completed by other original means, such as porous media located on the profiles, as well as vortex generator jets in order to drive active control.

#### **4.2.2. From polymer physics to rubber elasticity**

Our aim is to rigorously derive nonlinear elasticity theory from polymer physics. The starting point is the statistical physics description of polymer-chains. Under some proper rescaling, this discrete model converges to continuum nonlinear elasticity models in the sense of Gamma-convergence. The long-term goal of our approach is to derive practical constitutive laws for rubbers (to be used in nonlinear elasticity softwares) from the discrete model.

### **4.3. Corrosion models**

#### **4.3.1. Corrosion modelling of iron based alloy in nuclear waste repository**

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.* [32]. 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 worthy of interest.

#### **4.3.2. Corrosion modeling of Ni-base alloys in Pressurized Water Reactor primary water**

The understanding of the oxidation behavior of Ni-base alloys in Pressurized Water Reactor (PWR) primary water is of major importance due to the cations released due to corrosion of the steam generators which is a source of the radioactivity of the primary circuit. Moreover, the oxidation process is the reason of the initiation

of intergranular stress corrosion cracking in some alloys. A numerical model, called EKINOX (Estimation KINetics OXYdation), has been developed at CEA [33] in order to simulate the oxide scale growth. This model should be able to calculate the evolutions of concentration profiles of the species and of their point defects in the oxide and in the substrate. Numerical experiments have shown the limits of this existing numerical model, especially the need of very small time steps for the computations ; a macroscopic model has been developed and numerical methods proposed for its simulation.

## 5. Software and Platforms

### 5.1. ns2ddv-M

**Participants:** Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)].

Incompressible Navier-Stokes, Variable Density, Rayleigh-Taylor Instability The NS2DDV-M code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. This original approach for variable density flows is described in [41].

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A3, SO3-up4, SM2-up3, EM3, SDL4, DA1, CD4, MS4, TPM4.

Software web site : <http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html>

### 5.2. ns2ddv-C++

**Participants:** Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)], Thierry Goudon.

Incompressible Navier-Stokes, Variable Density, Kazhikhov-Smagulov model, Rayleigh-Taylor Instability, avalanches phenomena The NS2DVD-C++ code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. The code is developed around the GetFem++ and the Bang softwares. It allows in particular mesh refinement strategies so that very relevant simulations can be reached (as the falling droplet with very high density ratios, see for example [38]). The current version of the code consider the additional terms in the Kazhikhov-Smagulov model.

Webpage : <http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV>

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A1, SO3-up4, SM1, EM2, SDL1, DA1, CD4, MS4, TPM1.

### 5.3. RTcodes

**Participants:** Pauline Lafitte [correspondant (ECP)], Jean-François Coulombel [(CNRS & Univ. Nantes)], Christophe Besse [(Univ. Lille 1)], Thierry Goudon [(Inria)], Giovanni Samaey [(KU Leuven)].

Radiative Transfer, Radiative shocks, AP schemes

We have developed a set of numerical codes, written in Scilab, to compute the solutions of the system coupling the Euler equations to the radiation through energy exchanges, in the non equilibrium regime. This covers several situations in the hierarchy of asymptotic problems. The code treats the one-dimensional framework. In particular the code can be used to investigate radiative shocks profiles. The main advantage of our numerical codes is that they do not require any refinement near the singularities. The numerical tests show a very good agreement with the theoretical predictions. See reference [48].

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A2, SO3, SM2, EM1, SDL1.

## 5.4. FPcodes

**Participants:** Pauline Lafitte [correspondant (ECP)], Thierry Goudon [(Inria)], Benjamin Boutin [(Univ. Rennes)].

Fluid-Particles flows, Gravity driven flows, AP schemes

We have developed a numerical code, written in Scilab, to compute the solutions of the two-phase flows equations describing particles interacting with a fluid through friction forces. The code treats one-dimensional situation and is well adapted to describe gravity driven flows in either bubbling or flowing regimes. In particular, it can be used to describe the evolution of pollutants in the atmosphere. The numerical strategy, based on an asymptotic-based scheme, is described in details in [43].

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A2, SO3, SM2, EM1, SDL1.

## 5.5. CLAToolBox

**Participants:** Christophe Besse [correspondant (Univ. Lille 1)], Pauline Klein [Univ. Besançon].

Absorbant boundary conditions, Schrödinger equation

As a byproduct of the review paper [30], a user-friendly interface is offered <sup>1</sup> to trial and compare various numerical methods to solve the 1D Schrödinger equation with absorbant boundary conditions. We also mention [34] for a numerical investigation of blow-up phenomena in the nonlinear Schrödinger equation.

## 5.6. SPARCS

**Participants:** Christophe Besse [Univ. Lille 1], Thierry Goudon [correspondant (Inria)], Ingrid Lacroix-Violet [Univ. Lille 1].

Vlasov-Poisson system, Euler-Poisson system. Back-Trajectory method

SPARCS is the code developed by Thales Alenia Space for the simulation of the charge phenomena the spacecrafts are subject to. The current version of the code, according to the PhD thesis of O. Chanrion and M. Chane-Yook performed in collaboration with the team Caiman at Sophia Antipolis, is specialized to geostationary atmospheres. The model consists in the stationary Vlasov-Poisson system, but where instationary effects are taken into account with the boundary condition for the electric field. We participate, in particular through the post doc of N. Vauchelet, to the elaboration of an improved version of the code which includes parallization optimized procedures, the modelling of the natural difference of potential between different dielectric surfaces of the spacecraft, as well as the possible presence of devices emitting charged particles.

## 5.7. Code-Carmel3D

**Participant:** Emmanuel Creusé [correspondant (Univ. Lille 1)].

This numerical code, developed in collaboration between EDF R&D and Lille 1 University, is devoted to the electromagnetic fields computation by the use of finite element methods. This code allows in particular to perform nondestructive control by the use of Foucault currents in steam generator pipes, and should be soon coupled with the thermal simulation of Code-Aster. Code-Carmel3D uses the Salomé platform (mesh-generator and post-processing) and Open Turns (uncertainties computation). It will consequently allow to solve multi-physics problems, both for the temporal and harmonic formulations.

<sup>1</sup><http://math.univ-lille1.fr/~besse/site/recherche/logiciels/index.html>

## 6. New Results

### 6.1. Quantitative homogenization theory

In collaboration with S. Neukamm and F. Otto, A. Gloria developed in [46] and [45] a quantitative approach of the stochastic homogenization of discrete elliptic equations. There are two main achievements. In [46] we developed a general theory which quantifies optimally in time the decay of the non-constant coefficients semi-group associated with discrete random diffusion coefficients satisfying a spectral gap assumption (namely, the environment seen from the particle). Combined with spectral theory this allowed us to make a sharp numerical analysis of the popular periodization method to approximate homogenized coefficients. In [45], we obtained a quantitative two-scale expansion result, and essentially proved that the difference between the solution of a (discrete) elliptic equation with random coefficients on the torus and the first two terms of the two-scale expansion scales as in the periodic case (except in dimension 2, for which there is a logarithmic correction).

### 6.2. Corrosion

The Diffusion Poisson Coupled Model [32] 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 [44], 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 steady-state solution to this model. More recently, C. Chainais-Hillairet and I. Lacroix-Violet have also obtained an existence result for the time-dependent simplified model. This result is submitted for publication [47].

P.-L. Colin, C. Chainais-Hillairet and I. Lacroix-Violet have recently performed the numerical analysis of the numerical scheme presented in [31]. 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. T. Gallouët has proposed a new scheme in order to compute directly this pseudo-steady-state. This scheme has been implemented in the code CALIPSO (ANDRA). Validation is in progress, as the numerical analysis of the scheme.

### 6.3. New results on finite volume schemes

In [5], C. Chainais-Hillairet, S. Krell and A. Mouton develop Discrete Duality Finite Volume methods for the finite volume approximation of a system describing miscible displacement in porous media (Peaceman model). They establish relevant a priori estimates satisfied by the numerical solution and prove existence and uniqueness of the solution to the scheme. They show the efficiency of the schemes through numerical experiments. Recently, they also proved the convergence of the DDFV scheme for the Peaceman model. This work will be soon submitted for publication.

In [35], M. Bessemoulin-Chatard, C. Chainais-Hillairet and F. Filbet prove several discrete Gagliardo-Nirenberg-Sobolev and Poincaré-Sobolev inequalities for some approximations with arbitrary boundary values on finite volume meshes. The keypoint of their approach is to use the continuous embedding of the space  $BV(\Omega)$  into  $L^{N/(N-1)}(\Omega)$  for a Lipschitz domain  $\Omega \subset \mathbb{R}^N$ , with  $N \geq 2$ . Finally, they give several applications to discrete duality finite volume (DDFV) schemes which are used for the approximation of nonlinear and on isotropic elliptic and parabolic problems.

In [22], M. Bessemoulin-Chatard, C. Chainais-Hillairet and M.-H. Vignal consider the numerical approximation of the classical time-dependent drift-diffusion system near quasi-neutrality by a fully implicit in time and finite volume in space scheme, where the convection-diffusion fluxes are approximated by Scharfetter-Gummel fluxes. They establish that all the a priori estimates needed to prove the convergence of the scheme does not depend on the Debye length  $\lambda$ . This proves that the scheme is asymptotic preserving in the quasi-neutral limit  $\lambda \rightarrow 0$ .

In [24], 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.

## 6.4. New results in numerical fluid dynamics

In the case of compressible models, as the Euler equations, a careful analysis of sharp and practical stability conditions to ensure the positivity of both density and pressure variables was performed[4]. We are also concerned with the numerical simulation of certain multi-fluids flows, which in particular arises in the modeling of powder/snow avalanches. The hybrid scheme works on unstructured meshes and can be advantageously coupled to mesh refinements strategies in order to follow fronts of high density variation [42]. In particular, we investigate the influence of the characteristics Froude number, Schmidt number and Reynolds number on the front progression. In the context of the PhD thesis of Meriem Ezzoug (University of Monastir, Tunisia), co-advised by C. Calgaro and E. Zahrouni (University of Monastir, Tunisia), we investigate theoretically and numerically the influence of a specific stress tensor, introduced for the first time by Korteweg, in some diffuse interface models which allow to describe some phase transition phenomena, such as surface tension force formulation for multiphase fluid flows. In order to answer these questions, we have developed respectively a Fortran code, a C++ code (NS2DDV-C++, see the softwares section) and a MATLAB code (NS2DDV-M, see the softwares section).

## 6.5. New results on a posteriori estimates

Some residual-type a posteriori error estimators were developed in the context of magnetostatic and magnetodynamic Maxwell equations, given in their potential and harmonic formulations. Here, the task was to find a relevant decomposition of the error in order to obtain the reliability of the estimator, with the use of ad-hoc interpolations. This work was realized in collaboration with the L2EP Laboratory (Laboratoire d'Electrotechnique et d'Electronique de Puissance de Lille, Lille 1 University), and gave rise to several contributions [7], [18], [19], [20], [21], obtained in the context of the Ph-D thesis and of the Post-doc position of Zuqi Tang. Then, other results about a posteriori error estimators were obtained in other contexts [6], [8]. Recently, we started working on space/time error estimators for finite element methods, arising in the context of low-frequency Maxwell equations (PhD of R. Tittarelli, CIFRE EDF R&D, see [25]).

## 6.6. New results in control in fluid mechanics

Recently, we studied more particularly passive control techniques using porous media for incompressible aerodynamics on several bodies, with the use of the penalisation method [3].

# 7. Bilateral Contracts and Grants with Industry

## 7.1. Study of the EKINOX model of corrosion (CNRS Contract with CEA, Univ Lille1, Univ B. Pascal)

**Participants:** Claire Chainais-Hillairet, Antoine Gloria.

In collaboration with C.Desgranges and F. Lequien (CEA), F. Bouchon (Univ. B. Pascal), A. Gloria and C. Chainais-Hillairet are considering the model EKINOX developed at CEA for the study of the corrosion of Ni-base alloys in PWR primary water. Starting from this numerical model (leading to an explicit in time scheme), they have established a macroscopic model (a system of coupled partial differential equations). Based on this model, they have proposed a new numerical method based on an implicit discretization of the diffusion terms.

## 7.2. Numerical methods for the DPCM model (Inria/ANDRA Contract)

**Participants:** Claire Chainais-Hillairet, Thomas Gallouët, Antoine Gloria.

During his post-doc, Thomas Gallouët is working on the numerical approximation of the DPCM model, see [31]. He has designed a new scheme for the direct computation of a steady-state. This scheme has been implemented in the code CALIPSO developed at ANDRA. Validation is in progress, as the numerical analysis of the scheme. Further work will also be done in order to introduce in the code CALIPSO a second order in time scheme which remain unconditionally stable. This is work in collaboration with C. Bataillon (CEA), F. Bouchon (Univ B. Pascal) and J. Fuhrmann (WIAS Berlin).

# 8. Partnerships and Cooperations

## 8.1. Regional Initiatives

Collaboration with the laser physics department (PhLAM) of Université Lille 1 (C. Besse, S. De Bièvre, M. Gazeau, and G. Dujardin)

## 8.2. National Initiatives

### 8.2.1. Collaborations within Inria

REO (A. Gloria)  
COFFEE (E. Creusé and C. Calgaro)  
POEMS (C. Besse and I. Lacroix-Violet)  
CORIDA (C. Besse)  
IPSO (C. Besse)

### 8.2.2. ANR

#### 8.2.2.1. ANR IODISSEE (2009-2013)

**Participants:** Christophe Besse, Pauline Lafitte.

C. Besse has obtained a 4-years ANR grant, from the Cosinus proposal, for the project IODISSEE. P. Lafitte and C. Yang, also members of the EPI Simpaf, are involved in this project. The project IODISSEE also involves a team of mathematicians from Toulouse, a physicist team from Versailles and the Thales group. It deals with the elaboration of a physical model for helping the industrial partner for the new generation of Galileo satellites. For the last decade, satellite positioning devices became one of the most interesting means of navigation for the displacement of the goods and the people. The only current solution is based on the constellation of satellites Navstar GPS American system. Originally developed for military applications, its use was released under the Clinton administration. However, in order to guarantee its autonomy, Europe decided to launch a competitor program known as Galileo. Galileo system differs from the GPS thanks to its capability to provide real time integrity information to the user. In order to guarantee the stability of this system, it is fundamental to take into account the various problems which can affect the mission and to identify all the potential sources of system unavailability. One of the main source of data unavailability that has been identified is the phenomena of ionospheric scintillations. Indeed scintillation causes radio frequency signal amplitude fades and phase variations as satellite signals pass through the ionosphere. Such effects may induce



loss of lock or cycle slips on ranging signals broadcast by Galileo satellites making them totally useless for accurate integrity information determination. Scintillations are clearly identified like a source of disturbances. They appear as the turbulent aspect of a larger disturbance of the ionospheric plasma density which have the shape of a plasma bubble. The difficulty of their modelling is due to the lacks of in situ measurements with regard to them. However, some measurements recently acquired during the mission of satellite DEMETER make possible on the one hand the validation of the models existing but also, using techniques of data-models coupling, to reinforce them. The object of this proposal is therefore to provide a physical model making it possible to anticipate the attenuation of the signals during their propagation within the disturbed Earth ionosphere.

#### 8.2.2.2. ANR AMAM (2011-2014)

**Participant:** Antoine Gloria.

A. Gloria is involved in the 4-year ANR project “young researcher” AMAM, led by V. Millot (Paris 7). The aim of the project is to develop mathematical tools for the analysis of multiscale problems in material sciences (PDEs and variational methods). The fields of interest are primarily micromagnetics, dislocations, fatigue in nonlinear elasticity, and homogenization.

#### 8.2.2.3. ANR STAB (2013-2017)

**Participant:** Pauline Lafitte.

STAB : Most of the natural time-evolving systems that one encounters in Physics, Biology, Economics..., can be described by means of evolution equations, or systems of such equations. These equations may include randomness or not. During the last decade, a lot of progress has been made in the understanding of the stabilization of these dynamics, i.e. their convergence to equilibrium. In particular the picture of the qualitative description of the rate of convergence is now almost complete for symmetric models (reversible dynamics). However, the non-reversible setting is still insufficiently understood. One of the most fascinating features of this research area is the strong intricacy between the analysis of partial differential equations and stochastic methods, each approach enlightening the other one. The main goal of this project is to go further, developing tractable and efficient tools, in particular for numerical schemes and algorithms, based on the computation of explicit theoretical bounds. Hence, even if part of the project is devoted to the theoretical study of non-reversible or highly degenerate situations (we typically have to face kinetic or reaction-diffusion models for example), the heart of the project will include discretization schemes, approximating particle systems and concrete simulation situations (including boundary conditions). This concerns the stability of the discretization or numerical methods. The acronym STAB covers both aspects: stabilization and stability. Indeed, sensitivity to small perturbations (or to boundary conditions) is the first definition of large time stability for numerical schemes. The head of the project is I. Gentil (Univ. Lyon1).

#### 8.2.2.4. ANR BECASIM(2013-2017)

**Participants:** Christophe Besse, Guillaume Dujardin, Ingrid Lacroix-Violet.

C. Besse, G. Dujardin, and I. Lacroix-Violet are members of the new 4-years ANR "Modèles Numériques" project BECASIM. C. Besse is the Toulouse-node coordinator and I. Lacroix-Violet the Lille-node one. The scientific subject deals with mathematical modelling, numerical analysis and simulation of Bose-Einstein condensates (BEC). The goal of this ANR project is to : (i) develop new high-order numerical methods; (ii) develop an integrated and resilient open-source HPC software; (iii) apply these codes to numerically reproduce realistic physical configurations that are not possible to simulate with presently existing software.

### 8.2.3. Competitivity Clusters

#### 8.2.3.1. LABEX Centre Européen pour les Mathématiques, la Physique et leurs Interactions – CEMPI (2012-2019)

The “Laboratoire d’Excellence” CEMPI was created by the French government within the framework of its “Projets d’Investissement d’Avenir” program, in February 2012. It is a joint venture of the Laboratoire Paul Painlevé (mathematics) and the Laboratoire Physique des Lasers, Atomes et Molécules (PhLAM). Several members of CEMPI participate actively in the CEMPI research and training project, notably through the focus area “The interaction of mathematics and physics”. The corresponding research is described in Sections 3.2.3 and 3.4.



## 8.3. European Initiatives

### 8.3.1. FP7 Projects

ERC starting grant QUANTHOM (starting February 2014).

### 8.3.2. Collaborations with Major European Organizations

Felix Otto: Max Planck Institute for Mathematics in the Sciences (Germany)  
Quantitative stochastic homogenization theory.

## 8.4. International Research Visitors

### 8.4.1. Visits of International Scientists

- J.-C. Mourrat (EPFL, 1 week)
- D. Marahrens (MPIMS, 1 week)
- S. Neukamm (WIAS, 1 week)

### 8.4.2. Visits to International Teams

- A. Gloria, from September to December 2013, Math department, Stanford University

## 9. Dissemination

### 9.1. Scientific Animation

- A. Gloria organized of a mini-symposium at the SIAM Conference on Mathematical Aspects of Materials Science (Philadelphia, June 2013)

### 9.2. Teaching - Supervision - Juries

#### 9.2.1. Supervision

PhD : Émilie Soret, Accélération stochastique et thermalisation, 2011-2014, under the supervision of S. de Bièvre and T. Simon (Université Lille 1)

PhD : Pierre-Louis Colin, Theoretical and numerical study of some mathematical models of corrosion, Université Lille 1, 2012/09/01-2015/09/01, under the supervision of C. Chainais-Hillairet and I. Lacroix-Violet

#### 9.2.2. Juries

- A. Gloria, referee for the PhD thesis of F. Ouaki (Ecole polytechnique), December 2013

### 9.3. Popularization

C. Calgario is in charge of the communication of "Laboratoire Paul Painlevé" and she is in charge of the relation between the University of Lille and high schools. Accordingly, she organizes various events like « Les Mathématiques itinérantes » and « Stage de seconde à contenu scientifique ». With the help of the Communication Department of Inria, C. Calgario, E. Creusé and T. Goudon produced a documentary fiction (in French) for a general audience on how research in applied mathematics is being done. The title is "Avis de recherche" (see <http://www.inria.fr/avisderecherche>).

## 10. Bibliography

### Publications of the year

#### Articles in International Peer-Reviewed Journals

- [1] C. BESSE, R. CARLES, F. MÉHATS. *An asymptotic preserving scheme based on a new formulation for NLS in the semiclassical limit*, in "Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal", 2013, vol. 11, n<sup>o</sup> 4, pp. 1228-1260 [DOI : 10.1137/120899017], <http://hal.inria.fr/hal-00752011>
- [2] C. BESSE, J. COATLEVEN, S. FLISS, I. LACROIX-VIOLET, K. RAMDANI. *Transparent boundary conditions for locally perturbed infinite hexagonal periodic media*, in "Communications in Mathematical Sciences", 2013, vol. 11, n<sup>o</sup> 4, pp. 907-938, <http://hal.inria.fr/hal-00698916>
- [3] C.-H. BRUNEAU, E. CREUSÉ, P. GILLIÉRON, I. MORTAZAVI. *A glimpse on passive control using porous media for incompressible aerodynamics*, in "International Journal of Aerodynamics", 2014, vol. 4, n<sup>o</sup> 1/2, pp. 70-86, <http://hal.inria.fr/hal-00922032>
- [4] C. CALGARO, E. CREUSÉ, T. GOUDON, Y. PENEL. *Positivity-preserving schemes for Euler equations: Sharp and practical CFL conditions*, in "Journal of Computational Physics", 2013, vol. 234, n<sup>o</sup> 1, pp. 417-438 [DOI : 10.1016/J.JCP.2012.09.040], <http://hal.inria.fr/hal-00768479>
- [5] C. CHAINAIS-HILLAIRET, S. KRELL, A. MOUTON. *Study of discrete duality finite volume schemes for the Peaceman model*, in "SIAM Journal on Scientific Computing", 2013, vol. 35, n<sup>o</sup> 6, pp. A2928-A2952 [DOI : 10.1137/130910555], <http://hal.inria.fr/hal-00790449>
- [6] E. CREUSÉ, S. NICAISE. *A posteriori error estimator based on gradient recovery by averaging for convection-diffusion-reaction problems approximated by discontinuous Galerkin methods*, in "IMA Journal of Numerical Analysis", 2013, vol. 33, n<sup>o</sup> 1, pp. 212-241 [DOI : 10.1093/IMANUM/DRR052], <http://hal.inria.fr/hal-00531621>
- [7] E. CREUSÉ, S. NICAISE, Z. TANG, Y. LE MENACH, N. NEMITZ, F. PIRIOU. *Residual-based a posteriori estimators for the T/Omega magnetodynamic harmonic formulation of the Maxwell system*, in "International Journal of Numerical Analysis and Modeling", 2013, vol. 10, n<sup>o</sup> 2, pp. 411-429, <http://hal.inria.fr/hal-00777601>
- [8] E. CREUSÉ, S. NICAISE, E. VERHILLE. *Robust residual a posteriori error estimators for the Reissner-Mindlin eigenvalues system*, in "Journal of Numerical Mathematics", 2013, vol. 21, n<sup>o</sup> 2, pp. 89-134, <http://hal.inria.fr/hal-00777682>
- [9] M. DOUMIC JAUFFRET, L. M. TINE. *Estimating the Division Rate for the Growth-Fragmentation Equation*, in "Journal of Mathematical Biology", July 2013, vol. 67, n<sup>o</sup> 1, pp. 69-103 [DOI : 10.1007/s00285-012-0553-6], <http://hal.inria.fr/hal-00634539>
- [10] A. GLORIA. *Fluctuation of solutions to linear elliptic equations with noisy diffusion coefficients*, in "Communications in Partial Differential Equations", 2013, 1 p. [DOI : 10.1080/03605302.2012.715319], <http://hal.inria.fr/hal-00674445>

- [11] A. GLORIA, T. GOUDON, S. KRELL. *Numerical homogenization of a nonlinearly coupled elliptic-parabolic system, reduced basis method, and application to nuclear waste storage*, in "Mathematical Models and Methods in Applied Sciences", 2013, pp. 1-33, <http://hal.inria.fr/hal-00674519>
- [12] A. GLORIA, P. LE TALLEC, M. VIDRASCU. *Foundation, analysis, and numerical investigation of a variational network-based model for rubber*, in "Continuum Mechanics and Thermodynamics", 2013, pp. 1–31 [DOI : 10.1007/s00161-012-0281-6], <http://hal.inria.fr/hal-00673406>
- [13] A. GLORIA, J.-C. MOURRAT. *Quantitative version of the Kipnis-Varadhan theorem and Monte-Carlo approximation of homogenized coefficients*, in "Annals of Applied Probability", 2013, 31 p. , <http://hal.inria.fr/inria-00579424>
- [14] A. GLORIA, M. PENROSE. *Random parking, Euclidean functionals, and rubber elasticity*, in "Communications in Mathematical Physics", 2013, 1 p. , <http://hal.inria.fr/hal-00675037>
- [15] P. LAFITTE-GODILLON, K. RASCHEL, V. C. TRAN. *Extinction probabilities for a distylous plant population modeled by an inhomogeneous random walk on the positive quadrant*, in "SIAM Journal on Applied Mathematics", 2013, vol. 73, n<sup>o</sup> 2, pp. 700-722 [DOI : 10.1137/120864258], <http://hal.inria.fr/hal-00664536>
- [16] C. LIN, J.-F. COULOMBEL. *The strong relaxation limit of the multidimensional Euler equations*, in "Nonlinear Differential Equations and Applications", 2013, vol. 20, n<sup>o</sup> 3, pp. 447-461, <http://hal.inria.fr/hal-00622938>
- [17] A. RUGGERI, V. ROCHA, E. MASSON, M. LABOPIN, R. CUNHA, L. ABSI, A. BOUDIFA, B. COEFFIC, A. DEVYS, M. DE MATTEIS, V. DUBOIS, D. HANAU, F. HAU, I. JOLLET, D. MASSON, B. PEDRON, P. PERRIER, C. PICARD, A. RAMOUNEAU-PIGOT, F. VOLT, D. CHARRON, E. GLUCKMAN, P. LOISEAU. *Impact of donor-specific anti-HLA antibodies on graft failure and survival after reduced intensity conditioning-unrelated cord blood transplantation: a Eurocord, Société Francophone d'Histocompatibilité et d'Immunogénétique (SFHI) and Société Française de Greffe de Moelle et de Thérapie Cellulaire (SFGM-TC) analysis*, in "Haematologica", July 2013, vol. 98, n<sup>o</sup> 7, pp. 1154-60 [DOI : 10.3324/HAEMATOL.2012.077685], <http://hal.inria.fr/hal-00870805>
- [18] Z. TANG, Y. LE MENACH, E. CREUSÉ, S. NICAISE, F. PIRIOU, N. NEMITZ. *A posteriori error estimator for harmonic A/Phi formulation*, in "COMPEL: The International Journal for Computation and Mathematics in Electrical and Electronic Engineering", 2013, vol. 32, n<sup>o</sup> 4, pp. 1219-1229, <http://hal.inria.fr/hal-00910309>
- [19] Z. TANG, Y. LE MENACH, E. CREUSÉ, S. NICAISE, F. PIRIOU, N. NEMITZ. *Residual and Equilibrated Error Estimators for Magnetostatic Problems Solved by Finite Element Method*, in "IEEE Transactions on Magnetics", 2013, vol. 49, n<sup>o</sup> 12, pp. 5715-5723, <http://hal.inria.fr/hal-00910314>
- [20] Z. TANG, Y. LE MENACH, E. CREUSÉ, S. NICAISE, F. PIRIOU, N. NEMITZ. *Residual Based a Posteriori Error Estimators for Harmonic A/Phi and T/Omega Formulations in Eddy Current Problems*, in "IEEE Transactions on Magnetics", 2013, vol. 49, n<sup>o</sup> 5, pp. 1721-1724, <http://hal.inria.fr/hal-00910319>

### International Conferences with Proceedings

- [21] T. LELONG, Z. TANG, R. SCORRETTI, P. THOMAS, Y. LE MENACH, E. CREUSÉ, F. PIRIOU, N. BURAI, C. MIRY, I. MAGNE. *Error estimation in the Computation of Induced Current of Human Body in the Case of Low frequency Magnetic Field Excitation*, in "Compumag", Budapest, Hungary, June 2013, pp. PC1-11, <http://hal.inria.fr/hal-00829296>

## Other Publications

- [22] M. BESSEMOULIN-CHATARD, C. CHAINAIS-HILLAIRET, M.-H. VIGNAL. , *Study of a fully implicit scheme for the drift-diffusion system. Asymptotic behavior in the quasi-neutral limit*, 2013, <http://hal.inria.fr/hal-00801912>
- [23] C.-E. BRÉHIER, M. GAZEAU, L. GOUDENÈGE, M. ROUSSET. , *Analysis and simulation of rare events for SPDE*, January 2014, <http://hal.inria.fr/hal-00921680>
- [24] C. CHAINAIS-HILLAIRET, A. JÜNGEL, S. SCHUCHNIGG. , *Entropy-dissipative discretization of nonlinear diffusion equations and discrete Beckner inequalities*, 2013, <http://hal.inria.fr/hal-00924282>
- [25] E. CREUSÉ, S. NICAISE, R. TITTARELLI. , *Space-time residual-based a posteriori estimators for the A/Phi magneto dynamic formulation of the Maxwell system*, 2013, <http://hal.inria.fr/hal-00921116>
- [26] C. DAVID, G. DUJARDIN. , *Energy-preserving integrators for stochastic Poisson systems*, 2013, <http://hal.inria.fr/hal-00907890>
- [27] A. GLORIA, Z. HABIBI. , *Reduction of the resonance error in numerical homogenization II: correctors, extrapolation, and spectral theory*, January 2014, <http://hal.inria.fr/hal-00933234>
- [28] T. GOUDON, P. LAFITTE. , *The lovebirds problem: why solve Hamilton-Jacobi-Bellman equations matters in love affairs*, January 2013, <http://hal.inria.fr/hal-00780945>
- [29] V. GUDMUNDSSON, S. HAUSSON, A. JOHNSEN, G. REINISCH, A. MANOLESCU, C. BESSE, G. DUJARDIN. , *Excitation of radial collective modes in a quantum dot: Beyond linear response*, 2013, 12 p. , PDFLaTeX, RevTeX, <http://hal.inria.fr/hal-00907845>

## References in notes

- [30] X. ANTOINE, A. ARNOLD, C. BESSE, M. EHRHARDT, A. SCHÄDLE. *A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations*, in "Communications in Computational Physics", 2008, vol. 4, pp. 729–796
- [31] C. BATAILLON, F. BOUCHON, C. CHAINAIS-HILLAIRET, J. FUHRMANN, E. HOARAU, R. TOUZANI. *Numerical methods for simulation of a corrosion model with moving oxide layer*, in "Journal of Computational Physics", 2012, vol. 231, n<sup>o</sup> 18, pp. 6213–6231
- [32] C. BATAILLON, C. CHAINAIS-HILLAIRET, C. DESGRANGES, E. HOARAU, F. MARTIN, S. PERRIN, M. TURPIN, J. TALANDIER. *Corrosion modelling of iron based alloy in nuclear waste repository*, in "Electrochimica Acta", 2010, vol. 15, n<sup>o</sup> 55, pp. 4451–4467
- [33] N. BERTRAND, C. DESGRANGES, M. ÑASTAR, G. GIRARDIN, D. POQUILLON, D. MONCEAU. *Chemical evolution in the substrate due to oxidation : a numerical model with explicit treatment of vacancy fluxes*, in "Materials Science Forum", 2008, vol. 595-598, pp. 463–472

- [34] C. BESSE, R. CARLES, N. MAUSER, H.-P. STIMMING. *Monotonicity properties of blow-up time for nonlinear Schrödinger equation: numerical tests*, in "Discrete and Cont. Dyn. Syst. B", 2008, vol. 9, pp. 11–36
- [35] M. BESSEMOULIN-CHATARD, C. CHAINAIS-HILLAIRET, F. FILBET. , *On discrete functional inequalities for some finite volume schemes*, February 2012, <http://hal.archives-ouvertes.fr/hal-00672591>
- [36] C.-H. BRUNEAU, E. CREUSÉ, D. DEPEYRAS, P. GILLIÉRON, I. MORTAZAVI. *Coupling passive and active techniques to control the flow past the square back Ahmed body*, in "Computers and Fluids", 2010, vol. 39, n<sup>o</sup> 10, pp. 1875–1892
- [37] C.-H. BRUNEAU, E. CREUSÉ, D. DEPEYRAS, P. GILLIÉRON, I. MORTAZAVI. *Active and passive flow control around simplified ground vehicles*, in "Journal of Applied Fluid Mechanics", 2012, to appear
- [38] C. CALGARO, E. CHANE-KANE, E. CREUSÉ, T. GOUDON.  *$L^\infty$  stability of vertex-based MUSCL finite volume schemes on unstructured grids; simulation of incompressible flows with high density ratios*, in "Journal of Computational Physics", 2010, vol. 229, n<sup>o</sup> 17, pp. 6027–6046
- [39] C. CALGARO, E. CHANE-KANE, E. CREUSÉ, T. GOUDON.  *$L^\infty$ -stability of vertex-based MUSCL finite volume schemes on unstructured grids: simulation of incompressible flows with high density ratios*, in "J. Comput. Phys.", 2010, vol. 229, n<sup>o</sup> 17, pp. 6027–6046, <http://dx.doi.org/10.1016/j.jcp.2010.04.034>
- [40] C. CALGARO, J.-P. CHEHAB, Y. SAAD. *Incremental incomplete LU factorizations with applications*, in "Numer. Linear Algebra with Appl.", 2010, vol. 17, n<sup>o</sup> 5, pp. 811–817
- [41] C. CALGARO, E. CREUSÉ, T. GOUDON. *An hybrid finite volumes-finite elements method for variable density incompressible flows*, in "Journal of Computational Physics", 2008, vol. 227, n<sup>o</sup> 9, pp. 4671–4696
- [42] C. CALGARO, E. CREUSÉ, T. GOUDON. *Simulation of Mixture Flows: Pollution Spreading and Avalanches*, <http://hal.inria.fr/hal-00732112>
- [43] J. A. CARRILLO, T. GOUDON, P. LAFITTE. *Simulation of fluid and particles flows: asymptotic preserving schemes for bubbling and flowing regimes*, in "J. Comput. Phys.", 2008, vol. 227, n<sup>o</sup> 16, pp. 7929–7951
- [44] C. CHAINAIS-HILLAIRET, I. LACROIX-VIOLET. *The existence of solutions to a corrosion model*, in "Appl. Math. Lett.", 2012 [DOI : DOI:10.1016/j.AML.2012.02.012]
- [45] A. GLORIA, S. NEUKAMM, F. OTTO. , *An optimal quantitative two-scale expansion in stochastic homogenization of discrete elliptic equations*, <http://hal.inria.fr/hal-00863488>
- [46] A. GLORIA, S. NEUKAMM, F. OTTO. , *Quantification of ergodicity in stochastic homogenization: optimal bounds via spectral gap on Glauber dynamics — long version*, January 2013, 106 p. , <http://hal.inria.fr/hal-00782075>
- [47] I. LACROIX-VIOLET, C. CHAINAIS-HILLAIRET. , *On the existence of solutions for a drift-diffusion system arising in corrosion modelling*, December 2012, <http://hal.archives-ouvertes.fr/hal-00764239>

- [48] P. LAFITTE, G. SAMAËY. *Asymptotic-preserving projective integration schemes for kinetic equations in the diffusion limit*, in "SIAM Journal on Scientific Computing", 2012, vol. 34, n<sup>o</sup> 2, pp. A579-A602 [DOI : 10.1137/100795954], <http://arxiv.org/abs/1006.2603v1>