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# Activity Report 2014

# Project-Team IPSO

## Invariant Preserving SOlvers

IN COLLABORATION WITH: Institut de recherche mathématique de Rennes (IRMAR)

RESEARCH CENTER
**Rennes - Bretagne-Atlantique**

THEME
**Numerical schemes and simulations**

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# Project-Team IPSO

**Keywords:** Numerical Methods, Geometric Integration, Stochastic Methods, Fluid Dynamics

*Creation of the Project-Team:* 2004 December 06.

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# 2. Overall Objectives

## 2.1. An overview of geometric numerical integration

A fundamental and enduring challenge in science and technology is the quantitative prediction of time-dependent nonlinear phenomena. While dynamical simulation (for ballistic trajectories) was one of the first applications of the digital computer, the problems treated, the methods used, and their implementation have all changed a great deal over the years. Astronomers use simulation to study long term evolution of the solar system. Molecular simulations are essential for the design of new materials and for drug discovery. Simulation can replace or guide experiment, which often is difficult or even impossible to carry out as our ability to fabricate the necessary devices is limited.

During the last decades, we have seen dramatic increases in computing power, bringing to the fore an ever widening spectrum of applications for dynamical simulation. At the boundaries of different modeling regimes, it is found that computations based on the fundamental laws of physics are under-resolved in the textbook sense of numerical methods. Because of the vast range of scales involved in modeling even relatively simple biological or material functions, this limitation will not be overcome by simply requiring more computing power within any realistic time. One therefore has to develop numerical methods which capture crucial structures even if the method is far from "converging" in the mathematical sense. In this context, we are forced increasingly to think of the numerical algorithm as a part of the modeling process itself. A major step forward in this area has been the development of structure-preserving or "geometric" integrators which maintain conservation laws, dissipation rates, or other key features of the continuous dynamical model. Conservation of energy and momentum are fundamental for many physical models; more complicated invariants are maintained in applications such as molecular dynamics and play a key role in determining the long term stability of methods. In mechanical models (biodynamics, vehicle simulation, astrodynamics) the available structure may include constraint dynamics, actuator or thruster geometry, dissipation rates and properties determined by nonlinear forms of damping.
In recent years the growth of geometric integration has been very noticeable. Features such as *symplecticity* or *time-reversibility* are now widely recognized as essential properties to preserve, owing to their physical significance. This has motivated a lot of research [65], [62], [61] and led to many significant theoretical achievements (symplectic and symmetric methods, volume-preserving integrators, Lie-group methods, ...). In practice, a few simple schemes such as the Verlet method or the Störmer method have been used for years with great success in molecular dynamics or astronomy. However, they now need to be further improved in order to fit the tremendous increase of complexity and size of the models.

## 2.2. Overall objectives

To become more specific, the project *IPSO* aims at finding and implementing new structure-preserving schemes and at understanding the behavior of existing ones for the following type of problems:

- systems of differential equations posed on a manifold.
- systems of differential-algebraic equations of index 2 or 3, where the constraints are part of the equations.
- Hamiltonian systems and constrained Hamiltonian systems (which are special cases of the first two items though with some additional structure).
- highly-oscillatory systems (with a special focus of those resulting from the Schrödinger equation).

Although the field of application of the ideas contained in geometric integration is extremely wide (e.g. robotics, astronomy, simulation of vehicle dynamics, biomechanical modeling, biomolecular dynamics, geo-dynamics, chemistry...), *IPSO* will mainly concentrate on applications for *molecular dynamics simulation* and *laser simulation*:

- There is a large demand in biomolecular modeling for models that integrate microscopic molecular dynamics simulation into statistical macroscopic quantities. These simulations involve huge systems of ordinary differential equations over very long time intervals. This is a typical situation where the determination of accurate trajectories is out of reach and where one has to rely on the good qualitative behavior of structure-preserving integrators. Due to the complexity of the problem, more efficient numerical schemes need to be developed.
- The demand for new models and/or new structure-preserving schemes is also quite large in laser simulations. The propagation of lasers induces, in most practical cases, several well-separated scales: the intrinsically highly-oscillatory *waves* travel over long distances. In this situation, filtering the oscillations in order to capture the long-term trend is what is required by physicists and engineers.

# 3. Research Program

## 3.1. Structure-preserving numerical schemes for solving ordinary differential equations

**Participants:** François Castella, Philippe Chartier, Erwan Faou, Vilmart Gilles.

ordinary differential equation, numerical integrator, invariant, Hamiltonian system, reversible system, Lie-group system

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{1}$$

For a given $y_0$, the solution $y(t)$ at time $t$ is denoted $\varphi_t(y_0)$. For fixed $t$, $\varphi_t$ becomes a function of $y_0$ called the *flow* of (1). From this point of view, a numerical scheme with step size $h$ for solving (1) may be regarded as an approximation $\Phi_h$ of $\varphi_h$. One of the main questions of *geometric integration* is whether *intrinsic* properties of $\varphi_t$ may be passed on to $\Phi_h$.

This question can be more specifically addressed in the following situations:

### *3.1.1. Reversible ODEs*

The system (1) is said to be $\rho$-reversible if there exists an involutive linear map $\rho$ such that

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{2}$$

It is then natural to require that $\Phi_h$ satisfies the same relation. If this is so, $\Phi_h$ is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

### *3.1.2. ODEs with an invariant manifold*

The system (1) is said to have an invariant manifold $g$ whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{3}$$

is kept *globally* invariant by $\varphi_t$. In terms of derivatives and for sufficiently differentiable functions $f$ and $g$, this means that

$$\forall\, y \in \mathcal{M},\ g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [60] and divided into two classes, according to whether they use $g$ explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton's iterations.

### 3.1.3. Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{array}{rcccl} \dot{p}(t) & = & -\nabla_q H(p(t),q(t)) & \in & \mathbb{R}^d \\ \dot{q}(t) & = & \nabla_p H(p(t),q(t)) & \in & \mathbb{R}^d \end{array} \tag{4}$$

with some prescribed initial values $(p(0),q(0)) = (p_0,q_0)$ and for some scalar function $H$, called the Hamiltonian. In this situation, $H$ is an invariant of the problem. The evolution equation (4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p,q) \in \mathbb{R}^d \times \mathbb{R}^d; H(p,q) = H(p_0,q_0)\}.$$

Besides the Hamiltonian function, there might exist other invariants for such systems: when there exist $d$ invariants in involution, the system (4) is said to be *integrable*. Consider now the parallelogram $P$ originating from the point $(p,q) \in \mathbb{R}^{2d}$ and spanned by the two vectors $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$, and let $\omega(\xi,\eta)$ be the sum of the *oriented* areas of the projections over the planes $(p_i,q_i)$ of $P$,

$$\omega(\xi,\eta) = \xi^T J \eta,$$

where $J$ is the *canonical symplectic* matrix

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}.$$

A continuously differentiable map $g$ from $\mathbb{R}^{2d}$ to itself is called symplectic if it preserves $\omega$, i.e. if

$$\omega(g'(p,q)\xi, g'(p,q)\eta) = \omega(\xi,\eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

### 3.1.4. Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository section, it is enough to present the so-called index-2 systems

$$\begin{array}{rcl} \dot{y}(t) & = & f(y(t),z(t)), \\ 0 & = & g(y(t)), \end{array} \tag{5}$$

where initial values $(y(0),z(0)) = (y_0,z_0)$ are given and assumed to be consistent with the constraint manifold. By constraint manifold, we imply the intersection of the manifold

$$\mathcal{M}_1 = \{y \in \mathbb{R}^n, g(y) = 0\}$$

and of the so-called hidden manifold

$$\mathcal{M}_2 = \{(y,z) \in \mathbb{R}^n \times \mathbb{R}^m, \frac{\partial g}{\partial y}(y) f(y,z) = 0\}.$$

This manifold $\mathcal{M} = \mathcal{M}_1 \bigcap \mathcal{M}_2$ is the manifold on which the exact solution $(y(t), z(t))$ of (5) lives.

There exists a whole set of schemes which provide a numerical approximation lying on $\mathcal{M}_1$. Furthermore, this solution can be projected on the manifold $\mathcal{M}$ by standard projection techniques. However, it it worth mentioning that a projection destroys the symmetry of the underlying scheme, so that the construction of a symmetric numerical scheme preserving $\mathcal{M}$ requires a more sophisticated approach.

## 3.2. Highly-oscillatory systems

**Participants:** François Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Méhats, Mohammed Lemou, Gilles Vilmart.

second-order ODEs, oscillatory solutions, Schrödinger and wave equations, step size restrictions.

In applications to molecular dynamics or quantum dynamics for instance, the right-hand side of (1) involves *fast* forces (short-range interactions) and *slow* forces (long-range interactions). Since *fast* forces are much cheaper to evaluate than *slow* forces, it seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

A typical model of highly-oscillatory systems is the second-order differential equations

$$\ddot{q} \quad = \quad -\nabla V(q) \tag{6}$$

where the potential $V(q)$ is a sum of potentials $V = W + U$ acting on different time-scales, with $\nabla^2 W$ positive definite and $\|\nabla^2 W\| >> \|\nabla^2 U\|$. In order to get a bounded error propagation in the linearized equations for an explicit numerical method, the step size must be restricted according to

$$h\omega < C,$$

where $C$ is a constant depending on the numerical method and where $\omega$ is the highest frequency of the problem, i.e. in this situation the square root of the largest eigenvalue of $\nabla^2 W$. In applications to molecular dynamics for instance, *fast* forces deriving from $W$ (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from $U$ (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another prominent example of highly-oscillatory systems is encountered in quantum dynamics where the Schrödinger equation is the model to be used. Assuming that the Laplacian has been discretized in space, one indeed gets the *time*-dependent Schrödinger equation:

$$i\dot{\psi}(t) = \frac{1}{\varepsilon} H(t)\psi(t), \tag{7}$$

where $H(t)$ is finite-dimensional matrix and where $\varepsilon$ typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are faced once again with two different time-scales, 1 and $\varepsilon$. In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

## 3.3. Geometric schemes for the Schrödinger equation

**Participants:** François Castella, Philippe Chartier, Erwan Faou, Florian Méhats, Gilles Vilmart.

Schrödinger equation, variational splitting, energy conservation.

Given the Hamiltonian structure of the Schrödinger equation, we are led to consider the question of energy preservation for time-discretization schemes.

At a higher level, the Schrödinger equation is a partial differential equation which may exhibit Hamiltonian structures. This is the case of the time-dependent Schrödinger equation, which we may write as

$$i\varepsilon\frac{\partial\psi}{\partial t} = H\psi, \tag{8}$$

where $\psi = \psi(x,t)$ is the wave function depending on the spatial variables $x = (x_1, \cdots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, $\varepsilon$ is a (small) positive number representing the scaled Planck constant and $i$ is the complex imaginary unit. The Hamiltonian operator $H$ is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N}\frac{\varepsilon^2}{2m_k}\Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and $\Delta_{x_k}$ the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential $V$ acts as a multiplication operator on $\psi$.

The multiplication by $i$ in (8) plays the role of the multiplication by $J$ in classical mechanics, and the energy $\langle\psi|H|\psi\rangle$ is conserved along the solution of (8), using the physicists' notations $\langle u|A|u\rangle = \langle u, Au\rangle$ where $\langle\ ,\ \rangle$ denotes the Hermitian $L^2$-product over the phase space. In quantum mechanics, the number $N$ of particles is very large making the direct approximation of (8) very difficult.

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [64], [63] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

A particularly interesting case of study is given by symmetric splitting methods, such as the Strang splitting:

$$\psi_1 = \exp\left(-i(\delta t)V/2\right)\exp\left(i(\delta t)\Delta\right)\exp\left(-i(\delta t)V/2\right)\psi_0 \tag{9}$$

where $\delta t$ is the time increment (we have set all the parameters to 1 in the equation). As the Laplace operator is unbounded, we cannot apply the standard methods used in ODEs to derive long-time properties of these schemes. However, its projection onto finite dimensional submanifolds (such as Gaussian wave packets space or FEM finite dimensional space of functions in $x$) may exhibit Hamiltonian or Poisson structure, whose long-time properties turn out to be more tractable.

## 3.4. High-frequency limit of the Helmholtz equation

**Participant:** François Castella.

waves, Helmholtz equation, high oscillations.

The Helmholtz equation models the propagation of waves in a medium with variable refraction index. It is a simplified version of the Maxwell system for electro-magnetic waves.

The high-frequency regime is characterized by the fact that the typical wavelength of the signals under consideration is much smaller than the typical distance of observation of those signals. Hence, in the high-frequency regime, the Helmholtz equation at once involves highly oscillatory phenomena that are to be described in some asymptotic way. Quantitatively, the Helmholtz equation reads

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x) u_\varepsilon = f_\varepsilon(x). \tag{10}$$

Here, $\varepsilon$ is the small adimensional parameter that measures the typical wavelength of the signal, $n(x)$ is the space-dependent refraction index, and $f_\varepsilon(x)$ is a given (possibly dependent on $\varepsilon$) source term. The unknown is $u_\varepsilon(x)$. One may think of an antenna emitting waves in the whole space (this is the $f_\varepsilon(x)$), thus creating at any point $x$ the signal $u_\varepsilon(x)$ along the propagation. The small $\alpha_\varepsilon > 0$ term takes into account damping of the waves as they propagate.

One important scientific objective typically is to describe the high-frequency regime in terms of *rays* propagating in the medium, that are possibly refracted at interfaces, or bounce on boundaries, etc. Ultimately, one would like to replace the true numerical resolution of the Helmholtz equation by that of a simpler, asymptotic model, formulated in terms of rays.

In some sense, and in comparison with, say, the wave equation, the specificity of the Helmholtz equation is the following. While the wave equation typically describes the evolution of waves between some initial time and some given observation time, the Helmholtz equation takes into account at once the propagation of waves over *infinitely long* time intervals. Qualitatively, in order to have a good understanding of the signal observed in some bounded region of space, one readily needs to be able to describe the propagative phenomena in the whole space, up to infinity. In other words, the "rays" we refer to above need to be understood from the initial time up to infinity. This is a central difficulty in the analysis of the high-frequency behaviour of the Helmholtz equation.

## 3.5. From the Schrödinger equation to Boltzmann-like equations

**Participant:** François Castella.

Schrödinger equation, asymptotic model, Boltzmann equation.

The Schrödinger equation is the appropriate way to describe transport phenomena at the scale of electrons. However, for real devices, it is important to derive models valid at a larger scale.

In semi-conductors, the Schrödinger equation is the ultimate model that allows to obtain quantitative information about electronic transport in crystals. It reads, in convenient adimensional units,

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi + V(x)\psi, \tag{11}$$

where $V(x)$ is the potential and $\psi(t,x)$ is the time- and space-dependent wave function. However, the size of real devices makes it important to derive simplified models that are valid at a larger scale. Typically, one wishes to have kinetic transport equations. As is well-known, this requirement needs one to be able to describe "collisions" between electrons in these devices, a concept that makes sense at the macroscopic level, while it does not at the microscopic (electronic) level. Quantitatively, the question is the following: can one obtain the Boltzmann equation (an equation that describes collisional phenomena) as an asymptotic model for the Schrödinger equation, along the physically relevant micro-macro asymptotics? From the point of view of modelling, one wishes here to understand what are the "good objects", or, in more technical words, what are the relevant "cross-sections", that describe the elementary collisional phenomena. Quantitatively, the Boltzmann equation reads, in a simplified, linearized, form :

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v')\,[f(t,x,v') - f(t,x,v)]dv'. \tag{12}$$

Here, the unknown is $f(x,v,t)$, the probability that a particle sits at position $x$, with a velocity $v$, at time $t$. Also, $\sigma(v,v')$ is called the cross-section, and it describes the probability that a particle "jumps" from velocity $v$ to velocity $v'$ (or the converse) after a collision process.

# 4. Application Domains

## 4.1. Laser physics

Laser physics considers the propagation over long space (or time) scales of high frequency waves. Typically, one has to deal with the propagation of a wave having a wavelength of the order of $10^{-6}m$, over distances of the order $10^{-2}m$ to $10^{4}m$. In these situations, the propagation produces both a short-scale oscillation and exhibits a long term trend (drift, dispersion, nonlinear interaction with the medium, or so), which contains the physically important feature. For this reason, one needs to develop ways of filtering the irrelevant high-oscillations, and to build up models and/or numerical schemes that do give information on the long-term behavior. In other terms, one needs to develop high-frequency models and/or high-frequency schemes.

Generally speaking, the demand in developing such models or schemes in the context of laser physics, or laser/matter interaction, is large. It involves both modeling and numerics (description of oscillations, structure preserving algorithms to capture the long-time behaviour, etc).

In a very similar spirit, but at a different level of modelling, one would like to understand the very coupling between a laser propagating in, say, a fiber, and the atoms that build up the fiber itself.

The standard, quantum, model in this direction is called the Bloch model: it is a Schrödinger like equation that describes the evolution of the atoms, when coupled to the laser field. Here the laser field induces a potential that acts directly on the atom, and the link between this potential and the laser itself is given by the so-called dipolar matrix, a matrix made up of physical coefficients that describe the polarization of the atom under the applied field.

The scientific objective here is twofold. First, one wishes to obtain tractable asymptotic models that average out the high oscillations of the atomic system and of the laser field. A typical phenomenon here is the *resonance* between the field and the energy levels of the atomic system. Second, one wishes to obtain good numerical schemes in order to solve the Bloch equation, beyond the oscillatory phenomena entailed by this model.

## 4.2. Molecular Dynamics

In classical molecular dynamics, the equations describe the evolution of atoms or molecules under the action of forces deriving from several interaction potentials. These potentials may be short-range or long-range and are treated differently in most molecular simulation codes. In fact, long-range potentials are computed at only a fraction of the number of steps. By doing so, one replaces the vector field by an approximate one and alternates steps with the exact field and steps with the approximate one. Although such methods have been known and used with success for years, very little is known on how the "space" approximation (of the vector field) and the time discretization should be combined in order to optimize the convergence. Also, the fraction of steps where the exact field is used for the computation is mainly determined by heuristic reasons and a more precise analysis seems necessary. Finally, let us mention that similar questions arise when dealing with constrained differential equations, which are a by-product of many simplified models in molecular dynamics (this is the case for instance if one replaces the highly-oscillatory components by constraints).

## 4.3. Plasma physics

The development of efficient numerical methods is essential for the simulation of plasmas and beams at the kinetic level of description (Vlasov type equations). It is well known that plasmas or beams give rise to small scales (Debye length, Larmor radius, gyroperiod, mean free path...) which make numerical simulations challenging. Instead of solving the limit or averaged models by considering these small scales equal to zero, our aim is to explore a different strategy, which consists in using the original kinetic equation. Specific numerical scheme called 'Asymptotic Preserving" scheme is then built to discretize the original kinetic equation. Such a scheme allows to pass to the limit with no stability problems, and provide in the limit a consistent approximation of the limit or average model. A systematic and robust way to design such a scheme is the micro-macro decomposition in which the solution of the original model is decomposed into an averaged part and a remainder.

# 5. New Results

## 5.1. Highlights of the Year

- E. Faou was plenary speaker at the CANUM, Congrès d'analyse numérique, France, June 2014
- E. Faou was invited to give two presentations in the Analysis and applied mathematics seminars, Cambridge, UK, February 2014.

## 5.2. Multi-revolution composition methods for highly oscillatory differential equations

In [22], we introduce a new class of multi-revolution composition methods (MRCM) for the approximation of the $N$th-iterate of a given near-identity map. When applied to the numerical integration of highly oscillatory systems of differential equations, the technique benefits from the properties of standard composition methods: it is intrinsically geometric and well-suited for Hamiltonian or divergence-free equations for instance. We prove error estimates with error constants that are independent of the oscillatory frequency. Numerical experiments, in particular for the nonlinear Schrödinger equation, illustrate the theoretical results, as well as the efficiency and versatility of the methods.

## 5.3. Multiscale schemes for the BGK-Vlasov-Poisson system in the quasi-neutral and fluid limits. Stability analysis and first order schemes

In [51], in collaboration with G. Dimarco (University of Ferrara, Italy) and M.-H. Vignal (University of Toulouse), we deal with the development and the analysis of asymptotic stable and consistent schemes in the joint quasi-neutral and fluid limits for the collisional Vlasov-Poisson system. In these limits, the classical explicit schemes suffer from time step restrictions due to the small plasma period and Knudsen number. To solve this problem, we propose a new scheme stable for choices of time steps independent from the small scales dynamics and with comparable computational cost with respect to standard explicit schemes. In addition, this scheme reduces automatically to consistent discretizations of the underlying asymptotic systems. In this first work on this subject, we propose a first order in time scheme and we perform a relative linear stability analysis to deal with such problems. The framework we propose permits to extend this approach to high order schemes in the next future. We finally show the capability of the method in dealing with small scales through numerical experiments.

## 5.4. Asymptotic preserving scheme for a kinetic model describing incompressible fluids

In [52], in collaboration with M. Lemou (CNRS, Université de Rennes 1) and R. Rao, A. Ruhi, M. Sekhar (Indian Institute of Science, India), the kinetic theory of fluid turbulence modeling developed by Degond and Lemou is considered for further study, analysis and simulation. Starting with the Boltzmann like equation representation for turbulence modeling, a relaxation type collision term is introduced for isotropic turbulence. In order to describe some important turbulence phenomenology, the relaxation time incorporates a dependency on the turbulent microscopic energy and this makes difficult the construction of efficient numerical methods. To investigate this problem, we focus here on a multi-dimensional prototype model and first propose an appropriate change of frame that makes the numerical study simpler. Then, a numerical strategy to tackle the stiff relaxation source term is introduced in the spirit of Asymptotic Preserving Schemes. Numerical tests are performed in a one-dimensional framework on the basis of the developed strategy to confirm its efficiency.

## 5.5. Comparison of numerical solvers for anisotropic diffusion equations arising in plasma physics

In [39], in collaboration G. Latu (IRFM, Cadarache), we performed a comparison of numerical schemes to approximate anisotropic diffusion problems arising in tokamak plasma physics. We focus on the spatial approximation by using finite volume method and on the time discretization. This latter point is delicate since the use of explicit integrators leads to a severe restriction on the time step. Then, implicit and semi-implicit schemes are coupled to finite volumes space discretization and are compared for some classical problems relevant for magnetically confined plasmas. It appears that the semi-implicit approaches (using ARK methods or directional splitting) turn out to be the most efficient on the numerical results, especially when nonlinear problems are studied on refined meshes, using high order methods in space.

## 5.6. Asymptotic-Preserving scheme based on a Finite Volume/Particle-In-Cell coupling for Boltzmann- BGK-like equations in the diffusion scaling

In [38], in collaboration with A. Crestetto (University of Nantes), we are concerned with the numerical simulation of the collisional Vlasov equation in the diffusion limit using particles. To that purpose, we use a micro-macro decomposition technique introduced by Bennoune, Lemou and Mieussens. Whereas a uniform grid was used to approximate both the micro and the macro part of the full distribution function in their article, we use here a particle approximation for the kinetic (micro) part, the fluid (macro) part being always discretized by standard finite volume schemes. There are many advantages in doing so: (i) the so-obtained scheme presents a much less level of noise compared to the standard particle method; (ii) the computational cost of the micro-macro model is reduced in the diffusion limit since a small number of particles is needed for the micro part; (iii) the scheme is asymptotic preserving in the sense that it is consistent with the kinetic equation in the rarefied regime and it degenerates into a uniformly (with respect to the Knudsen number) consistent (and deterministic) approximation of the limiting equation in the diffusion regime.

## 5.7. Hamiltonian splitting for the Vlasov-Maxwell equations

In [23], in collaboration with L. Einkemmer (University of Innsbruck), a new splitting is proposed for solving the Vlasov-Maxwell system. This splitting is based on a decomposition of the Hamiltonian of the Vlasov-Maxwell system and allows for the construction of arbitrary high order methods by composition (independent of the specific deterministic method used for the discretization of the phase space). Moreover, we show that for a spectral method in space this scheme satisfies Poisson's equation without explicitly solving it. Finally, we present some examples in the context of the time evolution of an electromagnetic plasma instability which emphasizes the excellent behavior of the new splitting compared to methods from the literature.

## 5.8. A hybrid transport-diffusion model for radiative transfer in absorbing and scattering media

In [35], in collaboration with M. Roger (University of Lyon), C. Caliot (CNRS) and P. Coelho (Instituto Superior Tecnico of Lisboa), a new multi-scale hybrid transport-diffusion model for radiative transfer calculations is proposed. In this model, the radiative intensity is decomposed into a macroscopic component calculated by the diffusion equation, and a mesoscopic component. The transport equation for the mesoscopic component allows to correct the estimation of the diffusion equation, and then to obtain the solution of the linear radiative transfer equation. In this work, results are presented for stationary and transient radiative transfer cases, in examples which concern solar concentrated and optical tomography applications. The Monte Carlo and the discrete-ordinate methods are used to solve the mesoscopic equation. It is shown that the multi-scale model allows to improve the efficiency of the calculations when the medium is close to the diffusive regime. Moreover, the development of methods for coupling the radiative transfer equation with the diffusion equation becomes easier with this model than with the usual domain decomposition methods.

## 5.9. Charge conserving grid based methods for the Vlasov-Maxwell equations

In [26], in collaboration with P. Navaro (CNRS, Strasbourg) and E. Sonnendrücker (IPP Garching, Germany), In this article we introduce numerical schemes for the Vlasov-Maxwell equations relying on different kinds of grid based Vlasov solvers, as opposite to PIC schemes, that enforce a discrete continuity equation. The idea underlying this schemes relies on a time splitting scheme between configuration space and velocity space for the Vlasov equation and on the computation of the discrete current in a form that is compatible with the discrete Maxwell solver.

## 5.10. Improving conservation properties of a 5D gyrokinetic semi-Lagrangian code

In [32], in collaboration with G. Latu, V. Grandgirard, J. Abiteboul, G. Dif-Pradalier, X. Garbet, P. Ghendrih Y. Sarazin (IRFM, Cadarache), M. Mehrenberger (University of Strasbourg) and E. Sonnendrücker (IPP Garching, Germany), we are concerned with gyrokinetic turbulent simulations, where the knowledge of some stationary states can help reducing numerical artifacts. Considering long-term simulations, the qualities of the Vlasov solver and of the radial boundary conditions have an impact on the conservation properties. In order to improve mass and energy conservation mainly, the following methods are investigated: fix the radial boundary conditions on a stationary state, use a 4D advection operator that avoids a directional splitting, interpolate with a delta-f approach. The combination of these techniques in the semi-Lagrangian code gysela leads to a net improvement of the conservation properties in 5D simulations.

## 5.11. Simulations of Kinetic Electrostatic Electron Nonlinear (KEEN) Waves with Variable Velocity Resolution Grids and High-Order Time-Splitting

In [16], in collaboration with B. Afeyan (Polymath Research, USA), F. Casa (University Jaume, Spain), A. Dodhy, E. Sonnendrücker (IPP Garching, Germany) and M. Mehrenberger (University of Strasbourg), we are concerned with KEEN waves which are non-stationary, nonlinear, self-organized asymptotic states in Vlasov plasmas. They lie outside the precepts of linear theory or perturbative analysis, unlike electron plasma waves or ion acoustic waves. Steady state, nonlinear constructs such as BGK modes also do not apply. The range in velocity that is strongly perturbed by KEEN waves depends on the amplitude and duration of the ponderomotive force generated by two crossing laser beams, for instance, used to drive them. Smaller amplitude drives manage to devolve into multiple highly-localized vorticlets, after the drive is turned off, and may eventually succeed to coalesce into KEEN waves. Fragmentation once the drive stops, and potential eventual remerger, is a hallmark of the weakly driven cases. A fully formed (more strongly driven) KEEN wave has one dominant vortical core. But it also involves fine scale complex dynamics due to shedding and merging of smaller vortical structures with the main one. Shedding and merging of vorticlets are involved in either case, but at different rates and with different relative importance. The narrow velocity range in which one must maintain sufficient resolution in the weakly driven cases, challenges

fixed velocity grid numerical schemes. What is needed is the capability of resolving locally in velocity while maintaining a coarse grid outside the highly perturbed region of phase space. We here report on a new Semi-Lagrangian Vlasov-Poisson solver based on conservative non-uniform cubic splines in velocity that tackles this problem head on. An additional feature of our approach is the use of a new high-order time-splitting scheme which allows much longer simulations per computational effort. This is needed for low amplitude runs. There, global coherent structures take a long time to set up, such as KEEN waves, if they do so at all. The new code's performance is compared to uniform grid simulations and the advantages are quantified. The birth pains associated with weakly driven KEEN waves are captured in these simulations. Canonical KEEN waves with ample drive are also treated using these advanced techniques. They will allow the efficient simulation of KEEN waves in multiple dimensions, which will be tackled next, as well as generalizations to Vlasov-Maxwell codes. These are essential for pursuing the impact of KEEN waves in high energy density plasmas and in inertial confinement fusion applications. More generally, one needs a fully-adaptive grid-in-phase-space method which could handle all small vorticlet dynamics whether pealing off or remerging. Such fully adaptive grids would have to be computed sparsely in order to be viable. This two-velocity grid method is a concrete and fruitful step in that direction.

## 5.12. Gyroaverage operator on polar mesh

In [36], in collaboration with C. Steiner, M. Mehrenberger (University of Strasbourg) V. Grandgirard, G. Latu (IRFM, Cadarache). In this work, we are concerned with numerical approximation of the gyroaverage operators arising in plasma physics to take into account the effects of the finite Larmor radius corrections. The work initiated in [Crouseilles, Mehrenberger, Sellama, CiCP 2010] is extended here to polar geometries. A direct method is proposed in the space configuration which consists in integrating on the gyrocircles using interpolation operator (Hermite or cubic splines). Numerical comparisons with a standard method based on a Pade approximation are performed: (i) with analytical solutions, (ii) considering the 4D drift-kinetic model with one Larmor radius and (iii) on the classical linear DIII-D benchmark case [6]. In particular, we show that in the context of a drift-kinetic simulation, the proposed method has similar computational cost as the standard method and its precision is independent of the radius.

## 5.13. A new fully two-dimensional conservative semi-Lagrangian method: applications on polar grids, from diocotron instability to ITG turbulence

In [25], in collaboration with P. Glanc, S. Hirstoaga, E. Madaule, M. Mehrenberger, J. Pétri (University of Strasbourg), While developing a new semi-Lagrangian solver, the gap between a linear Landau run in 1dx1d and a 5D gyrokinetic simulation in toroidal geometry is quite huge. Intermediate test cases are welcome for checking the code. We consider here as building block, a 2D guiding-center type equation on an annulus. We first revisit a 2D test case previously done with a PIC approach and detail the boundary conditions. We then consider a 4D drift-kinetic slab simulation for which we give some first results of a new conservative method.

## 5.14. Uniformly accurate numerical schemes for highly oscillatory Klein-Gordon and nonlinear Schrödinger equations

In [21], we are interested in the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called "Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. The method is based on two main ingredients. First, we embed our problem in a suitable "two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog

expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

## 5.15. Asymptotic preserving schemes for the Wigner-Poisson-BGK equations in the diffusion limit

In [24], we focus on the numerical simulation of the Wigner-Poisson-BGK equation in the diffusion asymptotics. Our strategy is based on a "micro-macro" decomposition, which leads to a system of equations that couple the macroscopic evolution (diffusion) to a microscopic kinetic contribution for the fluctuations. A semi-implicit discretization provides a numerical scheme which is stable with respect to the small parameter $\varepsilon$ (mean free path) and which possesses the following properties: (i) it enjoys the asymptotic preserving property in the diffusive limit; (ii) it recovers a standard discretization of the Wigner-Poisson equation in the collisionless regime. Numerical experiments confirm the good behaviour of the numerical scheme in both regimes. The case of a spatially dependent $\varepsilon(x)$ is also investigated.

## 5.16. Models of dark matter halos based on statistical mechanics: II. The fermionic King model

In [49] we study the fermionic King model which may provide a relevant model of dark matter halos. The exclusion constraint can be due to quantum mechanics (for fermions such as massive neutrinos) or to Lynden- Bells statistics (for collisionless systems undergoing violent relaxation). This model has a finite mass. Dwarf and intermediate size halos are degenerate quantum objects stabilized against gravitational collapse by the Pauli exclusion principle. Large halos at sufficiently high energies are in a gaseous phase where quantum effects are negligible. They are stabilized by thermal motion. Below a critical energy Ec they undergo gravitational collapse (gravothermal catastrophe). This may lead to the formation of a central black hole that does not affect the structure of the halo. This may also lead to the formation of a compact degenerate object surrounded by a hot massive atmosphere extending at large distances. We argue that large dark matter halos should not contain a degenerate nucleus (fermion ball) because these nucleus-halo structures are thermodynamically unstable. We compare the rotation curves of the classical King model to observations of large dark matter halos (Burkert profile). Because of collisions and evaporation, the central density increases while the slope of the halo density profile decreases until an in- stability takes place. We find that the observations are compatible with a King profile at, or close to, the point of marginal stability in the micro- canonical ensemble. At that point, the King profile can be fitted by the modified Hubble profile. This is qualitatively similar to the Burkert profile and discrepancies between the King model and the observations are interpreted as a result of incomplete relaxation.

## 5.17. Models of dark matter halos based on statistical mechanics: I. The classical King model

In [48] we consider the possibility that dark matter halos are described by the Fermi-Dirac distribution at finite temperature. This is the case if dark matter is a self-gravitating quantum gas made of massive neutrinos at statistical equilibrium. This is also the case if dark matter can be treated as a self-gravitating collisionless gas experiencing Lynden-Bell?s type of violent relaxation. In order to avoid the infinite mass problem and carry out a rigorous stability analysis, we consider the fermionic King model. In this paper, we study the non-degenerate limit leading to the classical King model. This model was initially introduced to describe globular clusters and we propose to apply it also to large dark matter halos where quantum effects are negligible. We study the thermodynamical stability of the different configurations and compare the prediction of the classical King model to the observations of large dark matter halos. Because of collisions and evaporation, the central density increases while the slope of the halo density profile decreases until an instability takes place. We show that large dark matter halos are relatively well-described by the King model at, or close to, the point of marginal microcanonical stability. At that point, the King model generates a density profile that can be approximated

by the modified Hubble profile. This profile has a flat core and decreases as r?3 at large distances, like the observational Burkert profile. For large halos, the flat core is due to finite temperature effects, not to quantum mechanics. We argue that statistical mechanics may provide a good description of dark matter halos and interpret the discrepancies as a result of incomplete relaxation like in the case of stellar systems.

## 5.18. Analysis of models for quantum transport of electrons in graphene layers

In [28], two mathematical models for the self consistent quantum transport of electrons in a graphene layer are presented are analyzed. We treat two situations. First, when the particles can move in all the plane $R^2$, the model takes the form of a system of massless Dirac equations coupled together by a selfconsistent potential, which is the trace in the plane of the graphene of the 3D Poisson potential associated to surface densities. Second, we consider a situation where the particles are constrained in a regular bounded domain $\Omega$. In order to take into account Dirichlet boundary conditions which are not compatible with the Dirac Hamiltonian $H_0$, we propose a different model built on a modified Hamiltonian displaying the same energy band diagram as $H_0$ near the Dirac points.

## 5.19. Dimension reduction for anisotropic Bose-Einstein condensates in the strong interaction regime

The work [44] deals with the problem of dimension reduction for the three dimensional Gross-Pitaevskii equation (GPE) describing a Bose-Einstein condensate confined in a strongly anisotropic harmonic trap. Since the gas is assumed to be in a strong interaction regime, we have to analyze two combined singular limits: a semi-classical limit in the transport direction and the strong partial confinement limit in the transversal direction.

## 5.20. Superconvergence of Strang splitting for NLS in $T^d$

In [47], we investigate the convergence properties of semi-discretized approximations by Strang splitting method applied to fast-oscillating nonlinear Schrödinger equations. Our main contribution is to show that Strang splitting with constant step-sizes is unexpectedly more accurate by a factor $\varepsilon$ as compared to established results when the step-size is chosen as an integer fraction of the period, owing to an averaging effect.

## 5.21. Strong confinement limit for the nonlinear Schrödinger equation constrained on a curve

The preprint [58] is devoted to the cubic nonlinear Schrödinger equation in a two dimensional waveguide with shrinking cross section of order $\varepsilon$. For a Cauchy data living essentially on the first mode of the transverse Laplacian, we provide a tensorial approximation of the solution $\psi^\varepsilon$ in the limit $\varepsilon \to 0$, with an estimate of the approximation error, and derive a limiting nonlinear Schrödinger equation in dimension one with an additional effective potential depending on the curvature.

## 5.22. The fermionic King model

In [50], we study the fermionic King model which may provide a relevant model of dark matter halos.

## 5.23. Landau damping in Sobolev spaces for the Vlasov-HMF model

In [56], we consider the Vlasov-HMF (Hamiltonian Mean-Field) model. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that these solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping.

## 5.24. Collisions of vortex filament pairs

In [18], we consider the problem of collisions of vortex filaments for a model introduced by Klein, Majda and Damodaran, and Zakharov to describe the interaction of almost parallel vortex filaments in three-dimensional fluids. Since the results of Crow examples of collisions are searched as perturbations of antiparallel translating pairs of filaments, with initial perturbations related to the unstable mode of the linearized problem; most results are numerical calculations. In this article we first consider a related model for the evolution of pairs of filaments and we display another type of initial perturbation leading to collision in finite time. Moreover we give numerical evidence that it also leads to collision through the initial model. We finally study the self-similar solutions of the model.

## 5.25. Asymptotic preserving schemes for the Klein-Gordon equation in the non-relativistic limit regime

In [30], we consider the Klein-Gordon equation in the non-relativistic limit regime, i.e. the speed of light c tending to infinity. We construct an asymptotic expansion for the solution with respect to the small parameter depending on the inverse of the square of the speed of light. As the first terms of this asymptotic can easily be simulated our approach allows us to construct numerical algorithms that are robust with respect to the large parameter c producing high oscillations in the exact solution.

## 5.26. Analysis of a large number of Markov chains competing for transitions

In [17], we consider the behavior of a stochastic system composed of several identically distributed, but non independent, discrete-time absorbing Markov chains competing at each instant for a transition. The competition consists in determining at each instant, using a given probability distribution, the only Markov chain allowed to make a transition. We analyze the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyze the asymptotic behavior of the system for an arbitrary probability mass function governing the competition. We give conditions for the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed systems when the competition between the Markov chains is handled by using a geometric distribution.

## 5.27. Coexistence phenomena and global bifurcation structure in a chemostat-like model with species-dependent diffusion rates

In [20], we study the competition of two species for a single resource in a chemostat. In the simplest space-homogeneous situation, it is known that only one species survives, namely the best competitor. In order to exhibit coexistence phenomena, where the two competitors are able to survive, we consider a space dependent situation: we assume that the two species and the resource follow a diffusion process in space, on top of the competition process. Besides, and in order to consider the most general case, we assume each population is associated with a distinct diffusion constant. This is a key difficulty in our analysis: the specific (and classical) case where all diffusion constants are equal, leads to a particular conservation law, which in turn allows to eliminate the resource in the equations, a fact that considerably simplifies the analysis and the qualitative phenomena. Using the global bifurcation theory, we prove that the underlying 2-species, stationary, diffusive, chemostat-like model, does possess coexistence solutions, where both species survive. On top of that, we identify the domain, in the space of the relevant bifurcation parameters, for which the system does have coexistence solutions.

## 5.28. Global behavior of N competing species with strong diffusion: diffusion leads to exclusion

In [46], we study the following problem. For a large class of models involving several species competing for a single resource in a *homogeneous* environment, it is known that the competitive exclusion principle holds: only

one species survives eventually. Various works indicate though that coexistence of many species is possible when the competition occurs in a *heterogeneous* environment. We propose here a spatially heterogeneous system modeling several species competing for a single resource, and migrating in the spatial domain. For this model, it is known, at least in particular cases, that if migrations are *slow* enough, then coexistence occurs. In this paper we show at variance that if the spatial migrations are *fast* enough, then our system can be approximated by a spatially homogeneous system, called aggregated model, which can be explicitly computed, and we show that if the competitive exclusion principle holds for the aggregated model, then it holds as well for the original, spatially heterogeneous model. In other words, we show the persistence of the competitive exclusion principle in the spatially heterogeneous situation when migrations are fast. As a consequence, for fast migrations only one species may survive, namely the best competitor *in average*. We last study which is the best competitor *in average* on some examples, and draw some ecological consequences.

## 5.29. Randomized Message-Passing Test-and-Set

In [42] we present a solution to the well-known Test&Set operation in an asynchronous system prone to process crashes. Test&Set is a synchronization operation that, when invoked by a set of processes, returns yes to a unique process and returns no to all the others. Recently many advances in implementing Test&Set objects have been achieved, however all of them target the shared memory model. In this paper we propose an implementation of a Test&Set object in the message passing model. This implementation can be invoked by any number $p \leq n$ of processes where $n$ is the total number of processes in the system. It has an expected individual step complexity in O(log p) against an oblivious adversary, and an expected individual message complexity in O(n). The proposed Test&Set object is built atop a new basic building block, called selector, that allows to select a winning group among two groups of processes. We propose a message-passing implementation of the selector whose step complexity is constant. We are not aware of any other implementation of the Test&Set operation in the message passing model.

## 5.30. Existence of densities for the 3D Navier–Stokes equations driven by Gaussian noise

In [27], we prove three results on the existence of densities for the laws of finite dimensional functionals of the solutions of the stochastic Navier-Stokes equations in dimension 3. In particular, under very mild assumptions on the noise, we prove that finite dimensional projections of the solutions have densities with respect to the Lebesgue measure which have some smoothness when measured in a Besov space. This is proved thanks to a new argument inspired by an idea introduced by N. Fournier and J. Printems.

## 5.31. Diffusion limit for the radiative transfer equation perturbed by a Markovian process

In [54], we study the stochastic diffusive limit of a kinetic radiative transfer equation, which is non linear, involving a small parameter and perturbed by a smooth random term. Under an appropriate scaling for the small parameter, using a generalization of the perturbed test-functions method, we show the convergence in law to a stochastic non linear fluid limit.

## 5.32. Diffusion limit for the radiative transfer equation perturbed by a Wiener process

In [55], we consider the rigorous derivation of a stochastic non-linear diffusion equation from a radiative transfer equation perturbed with a random noise of white noise type. The proof of the convergence relies on a formal Hilbert expansion and the estimation of the remainder. The Hilbert expansion has to be done up to order 3 to overcome some difficulties caused by the random noise.

# 6. Partnerships and Cooperations

## 6.1. National Initiatives

### *6.1.1. ANR Programme blanc international (BLAN) LODIQUAS 2012-2015*

**Participants:** Philippe Chartier, Florian Méhats, Francois Castella, Mohammed Lemou.

The project, entitled "LODIQUAS" (for: Low DImensional QUANtum Systems), received fundings for 4 postdocs (48 months) and one pre-doc (36 months). The whole project involves the following researchers : Norbert Mauser (Vienna), Erich Gornik (Vienna), Mechthild Thalhammer (Innsbruck), Christoph Naegerl (Innsbruck), Jörg Schmiedmayer (Vienna), Hans-Peter Stimming (Vienna),Francis Nier (Rennes), Raymond El Hajj (Rennes), Claudia Negulescu (Toulouse), Fanny Delebecque (Toulouse), Stéphane Descombes (Nice), Christophe Besse (Lille).
Quantum technology as the application of quantum effects in macroscopic devices has an increasing importance, not only for far future goals like the quantum computer, but already now or in the near future. The present project is mainly concerned with the mathematical and numerical analysis of these objects, in conjunction with experimental physicists.

### *6.1.2. ANR MOONRISE: 2015-2019*

**Participants:** Nicolas Crouseilles, Philippe Chartier, Florian Méhats, Francois Castella, Mohammed Lemou.

The project *Moonrise* submitted by F. Méhats has been funded by the ANR for 4 years, for the period 2015-2019. This project aims at exploring modeling, mathematical and numerical issues originating from the presence of high-oscillations in nonlinear PDEs from the physics of nanotechnologies (quantum transport) and from the physics of plasmas (magnetized transport in tokamaks). The partners of the project are the IRMAR (Rennes), the IMT (Toulouse) and the CEA Cadarache. In the IPSO team, F. Castella, P. Chartier, N. Crouseilles and M. Lemou are members of the project Moonrise.

### *6.1.3. ANR Programme blanc GYPSI: 2010-2014*

**Participant:** Nicolas Crouseilles.

Leader: Ph. Gendrih.

The full description is available at https://sites.google.com/site/anrgypsi/

### *6.1.4. ANR Programme blanc E2T2: 2010-2014*

**Participant:** Nicolas Crouseilles.

Leader: P. Beyer

## 6.2. European Initiatives

### *6.2.1. FP7 & H2020 Projects*

#### *6.2.1.1. Geopardi*

Type: FP7

Defi: NC

Instrument: ERC Starting Grant

Objectif: NC

Duration: September 2011 - August 2016

Coordinator: E. Faou

Inria contact: E. Faou

### 6.2.2. Collaborations in European Programs, except FP7 & H2020

*6.2.2.1. Verification of global gyrokinetic codes and development of new algorithms for gyrokinetic and kinetic codes*

Project acronym: EUROFusion CfP-WP14-ER-01/IPP-03: 2014

Project title: verification of global gyrokinetic codes and development of new algorithms for gyrokinetic and kinetic codes

Duration: 2013-2014

Participants: N. Crouseilles and M. Lemou

Coordinator:E. Sonnendrücker

*6.2.2.2. Enabling Research Project for the implementation of the fusion roadmap*

Project acronym: EUROFusion

Project title: Enabling Research Project for the implementation of the fusion roadmap

Duration: 2015-2017

Participants: N. Crouseilles and M. Lemou

Coordinator:E. Sonnendrücker

## 6.3. International Research Visitors

### 6.3.1. Visits of International Scientists

- L. Einkemmer, University of Innsbruck, two weeks, november 2014.
- Y. Zhang, WPI, Vienna, 3 months.

### 6.3.2. Visits to International Teams

*6.3.2.1. Research stays abroad*

- N. Crouseilles visited the group of P. Coelho (Universitad tecnico de Lisboa, Portugal), one week (november 2014).
- M. Lemou and N. Crouseilles visited the India Institute of Science at Bangalore (India): from december 2d to december 17th, 2013. Visited team: around Raghurama Rao.
- M. Lemou visited the Wisconsin university, Madison (USA): from February 1st to February 16th, 2014. Visited team: around Shi Jin.
- P. Chartier, M. Lemou and F. Méhats visited the university of San Sebastien, Pays Basque (Spain): from June 8th to June 13th 2014.

# 7. Dissemination

## 7.1. Promoting Scientific Activities

### 7.1.1. Scientific events organisation

*7.1.1.1. Member of the organizing committee*

- F. Castella organised, jointly with P. Chartier, a meeting held in Saint-Malo (25 participants) in the framework of the european ANR project Lodiquas.

### 7.1.2. Scientific events selection

*7.1.2.1. Member of the conference program committee*

- A. Debussche was member of the scientific committee of the conference *Stochastic Partial Differential Equations and Applications - IX*, Trento, Italy, january 7-11, 2014.

### *7.1.3. Journal*

*7.1.3.1. Member of the editorial board*

- N. Crouseilles is member of the editorial board of Hindawi review "International Journal of Analysis"
  http://www.hindawi.com/journals/analysis/
- M. Lemou is associate editor in the journal "Annales de la faculté des sciences de Toulouse"
- A. Debussche is editor in Chief of "Stochastic Partial Differential Equations: analysis and computations".
- A. Debussche is member of the editorial board of "Potential Analysis".
- A. Debussche is member of the editorial board of the "Journal of Evolution Equations".
- A. Debussche is member of the editorial board of "Differential and Integral Equations".
- A. Debussche is member of the editorial board of "ESAIM: Proceedings".
- A. Debussche is member of the editorial board of the collection: "Mathématiques et Applications", SMAI, Springer.
- P. Chartier is member of the editorial board of M2AN (Mathematical Modelling and Numerical Analysis).
- P. Chartier is member of the editorial board of ISRN Mathematical Analysis.

## 7.2. Teaching - Supervision - Juries

### *7.2.1. Teaching*

Master 2 lectures: N. Crouseilles, Numerical methods for kinetic equations.

Master 1 lectures: M. Lemou, Theory of distributions, University of Rennes 1 and ENS Cachan (Ker Lann), 24 hours.

Master 2: M. Lemou was the manager of Master 2 courses in "Analysis and Applications", university of Rennes 1.

E. Faou gave a series of lectures on *Stochastic methods for PDEs*, Heriot-Watt University, Edinburgh, UK, october 2014.

E. Faou gave a series of lectures on *Geometric Numerical Integration for PDE*, KIT, Karlsruhe, Germany, August 2014.

E. Faou gave a series of lectures on *Stochastic computation* and on *Geometric Numerical Integration for PDE*, Chinese Academy of Sciences, Beijing, May 2014

A. Debussche gave a mini-course on *Introduction aux EDPS* in the school *EDP avec conditions aleatoires*, Toulouse, April 22-25, 2014.

Licence 3: P. Chartier gave a lecture on ODEs at ENS Rennes, september-december, 24 hours.

### *7.2.2. Supervision*

N. Crouseilles and M. Lemou co-advise H. Hivert's PhD (first year in Rennes university), ENS grant.

N. Crouseilles and M. Lemou co-advise (with R. Raghurama and M. Lemou) A. Ruhi's PhD (third year in IISc), Indian grant.

M. Lemou and F. Méhats co-advised P. Carcaud's PhD: University of Rennes 1. Thesis defense on june 2nd 2014.

P. Chartier and F. Méhats co-supervise the PhD thesis of G. Leboucher.

P. Chartier and F. Castella co-supervise the PhD thesis of J. Sauzeau.

A. Debussche and F. Méhats co-supervise the PhD thesis of M. Tusseau.

E. Faou co-supervises the PhD thesis of R. Horsin.

A. Debussche and E. Faou co-supervised the thesis of M. Kopec, ENS Rennes.

### *7.2.3. Juries*

N. Crouseilles: member of the PHD jury of P. Glanc, 20 january 2014 (Strasbourg); co-advising (with M. Mehrenberger) of Pierre Glanc PhD (Strasbourg University), Inria-Cordi grant.

N. Crouseilles: member of the PHD jury of Ch. Steiner, 11 december 2014 (Strasbourg); co-advising (with M. Mehrenberger) of Christophe Steiner PhD (Strasbourg University), ministry grant.

N. Crouseilles: member of the PHD jury of M. Kuhn, 29 september 2014 (Strasbourg); co-advising (with S. Genaud) of Matthieu Kuhn PhD (Strasbourg University and Inria IPSO), ANR "E2T2" grant.

N. Crouseilles: member of the Master 2 jury of P. Pereira, 26 november 2014 (Lisboa, Portugal).

F. Méhats was referee of the thesis of L. Hari (Cergy, supervised by T. Duyckaerts and C. Fermanian).

F. Méhats was referee of the thesis of X. Zhao (Singapore, supervised by W. Bao).

P. Chartier was referee of the PhD thesis of Philipp Bader, University of Valencia, june.

# 8. Bibliography

## Major publications by the team in recent years

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[4] P. CHARTIER, E. FAOU, A. MURUA. *An algebraic approach to invariant preserving integators: the case of quadratic and Hamiltonian invariants*, in "Numer. Math.", 2006, vol. 103, n$^{o}$ 4, pp. 575-590, http://dx.doi.org/10.1007/s00211-006-0003-8

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