IN PARTNERSHIP WITH:
CNRS

Université Rennes 1

École normale supérieure de Rennes

Activity Report 2017

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

Creation of the Project-Team: 2004 December 06, end of the Project-Team: 2017 December 31

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Other Research Topics and Application Domains:

B1. - Life sciences
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B1.1.10. - Mathematical biology
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1. Personnel

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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 [42], [39], [38] 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, geodynamics, 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: Francois Castella, Philippe Chartier, Erwan Faou.

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, φ_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 Φ_h of φ_h. One of the main questions of *geometric integration* is whether *intrinsic* properties of φ_t may be passed on to Φ_h.

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

3.1.1. Reversible ODEs

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

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

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_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 φ_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 [37] 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 ω, 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

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

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: Francois Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Mehats, Mohammed Lemou.

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

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

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 ω 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 ε 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 ε. 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: Francois Castella, Philippe Chartier, Erwan Faou, Florian Mehats.

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, ε 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 Δ_{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 ψ.

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 [41], [40] 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 δt 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: Francois 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, ε 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 ε) 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: Francois 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. New Results

4.1. Multiscale numerical methods

4.1.1. Asymptotic preserving and time diminishing schemes for rarefied gas dynamic

In [10], we introduce a new class of numerical schemes for rarefied gas dynamic problems described by collisional kinetic equations. The idea consists in reformulating the problem using a micro-macro decomposition and successively in solving the microscopic part by using asymptotic preserving Monte Carlo methods. We consider two types of decompositions, the first leading to the Euler system of gas dynamics while the second to the Navier-Stokes equations for the macroscopic part. In addition, the particle method which solves the microscopic part is designed in such a way that the global scheme becomes computationally less expensive as the solution approaches the equilibrium state as opposite to standard methods for kinetic equations which computational cost increases with the number of interactions. At the same time, the statistical error due to the particle part of the solution decreases as the system approach the equilibrium state. This causes the method to degenerate to the sole solution of the macroscopic hydrodynamic equations (Euler or Navier-Stokes) in the limit of infinite number of collisions. In a last part, we will show the behaviors of this new approach in comparisons to standard Monte Carlo techniques for solving the kinetic equation by testing it on different problems which typically arise in rarefied gas dynamic simulations.

4.1.2. An exponential integrator for the drift-kinetic model

In [30], we propose an exponential integrator for the drift-kinetic equations in polar geometry. This approach removes the CFL condition from the linear part of the system (which is often the most stringent requirement in practice) and treats the remainder explicitly using Arakawa's finite difference scheme. The present approach is mass conservative, up to machine precision, and significantly reduces the computational effort per time step. In addition, we demonstrate the efficiency of our method by performing numerical simulations in the context of the ion temperature gradient instability. In particular, we find that our numerical method can take time steps comparable to what has been reported in the literature for the (predominantly used) splitting approach. In addition, the proposed numerical method has significant advantages with respect to conservation of energy and efficient higher order methods can be obtained easily. We demonstrate this by investigating the performance of a fourth order implementation.

4.1.3. Multiscale Particle-in-Cell methods and comparisons for the long-time two-dimensional Vlasov-Poisson equation with strong magnetic field

In [11], we applied different kinds of multiscale methods to numerically study the long-time Vlasov-Poisson equation with a strong magnetic field. The multiscale methods include an asymptotic preserving Runge-Kutta scheme, an exponential time differencing scheme, stroboscopic averaging method and a uniformly accurate two-scale formulation. We briefly review these methods and then adapt them to solve the Vlasov-Poisson equation under a Particle-in-Cell discretization. Extensive numerical experiments are conducted to investigate and compare the accuracy, efficiency, and long-time behavior of all the methods. The methods with the best performance under different parameter regimes are identified.

4.1.4. Nonlinear Geometric Optics based multiscale stochastic Galerkin methods for highly oscillatory transport equations with random inputs

In [31], we develop generalized polynomial chaos (gPC) based stochastic Galerkin (SG) methods for a class of highly oscillatory transport equations that arise in semiclassical modeling of non-adiabatic quantum dynamics. These models contain uncertainties, particularly in coefficients that correspond to the potentials of the molecular system. We first focus on a highly oscillatory scalar model with random uncertainty. Our method is built upon the nonlinear geometrical optics (NGO) based method, developed in [12] for numerical approximations of deterministic equations, which can obtain accurate pointwise solution even without numerically resolving spatially and temporally the oscillations. With the random uncertainty, we show that such a method has oscillatory higher order derivatives in the random space, thus requires a frequency dependent discretization in the random space. We modify this method by introducing a new " time " variable based on the phase, which is shown to be non-oscillatory in the random space, based on which we develop a gPC-SG method that can capture oscillations with the frequency-independent time step, mesh size as well as the degree of polynomial chaos. A similar approach is then extended to a semiclassical surface hopping model system with a similar numerical conclusion. Various numerical examples attest that these methods indeed capture accurately the solution statistics pointwisely even though none of the numerical parameters resolve the high frequencies of the solution.

4.1.5. Nonlinear Geometric Optics method based multi-scale numerical schemes for highly-oscillatory transport equations

In [12], we introduce a new numerical strategy to solve a class of oscillatory transport PDE models which is able to capture accurately the solutions without numerically resolving the high frequency oscillations *in both space and time*. Such PDE models arise in semiclassical modeling of quantum dynamics with band-crossings, and other highly oscillatory waves. Our first main idea is to use the nonlinear geometric optics ansatz, which builds the oscillatory phase into an independent variable. We then choose suitable initial data, based on the Chapman-Enskog expansion, for the new model. For a scalar model, we prove that so constructed model will have certain smoothness, and consequently, for a first order approximation scheme we prove uniform error estimates independent of the (possibly small) wave length. The method is extended to systems arising

from a semiclassical model for surface hopping, a non-adiabatic quantum dynamic phenomenon. Numerous numerical examples demonstrate that the method has the desired properties.

4.1.6. High-order Hamiltonian splitting for Vlasov-Poisson equations

In [5], we consider the Vlasov-Poisson equation in a Hamiltonian framework and derive new time splitting methods based on the decomposition of the Hamiltonian functional between the kinetic and electric energy. Assuming smoothness of the solutions, we study the order conditions of such methods. It appears that these conditions are of Runge-Kutta-Nyström type. In the one dimensional case, the order conditions can be further simplified, and efficient methods of order 6 with a reduced number of stages can be constructed. In the general case, high-order methods can also be constructed using explicit computations of commutators. Numerical results are performed and show the benefit of using high-order splitting schemes in that context. Complete and self-contained proofs of convergence results and rigorous error estimates are also given.

4.1.7. A particle micro-macro decomposition based numerical scheme for collisional kinetic equations in the diffusion scaling

In [29], we derive particle schemes, based on micro-macro decomposition, for linear kinetic equations in the diffusion limit. Due to the particle approximation of the micro part, a splitting between the transport and the collision part has to be performed, and the stiffness of both these two parts prevent from uniform stability. To overcome this difficulty, the micro-macro system is reformulated into a continuous PDE whose coefficients are no longer stiff, and depend on the time step Δt in a consistent way. This non-stiff reformulation of the micro-macro system allows the use of standard particle approximations for the transport part, and extends a previous work where a particle approximation has been applied using a micro-macro decomposition on kinetic equations in the fluid scaling. Beyond the so-called asymptotic-preserving property which is satisfied by our schemes, they significantly reduce the inherent noise of traditional particle methods, and they have a computational cost which decreases as the system approaches the diffusion limit.

4.1.8. Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equation

This work [13] is devoted to the numerical simulation of a Vlasov-Poisson equation modeling charged particles in a beam submitted to a highly oscillatory external electric field. A numerical scheme is constructed for this model. This scheme is uniformly accurate with respect to the size of the fast time oscillations of the solution, which means that no time step refinement is required to simulate the problem. The scheme combines the forward semi-Lagrangian method with a class of Uniformly Accurate (UA) time integrators to solve the characteristics. These UA time integrators are derived by means of a two-scale formulation of the characteristics, with the introduction of an additional periodic variable. Numerical experiments are done to show the efficiency of the proposed methods compared to conventional approaches.

4.1.9. Uniformly accurate multiscale time integrators for second order oscillatory differential equations with large initial data

In [23], we apply the modulated Fourier expansion to a class of second order differential equations which consists of an oscillatory linear part and a nonoscillatory nonlinear part, with the total energy of the system possibly unbounded when the oscillation frequency grows. We comment on the difference between this model problem and the classical energy bounded oscillatory equations. Based on the expansion, we propose the multiscale time integrators to solve the ODEs under two cases: the nonlinearity is a polynomial or the frequencies in the linear part are integer multiples of a single generic frequency. The proposed schemes are explicit and efficient. The schemes have been shown from both theoretical and numerical sides to converge with a uniform second order rate for all frequencies. Comparisons with popular exponential integrators in the literature are done.

4.1.10. Unconditional and optimal H^2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrödinger equation in high dimensions

In [21], we focus on the optimal error bounds of two finite difference schemes for solving the d-dimensional ($d = 2, 3$) nonlinear Klein-Gordon-Schrödinger (KGS) equations. The proposed finite difference schemes not only conserve the mass and energy in the discrete level but also are efficient in practical computation because only two linear systems need to be solved at each time step. Besides the standard energy method, an induction argument as well as a 'lifting' technique are introduced to establish rigorously the optimal H^2-error estimates without any restrictions on the grid ratios, while the previous works either are not rigorous enough or often require certain restriction on the grid ratios. The convergence rates of the proposed schemes are proved to beat $O(h^2 + \tau^2)$ with mesh size h and time step τ in the discrete H^2-norm. The analysis method can be directly extended to other linear finite difference schemes for solving the KGS equations in high dimensions. Numerical results are reported to confirm the theoretical analysis for the proposed finite difference schemes

4.1.11. A combination of multiscale time integrator and two-scale formulation for the nonlinear Schrödinger equation with wave operator

In [22], we consider the nonlinear Schrödinger equation with wave operator (NLSW), which contains a dimensionless parameter $0 < \varepsilon \leq 1$. As $0 < \varepsilon << 1$, the solution of the NLSW propagates fast waves in time with wavelength $O(\varepsilon^2)$ and the problem becomes highly oscillatory in time. The oscillations come from two parts. One part is from the equation and another part is from the initial data. For the ill-prepared initial data case as described in Bao and Cai (2014) which brings inconsistency in the limit regime, standard numerical methods have strong convergence order reduction in time when becomes small. We review two existing methods to solve the NLSW: an exponential integrator and a two-scale method. We comment on their order reduction issues. Then we derive a multiscale decomposition two-scale method for solving the NLSW by first performing a multiscale decomposition on the NLSW which decomposes it into a well-behaved part and an energy-unbounded part, and then applying an exponential integrator for the well-behaved part and a two-scale approach for the energy-unbounded part. Numerical experiments are conducted to test the proposed method which shows uniform second order accuracy without significant order reduction for all $0 < \varepsilon \leq 1$. Comparisons are made with the existing methods.

4.1.12. Uniformly accurate numerical schemes for the nonlinear Dirac equation in the nonrelativistic limit regime

In [18], we apply the two-scale formulation approach to propose uniformly accurate (UA) schemes for solving the nonlinear Dirac equation in the nonrelativistic limit regime. The nonlinear Dirac equation involves two small scales ε and ε^2 with epsilon $\to 0$ in the nonrelativistic limit regime. The small parameter causes high oscillations in time which brings severe numerical burden for classical numerical methods. We transform our original problem as a two-scale formulation and present a general strategy to tackle a class of highly oscillatory problems involving the two small scales ε and ε^2. Suitable initial data for the two-scale formulation is derived to bound the time derivatives of the augmented solution. Numerical schemes with uniform (with respect to $\varepsilon \in (0; 1]$) spectral accuracy in space and uniform first order or second order accuracy in time are proposed. Numerical experiments are done to confirm the UA property.

4.1.13. A formal series approach to the center manifold theorem

In [6], we consider near-equilibrium systems of ordinary differential equations with explicit separation of the slow and stable manifolds. Formal B-series like those previously used to analyze highly-oscillatory systems or to construct modified equations are employed here to construct expansions of the change of variables, the center invariant manifold and the reduced model. The new approach may be seen as a process of reduction to a normal form, with the main advantage, as compared to the standard view conveyed by the celebrated center manifold theorem, that it is possible to recover the complete solution at any time through an explicit change of variables.

4.1.14. Convergence of multi-revolution composition time-splitting methods for highly oscillatory differential equations of Schrödinger type

In [8], the convergence behaviour of multi-revolution composition methods combined with time-splitting methods is analysed for highly oscillatory linear differential equations of Schrödinger type. Numerical experiments illustrate and complement the theoretical investigations.

4.1.15. Highly-oscillatory evolution equations with multiple frequencies: averaging and numerics

In [7], we are concerned with the application of the recently introduced multi-revolution composition methods, on the one hand, and two-scale methods, on the other hand, to a class of highly-oscillatory evolution equations with multiple frequencies. The main idea relies on a well-balanced reformulation of the problem as an equivalent mono-frequency equation which allows for the use of the two aforementioned techniques.

4.1.16. Optimality and resonances in a class of compact finite difference schemes of high order

In [25], we revisit the old problem of compact finite difference approximations of the homogeneous Dirichlet problem in dimension 1. We design a large and natural set of schemes of arbitrary high order, and we equip this set with an algebraic structure. We give some general criteria of convergence and we apply them to obtain two new results. On the one hand, we use Padé approximant theory to construct, for each given order of consistency, the most efficient schemes and we prove their convergence. On the other hand, we use diophantine approximation theory to prove that almost all of these schemes are convergent at the same rate as the consistency order, up to some logarithmic correction.

4.2. mathematical analysis of multiscale partial differential equations

4.2.1. Collision of almost parallel vortex filaments

In [3], we investigate the occurrence of collisions in the evolution of vortex filaments through a system introduced by Klein, Majda and Damodaran and Zakharov. We first establish rigorously the existence of a pair of almost parallel vortex filaments, with opposite circulation, colliding at some point in finite time. The collision mechanism is based on the one of the self-similar solutions of the model, described in a previous work. In the second part of this paper we extend this construction to the case of an arbitrary number of filaments, with polygonial symmetry, that are perturbations of a configuration of parallel vortex filaments forming a polygon, with or without its center, rotating with constant angular velocity.

4.2.2. Free vibrations of axisymmetric shells: parabolic and elliptic cases

In [9], approximate eigenpairs (quasimodes) of axisymmetric thin elastic domains with laterally clamped boundary conditions (Lamé system) are determined by an asymptotic analysis as the thickness (2ε) tends to zero. The departing point is the Koiter shell model that we reduce by asymptotic analysis to a scalar model that depends on two parameters: the angular frequency k and the half-thickness ε. Optimizing k for each chosen ε, we find power laws for k in function of ε that provide the smallest eigenvalues of the scalar reductions. Corresponding eigenpairs generate quasimodes for the 3D Lamé system by means of several reconstruction operators, including boundary layer terms. Numerical experiments demonstrate that in many cases the constructed eigenpair corresponds to the first eigenpair of the Lamé system. Geometrical conditions are necessary to this approach: The Gaussian curvature has to be nonnegative and the azimuthal curvature has to dominate the meridian curvature in any point of the midsurface. In this case, the first eigenvector admits progressively larger oscillation in the angular variable as ε tends to 0 . Its angular frequency exhibits a power law relation of the form $k = \gamma\varepsilon^{\beta}$ with $\beta = \frac{1}{4}$ in the parabolic case (cylinders and trimmed cones), and the various β's ($\frac{2}{5}$, $\frac{3}{7}$ and $\frac{1}{3}$ in the elliptic case. For these cases where the mathematical analysis is applicable, numerical examples that illustrate the theoretical results are presented.

4.2.3. High frequency oscillations of first eigenmodes in axisymmetric shells as the thickness tends to zero

In [24], the lowest eigenmode of thin axisymmetric shells is investigated for two physical models (acoustics and elasticity) as the shell thickness (2ε) tends to zero. Using a novel asymptotic expansion we determine the behavior of the eigenvalue $\lambda(\varepsilon)$ and the eigenvector angular frequency $k(\varepsilon)$ for shells with Dirichlet boundary conditions along the lateral boundary, and natural boundary conditions on the other parts. First, the scalar Laplace operator for acoustics is addressed, for which $k(\varepsilon)$ is always zero. In contrast to it, for the Lamé system of linear elasticity several different types of shells are defined, characterized by their geometry, for which $k(\varepsilon)$ tends to infinity as ε tends to zero. For two families of shells: cylinders and elliptical barrels we explicitly provide $\lambda(\varepsilon)$ and $k(\varepsilon)$ and demonstrate by numerical examples the different behavior as ε tends to zero.

4.2.4. Semiclassical Sobolev constants for the electro-magnetic Robin Laplacian

This paper [15] is devoted to the asymptotic analysis of the optimal Sobolev constants in the semiclassical limit and in any dimension. We combine semiclassical arguments and concentration-compactness estimates to tackle the case when an electromagnetic field is added as well as a smooth boundary carrying a Robin condition. As a byproduct of the semiclassical strategy, we also get exponentially weighted localization estimates of the minimizers.

4.2.5. On the MIT Bag Model in the Non-relativistic Limit

This paper [2] is devoted to the spectral investigation of the MIT bag model, that is, the Dirac operator on a smooth and bounded domain of $\mathbb{R}^3$ with certain boundary conditions. When the mass m goes to $\pm\infty$, we provide spectral asymptotic results.

4.2.6. Dimension reduction for dipolar Bose-Einstein condensates in the strong interaction regime

In [4], we study dimension reduction for the three-dimensional Gross-Pitaevskii equation with a long-range and anisotropic dipole-dipole interaction modeling dipolar Bose-Einstein condensation in a strong interaction regime. The cases of disk shaped condensates (confinement from dimension three to dimension two) and cigar shaped condensates (confinement to dimension one) are analyzed. In both cases, the analysis combines averaging tools and semiclassical techniques. Asymptotic models are derived, with rates of convergence in terms of two small dimensionless parameters characterizing the strength of the confinement and the strength of the interaction between atoms.

4.2.7. Nonlinear stability criteria for the HMF Model

In [17], we study the nonlinear stability of a large class of inhomogeneous steady state solutions to the Hamiltonian Mean Field (HMF) model. Under a specific criterion, we prove the nonlinear stability of steady states which are decreasing functions of the microscopic energy. To achieve this task, we extend to this context the strategy based on generalized rearrangement techniques which was developed recently for the gravitational Vlasov-Poisson equation. Explicit stability inequalities are established and our analysis is able to treat non compactly supported steady states to HMF, which are physically relevant in this context but induces additional difficulties, compared to the Vlasov-Poisson system.

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

This paper [20] is devoted to the cubic nonlinear Schrödinger equation in a two dimensional waveguide with shrinking cross section. For a Cauchy data living essentially on the first mode of the transverse Laplacian, we provide a tensorial approximation of the solution in this limit, with an estimate of the approximation error, and derive a limiting nonlinear Schrödinger equation in dimension one.

4.2.9. Stable ground states for the HMF Poisson Model

In [36], we prove the nonlinear orbital stability of a large class of steady states solutions to the Hamiltonian Mean Field (HMF) system with a Poisson interaction potential. These steady states are obtained as minimizers of an energy functional under one, two or infinitely many constraints. The singularity of the Poisson potential prevents from a direct run of the general strategy which was based on generalized rearrangement techniques, and which has been recently extended to the case of the usual (smooth) cosine potential. Our strategy is rather based on variational techniques. However, due to the boundedness of the space domain, our variational problems do not enjoy the usual scaling invariances which are, in general, very important in the analysis of variational problems. To replace these scaling arguments, we introduce new transformations which, although specific to our context, remain somehow in the same spirit of rearrangements tools introduced in the references above. In particular, these transformations allow for the incorporation of an arbitrary number of constraints, and yield a stability result for a large class of steady states.

4.2.10. The quantum Liouville-BGK equation and the moment problem

This work [19] is devoted to the analysis of the quantum Liouville-BGK equation. This equation arises in the work of Degond and Ringhofer on the derivation of quantum hydrodynamical models from first principles. Their theory consists in transposing to the quantum setting the closure strategy by entropy minimization used for kinetic equations. The starting point is the quantum Liouville-BGK equation, where the collision term is defined via a so-called quantum local equilibrium, defined as a minimizer of the quantum free energy under a local density constraint. We then address three related problems: we prove new results about the regularity of these quantum equilibria; we prove that the quantum Liouville-BGK equation admits a classical solution; and we investigate the long-time behavior of the solutions. The core of the proofs is based on a fine analysis of the properties of the minimizers of the free energy.

4.2.11. Averaging of nonlinear Schrödinger equations with strong magnetic confinement

In [16], we consider the dynamics of nonlinear Schrödinger equations with strong constant magnetic fields. In an asymptotic scaling limit the system exhibits a purely magnetic confinement, based on the spectral properties of the Landau Hamiltonian. Using an averaging technique we derive an associated effective description via an averaged model of nonlinear Schrödinger type. In a special case this also yields a derivation of the LLL equation.

4.3. mathematical analysis of stochastic partial differential equations

4.3.1. Large deviations for the dynamic Φ_d^{2n} model

In [27], we are dealing with the validity of a large deviation principle for a class of reaction-diffusion equations with polynomial non-linearity, perturbed by a Gaussian random forcing. We are here interested in the regime where both the strength of the noise and its correlation are vanishing, on a length scale ρ and $\delta(\rho)$, respectively, with $0 < \rho, \delta(\rho) << 1$. We prove that, under the assumption that ρ and $\delta(\rho)$ satisfy a suitable scaling limit, a large deviation principle holds in the space of continuous trajectories with values both in the space of square-integrable functions and in Sobolev spaces of negative exponent. Our result is valid, without any restriction on the degree of the polynomial nor on the space dimension.

4.3.2. Solution to the stochastic Schrödinger equation on the full space

In [33], we show how the methods recently applied by Debussche and Weber to solve the stochastic nonlinear Schrödinger equation on $\mathbb{T}^2$ can be enhanced to yield solutions on $\mathbb{R}^2$ if the non-linearity is weak enough. We prove that the solutions remains localized on compact time intervals which allows us to apply energy methods on the full space.

4.3.3. A law of large numbers in the supremum norm for a multiscale stochastic spatial gene network

In [34], we study the asymptotic behavior of multiscale stochastic spatial gene networks. Multiscaling takes into account the difference of abundance between molecules, and captures the dynamic of rare species at a mesoscopic level. We introduce an assumption of spatial correlations for reactions involving rare species and a new law of large numbers is obtained. According to the scales, the whole system splits into two parts with different but coupled dynamics. The high scale component converges to the usual spatial model which is the solution of a partial differential equation, whereas, the low scale component converges to the usual homogeneous model which is the solution of an ordinary differential equation. Comparisons are made in the supremum norm.

4.3.4. Long time behavior of Gross-Pitaevskii equation at positive temperature

In [32], the stochastic Gross-Pitaevskii equation is used as a model to describe Bose-Einstein condensation at positive temperature. The equation is a complex Ginzburg Landau equation with a trapping potential and an additive space-time white noise. Two important questions for this system are the global existence of solutions in the support of the Gibbs measure, and the convergence of those solutions to the equilibrium for large time. In this paper, we give a proof of these two results in one space dimension. In order to prove the convergence to equilibrium, we use the associated purely dissipative equation as an auxiliary equation, for which the convergence may be obtained using standard techniques.

4.3.5. An integral inequality for the invariant measure of a stochastic reaction–diffusion equation

In [14], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove an integral inequality for the invariant measure ν of a stochastic reaction-diffusion equation. Then we discuss some consequences as an integration by parts formula which extends to ν a basic identity of the Malliavin Calculus. Finally, we prove the existence of a surface measure for a ball and a half-space of $\mathcal{H}$.

4.3.6. Kolmogorov equations and weak order analysis for SPDES with nonlinear diffusion coefficient

In [26], we provide new regularity results for the solutions of the Kolmogorov equation associated to a SPDE with nonlinear diffusion coefficients and a Burgers type nonlinearity. This generalizes previous results in the simpler cases of additive or affine noise. The basic tool is a discrete version of a two sided stochastic integral which allows a new formulation for the derivatives of these solutions. We show that this can be used to generalize the weak order analysis performed by Debussche in 2011. The tools we develop are very general and can be used to study many other examples of applications.

4.3.7. Approximation-diffusion in stochastically forced kinetic equations

In [35], we derive the hydrodynamic limit of a kinetic equation where the interactions in velocity are modelled by a linear operator (Fokker-Planck or Linear Boltzmann) and the force in the Vlasov term is a stochastic process with high amplitude and short-range correlation. In the scales and the regime we consider, the hydrodynamic equation is a scalar second-order stochastic partial differential equation. Compared to the deterministic case, we also observe a phenomenon of enhanced diffusion.

5. Partnerships and Cooperations

5.1. Regional Initiatives

- A. Crestetto is member of the project "Pari Scientifique Régional Exprodil".
- M. Lemou is member of the project "Défis" of the University of Rennes 1, leader Nicolas Seguin.

5.2. National Initiatives

5.2.1. ANR MOONRISE: 2015-2019

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

The project *Moonrise* submitted by Florian 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, François Castella, Philippe Chartier, Nicolas Crouseilles and Mohammed Lemou are members of the project Moonrise.

Postdocs

- Loïc Le Treust has been hired as a Postdoc, under the supervision of Philippe Chartier and Florian Méhats. His contract started in september 2015 and ended in august 2016. Loïc Le Treust is now assistant professor at the university of Marseille.
- Xiaofei Zhao has been hired as a Postdoc from september 2015 to september 2016 under the supervision of Florian Méhats.

5.2.2. ANR MFG: 2016-2020

Participant: Arnaud Debussche.

Mean Field Games (MFG) theory is a new and challenging mathematical topic which analyzes the dynamics of a very large number of interacting rational agents. Introduced ten years ago, the MFG models have been used in many areas such as, e.g., economics (heterogeneous agent models, growth modeling,...), finance (formation of volatility, models of bank runs,...), social sciences (crowd models, models of segregation) and engineering (data networks, energy systems...). Their importance comes from the fact that they are the simplest (“stochastic control"-type) models taking into account interactions between rational agents (thus getting beyond optimization), yet without entering into the issues of strategic interactions. MFG theory lies at the intersection of mean field theories (it studies systems with a very large number of agents), game theory, optimal control and stochastic analysis (the agents optimize a payoff in a possibly noisy setting), calculus of variations (MFG equilibria may arise as minima of suitable functionals) and partial differential equations (PDE): In the simplest cases, the value of each agent is found by solving a backward Hamilton-Jacobi equation whereas the distribution of the agents’ states evolves according to a forward Fokker-Planck equation. The “Master" equation (stated in the space of probability measures) subsumes the individual and collective behaviors. Finally, modeling, numerical analysis and scientific computing are crucial for the applications. French mathematicians play a world-leading role in the research on MFG: The terminology itself comes from a series of pioneering works by J.-M. Lasry and P.-L. Lions who introduced most of the key ideas for the mathematical analysis of MFG; the last conference on MFG was held last June in Paris and organized by Y. Achdou, P. Cardaliaguet and J.-M. Lasry. As testifies the proposal, the number of researchers working on MFG in France (and also abroad) is extremely fast-growing, not only because the theoretical aspects are exciting and challenging, but also because MFG models find more and more applications. The aim of the project is to better coordinate the French mathematical research on MFG and to achieve significant progress in the theory and its applications.

The partners of the project are the CEREMADE laboratory (Paris Dauphine), the IRMAR laboratory (Rennes I), the university of Nice and of Tours.

5.2.3. ANR ACHYLLES: 2014-2018

Participant: Anais Crestetto.

The ACHYLLES project focuses on Long-Time Asymptotic-Preserving (LTAP) numerical schemes for hyperbolic systems of conservation laws supplemented by potentially stiff source terms. It ambitions to perform a breakthrough in the understanding and efficiency of LTAP scheme.

The partners are IMB (Bordeaux), LMV (Versailles) and LMJL (Nantes).

5.2.4. IPL FRATRES

IPSO is associated to IPL FRATRES which started in june 2015. The aim of this project is to organize Inria teams activities which develop mathematical and numerical tools in magnetically confined nuclear fusion. The ambition is to prepare the next generation of numerical modeling methodologies able to use in an optimal way the processing capabilities of modern massively parallel architectures. This objective requires close collaboration between a) applied mathematicians and physicists that develop and study mathematical models of PDE; b) numerical analysts developing approximation schemes; c) specialists of algorithmics proposing solvers and libraries using the many levels of parallelism offered by the modern architecture and d) computer scientists. The project road map ambitions to contribute in close connection with National and European initiatives devoted to nuclear Fusion to the improvement and design of numerical simulation technologies applied to plasma physics and in particular to the ITER project for magnetic confinement fusion.

Postdoc

- Xiaofei Zhao has been hired as a Postdoc, under the supervision of Nicolas Crouseilles and Sever Hirstoaga (Inria-Nancy). His contract started in october 2016 and ended in september 2017.

5.3. European Initiatives

5.3.1. Collaborations in European Programs, Except FP7 & H2020

Program: EUROFusion Enabling Research

Project acronym: WPENR

Project title: Verification and development of new algorithms for gyrokinetic codes

Duration: january 2015 - december 2017.

Coordinator: E. Sonnendrücker (Max-Planck IPP, Germany)

Other partners: IPP, EPFL, CEA-Cadarache, university of Strasbourg, Toulouse, Marseille, Paris 6.

Abstract: Gyrokinetic codes play a major role in understanding the development and saturation of micro-turbulence in a magnetic fusion plasma and its influence on energy confinement time. The first aim of this proposal is to assess the reliability of gyrokinetic codes by extensive verification and benchmarking. All the major european gyrokinetic codes are involved in the proposal and this will enable them to define comparison elements, which ultimately will also facilitate the cross-validation of new physics. On the other hand we will develop new algorithms for extending the physics capabilities or the computational efficiency of different gyrokinetic codes. Finally we will also perform a prospective investigation of models and numerical methods that could help in the future to address physics where kinetic effects might play an important role but that cannot be handled with today's gyrokinetic codes, like L-H (low to high confinement) transition, edge physics or MHD time scales simulations.

5.4. International Initiatives

5.4.1. Informal International Partners

Members of the IPSO team have several international collaborations

- the group of S. Jin (university of Wisconsin, US).
- the group of W. Bao (university of Singapore).
- G. Vimart (university of Geneva, Swizerland).
- the group of A. Ostermann (university of Innsbrück).
- the SNS of Pisa (G. Da Prato).
- several US universities: Maryland (S. Cerrai), Chicago (C. Sparber), Colorado (O. Pinaud), $\cdots$
- $\cdots$

5.4.2. Participation in Other International Programs

- A. Crestetto is involved in the project PHC PROCOPE "Hétérogénéités Fortes dans les Modèles d'Ecoulement Fluide".

5.5. International Research Visitors

5.5.1. Visits to International Teams

- P. Chartier was invited by Fernando Casas, University of Castellon, Spain, July 6-9 2017.
- A. Crestetto was invited by Christian Klingenberg, Institute of Mathematics, Würzburg University, July 10-14 2017.
- M. Lemou was invited by Shi Jin, Jiao Tong university Shanghai, China, July 5-15 2017.
- M. Lemou was invited by Hao Wu, Tsinghua university Beijing, China, July 15-20 2017.

6. Dissemination

6.1. Promoting Scientific Activities

6.1.1. Scientific Events Organisation

6.1.1.1. Member of the Organizing Committees

- F. Castella organized the workshop "Multiscale numerical methods", Saint-Malo, december 13-15 2017. [15 participants]
- N. Crouseilles co-organized the weekly seminar "Mathematic and applications", ENS Rennes.
- N. Crouseilles co-organized the Nantes-Rennes meeting at the university of Nantes, january 19 2017. [50 participants]
- N. Crouseilles organized the IPL FRATRES meeting at Inria Rennes, november 27-28 2017. [30 participants]
- N. Crouseilles and M. Lemou co-organized (with C. Cheverry and K. Pravda-Starov) the international workshop "Analysis of transport equations: Vlasov and related models", Rennes, may 16-19 2017. [50 participants]
- E. Faou organizes a work-group on "Mathematics of deep learning" (Inria, IRMAR and Technicolor), Rennes, France.
- E. Faou organized the mini-sympositum "Methods for the nonlinear Schrödinger equations, solitary waves and discrete patterns", with T. Matsuo (University of Tokyo), at the Scicade international conference, Bath (UK), september 11-15 2017.
- E. Faou co-organized the conference ANSIVAL on the occation of the 60th birthday of M. Dauge (IRMAR), Rennes, France, february 8-10 2017. [70 participants]

6.1.2. Journal

6.1.2.1. Member of the Editorial Boards

- P. Chartier is associate editor of M2AN (2007-).
- A. Debussche is editor in chief of Stochastic Partial Differential Equations: analysis and computations (2013-).
- A. Debussche is associate editor of Differential and Integral Equations (2002-).
- A. Debussche is associate editor of Potential Analysis (2011-).
- A. Debussche is associate editor of ESAIM:PROC (2012-).
- A. Debussche is associate editor of Journal of Evolution Equation (2014-).
- A. Debussche is associate editor of Applied Mathematics & Optimization (2014-).
- A. Debussche is associate editor of SIAM JUQ (2017-).
- A. Debussche is member of the editorial board of the collection "Mathématiques & Applications de la SMAI", Springer.

6.1.2.2. Reviewer - Reviewing Activities

The members of the IPSO team are reviewers for almost all the journals in which they publish.

6.1.3. Invited Talks

National conferences

- A. Crestetto gave talk at Congrès SMAI 2017, La Tremblade, june 5-9 2017.
- The members of the team gave several seminars in french institutions (Marseille, Cergy, Toulouse, Nancy, CEA Cadarache, $\cdots$).

International conferences

- P. Chartier was invited speaker at FoCM 2017, workshop on "Geometric Integration and Computational Mechanics" (july 10-12), Barcelona, Spain.
- P. Chartier was invited speaker at "Mathematical and Computational Methods for Quantum and Kinetic Problems", (june 12-14), Beijing, China.
- P. Chartier was invited speaker at "Kinema 2017: Numerical Modelling of Kinetic Magnetized Plasmas", spring school, Institut d'études scientifiques de Cargèse, (april 3-7), Cargèse, France.
- A. Crestetto gave talk at the workshop "NumKin 2017" (october 23-27), IPP Garching, Germany.
- A. Crestetto gave a talk at the Oberseminar (july 11), Würzburg, Germany.
- N. Crouseilles gave a talk at the workshop on "Mathematical and Computational methods for Quantum and Kinetic Problems, (june 12-14), Beijing, China.
- A. Debussche gave a talk at "Stochastic PDEs: Analysis and Computation", (march 27-31), Warwick, England.
- A. Debussche gave a talk at "Probabilistic Perspectives in Nonlinear PDEs", (june 5-9), International Centre for Mathematical Sciences (ICMS), Edinburgh, Scotland.
- A. Debussche gave a talk at FoCM2017, workshop on "Stochastic Computation", (july 10-12), Barcelona, Spain.
- A. Debussche gave a talk at "2017 Fields Medal Symposium", (october 16-19), Toronto, Canada.
- E. Faou gave a talk at the mini-symposium "Modelling, theory and approximation of nonlinear waves", Scicade international conference, (september 11-15), University of Bath, UK.
- E. Faou gave a talk at the conference "Asymptotic analysis of evolution equations", (july 3-7), CIRM, Marseille.
- E. Faou gave a talk at the seminar at the University of Cambridge, (june 2017), UK.
- E. Faou gave a talk at the workshop "Mathematical questions in wave turbulence theory", (may 15-19), San Jose, California.
- E. Faou gave a talk at the workshop "Modern Numerical Methods for Quantum Mechanics", (march 20-22) Polish Academy of sciences, Warsaw, Poland.
- M. Lemou gave a talk at International workshop "Geometric Transport Equations in General Relativity", (february 20-24), ESI, Vienna, Austria.
- M. Lemou gave a course in the summer school "Applied and Stochastic Analysis for Partial Differential Equations". Institute of Natural Science, Shanghai Jiao Tong University, (july 12-22), Shanghai, China.
- M. Lemou gave a talk at WPI workshop on "Quantum Dynamics and Uncertainty Quantification", (june 20-25), Vienna, Austria,
- M. Lemou gave a talk at the workshop on "Mathematical and Computational methods for Quantum and Kinetic Problems, (june 12-14), Beijing, China.
- M. Lemou gave a course at "Kinema 2017: Numerical Modelling of Kinetic Magnetized Plasmas", spring school, Institut d'études scientifiques de Cargèse, (april 3-7), Cargèse, France.
- M. Lemou gave a talk at the workshop on "Kinetic Theory and Fluid Mechanics : theoretical and computational aspects", (november 6-10), Toulouse, France.

- F. Méhats gave a talk at SIAM Conference on "Analysis of Partial Differential Equations", (december 10-12), Baltimore, USA.
- F. Méhats gave a talk at the workshop on "Mathematical and Computational methods for Quantum and Kinetic Problems, (june 12-14), Beijing, China.
- F. Méhats gave a talk at the conference "Advances in Mathematics for Technology", (october 9-11) Catania, Italy.

6.1.4. Scientific Expertise

- P. Chartier is member of the promotion committees DR1 and DR0 Inria.
- N. Crouseilles was reviewer for ANR project.
- A. Debussche participated to the report projet EUR Centre Henri Lebesgue.
- A. Debussche was reviewer for ERC projects, "Philip Leverhulme" (GB) fundation, Austrian Science Fundation.
- A. Debussche was president of the visiting committee HCERES of the Centre d'Analyses et de Mathématique Sociales (Paris, EHESS).

6.1.5. Research Administration

- P. Chartier is scientific vice-deputy of the Inria Rennes center.
- P. Chartier is member of the Inria evaluation committee.
- P. Chartier is member of the Inria Scientific Committee (COSI).
- P. Chartier is member of the Bureau du Comité des Projets (BCP).
- A. Crestetto is member of the mathematic department council of the university of Nantes.
- A. Crestetto is member of the scientific council of "UFR Sciences et Techniques" of the university of Nantes.
- N. Crouseilles is member of the scientific council of ENS Rennes.
- N. Crouseilles is member of the mathematic laboratory (IRMAR) council.
- N. Crouseilles is member of the Fédération de Fusion council (University of Rennes representative).
- A. Debussche is member of the scientific council of the Fédération Denis Poisson.
- A. Debussche is member of the administrative council of ENS Paris-Saclay.
- A. Debussche if scientific vice-deputy and international relations of ENS Rennes.
- A. Debussche is vice-head ot the Centre Henri Lebesgue.
- A. Debussche is vice-head of the Lebesgue agency for Mathematic and Innovation.
- E. Faou is member of the scientific council of the Pôle Universitaire Léonard de Vinci.
- E. Faou is member of the CNU section 26.
- E. Faou is head of organization of the semester *scientific computing* sponsored by the Labex Lebesgue (2 international summer schools, 7 workshops and international conferences).
- M. Lemou is member of the scientific council of the Center Henri Lebesgue.
- M. Lemou is member of the scientific council of ENS Rennes.
- M. Lemou is the head of the numerical analysis team of IRMAR laboratory. [46 members].
- F. Méhats was head of the mathematic laboratory IRMAR (2015-2017). [250 members].

6.2. Teaching - Supervision - Juries

6.2.1. Teaching

- Master : F. Castella, "Equations de transport et Phenomenes de Propagation", 48h, M1, university of Rennes 1, France.

- Master : F. Castella, "Analyse Numerique Generale", 48h, M1, university of Rennes 1, France.
- Master : P. Chartier, "Semi-lagrangian methods for Vlasov-Poisson equations", 18h, M2, university of Rennes 1, France.
- Master : A. Crestetto, "Méthodes numériques pour les fluides incompressibles", 64h, M2, university of Nantes, France.
- Master : A. Crestetto, "Compléments de modélisation pour l'agrégation", 26h, M2, university of Nantes, France.
- Master : N. Crouseilles, "Analyse numérique", 30h, M1, ENS Rennes, France.
- Master : A. Debussche, "Distribution et analyse fonctionnelle", 30h, M1, ENS Rennes, France.
- Master : A. Debussche, "Introduction aux EDP Stochastiques", 48h, M2, university of Rennes 1, France.
- Master : A. Debussche, "Compléments pour l'agrégation", 26h, M2, ENS Rennes, France.
- Master : M. Lemou, "Equations aux dérivées partielles elliptiques", 30h, M1, ENS de Rennes.
- Master : F. Méhats, "Equations hyperboliques", 30h, M2, university of Rennes 1, France.

6.2.2. Supervision

- PhD : R. Horsin, Comportement en temps long d'équations de type Vlasov: Etudes mathématiques et numériques, university of Rennes 1, december 1st 2017, E. Faou and F. Rousset (university Paris Sud).
- PhD : V. Doli, Phénomènes de propagation de champignons parasites de plantes, par couplage de diffusion spatiale et de reproduction sexuée, december 23th 2017, F. Castella and F. Hamelin (IGEPP, Agrocampus).
- PhD in progress : M. Malo, Equations cinétiques non collisionnelles : stabilité, oscillations, september 2015, M. Lemou and F. Méhats.
- PhD in progress : J. Bernier, Mathematical and numerical anaysis of nonlinear transport equations, (2016-), september 2016, N. Crouseilles and E. Faou.
- PhD in progress : M. Tusseau, Sur l'équation de Schrödinger non linéaire hautement oscillante avec potentiel aléatoire, september 2013, A. Debussche and F. Méhats.
- PhD in progress : M. Jugal Nguepedja Nankep, Modèles spatiaux stochastiques de systèmes multi-échelle de particules en interactions, september 2014, A. Debussche.
- PhD in progress : A. Rosello, Approximation-diffusion pour des équations cinétiques pour les modèles de type "spray", september 2017, A. Debussche.

6.2.3. Juries

- A. Crestetto was member of the jury of the thesis of T. Blanc, "Etude mathématique de problèmes paraboliques fortement anisotropes", Marseille, december 4th 2017.
- N. Crouseilles was member of the jury of the thesis of A. Finot, "Analyse mathématique des modèles cinétiques en présence d'un champ magnétique intense", Marseille, january 26th 2017.
- N. Crouseilles was member of the jury of the thesis of T. Hardy, "Traitement des conditions aux limites spéculaires pour l'étude du transfert radiatif dans des matériaux à géométrie complexe", Nantes, january 31th 2017.
- E. Faou was member of the jury of the thesis of S. Dieckmann, "Dynamics of patterns in equivariant Hamiltonian partial differential equations", Bielefeld (Germany), april 2017.
- E. Faou was member of the jury of the thesis of P. Krämer, "Numerical integrators for Maxwell-Klein-Gordon and Maxwell-Dirac systems in highly to slowly oscillatory regimes", Karlsruhe (Germany), august 2017.

- M. Lemou was member of the jury of the thesis of R. Horsin Blanc, "Comportement en temps long d'équations de type Vlasov: Etudes mathématiques et numériques", Rennes, december 1st 2017.
- M. Lemou was member of the jury (reviewer) of the thesis of T. Blanc, "Etude mathématique de problèmes paraboliques fortement anisotropes", Marseille, december 4th 2017.
- F. Méhats was member of the jury of the thesis of A. Finot, "Analyse mathématique des modèles cinétiques en présence d'un champ magnétique intense", Marseille, january 26th 2017.

7. Bibliography

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[1] R. HORSIN. *On long time behavior of certain Vlasov equations: Mathematics and Numerics*, Université de Rennes 1, December 2017, https://tel.archives-ouvertes.fr/tel-01670352

Articles in International Peer-Reviewed Journals

[2] N. ARRIZABALAGA, L. LE TREUST, N. RAYMOND. *On the MIT Bag Model in the Non-relativistic Limit*, in "Communications in Mathematical Physics", 2017, vol. 354, n° 2, pp. 641-669 [*DOI :* 10.1007/s00220-017-2916-8], https://hal.archives-ouvertes.fr/hal-01343717

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