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Activity Report 2016

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

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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 [53], [50], [49] 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: François 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 [48] 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: François Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Méhats, 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: François Castella, Philippe Chartier, Erwan Faou, Florian Méhats.

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 [52], [51] 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: 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, 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: 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. New Results

4.1. List of results

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

In [25], the authors consider the Vlasov-HMF (Hamiltonian Mean-Field) model. They consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). They prove that these solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping.

4.1.2. Fast Weak-Kam Integrators for separable Hamiltonian systems

In [4], the authors consider a numerical scheme for Hamilton-Jacobi equations based on a direct discretization of the Lax-Oleinik semi-group. They prove that this method is convergent with respect to the time and space stepsizes provided the solution is Lipschitz, and give an error estimate. Moreover, They prove that the numerical scheme is a *geometric integrator* satisfying a discrete weak-KAM theorem which allows to control its long time behavior. Taking advantage of a fast algorithm for computing min–plus convolutions based on the decomposition of the function into concave and convex parts, they show that the numerical scheme can be implemented in a very efficient way.

4.1.3. The weakly nonlinear large-box limit of the 2D cubic nonlinear Schrödinger equation

In [23], the authors consider the cubic nonlinear Schrödinger (NLS) equation set on a two dimensional box of size L with periodic boundary conditions. By taking the large box limit $L \to \infty$ in the weakly nonlinear regime (characterized by smallness in the critical space), we derive a new equation set on $\mathbb{R}^2$ that approximates the dynamics of the frequency modes. This nonlinear equation turns out to be Hamiltonian and enjoys interesting symmetries, such as its invariance under Fourier transform, as well as several families of explicit solutions. A large part of this work is devoted to a rigorous approximation result that allows to project the long-time dynamics of the limit equation into that of the cubic NLS equation on a box of finite size.

4.1.4. An asymptotic preserving scheme for the relativistic Vlasov–Maxwell equations in the classical limit

In [13], the authors consider the relativistic Vlasov–Maxwell (RVM) equations in the limit when the light velocity c goes to infinity. In this regime, the RVM system converges towards the Vlasov–Poisson system and the aim of this work is to construct asymptotic preserving numerical schemes that are robust with respect to this limit. A number of numerical simulations are conducted in order to investigate the performances of our numerical scheme both in the relativistic as well as in the classical limit regime. In addition, they derive the dispersion relation of the Weibel instability for the continuous and the discretized problem.

4.1.5. Free Vibrations of Axisymmetric Shells: Parabolic and Elliptic cases

In [41], 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 βs $\frac{2}{5}$, $\frac{3}{7}$, 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.

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

In [30], 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.

4.1.7. On numerical Landau damping for splitting methods applied to the Vlasov-HMF model

In [24], we consider time discretizations of the Vlasov-HMF (Hamiltonian Mean-Field) equation based on splitting methods between the linear and non-linear parts. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that the numerical solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping. Moreover, we prove that the modified state is close to the continuous one and provide error estimates with respect to the time stepsize.

4.1.8. 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.

4.1.9. Uniformly accurate exponential-type integrators for Klein-Gordon equations with asymptotic convergence to classical splitting schemes in the nonlinear schrödinger limit

In [34], we introduce efficient and robust exponential-type integrators for Klein-Gordon equations which resolve the solution in the relativistic regime as well as in the highly-oscillatory non-relativistic regime without any step-size restriction under the same regularity assumptions on the initial data required for the integration of the corresponding nonlinear Schrödinger limit system. In contrast to previous works we do not employ any asymptotic or multiscale expansion of the solution. This allows us to derive uniform convergent schemes under far weaker regularity assumptions on the exact solution. In addition, the newly derived first- and second-order exponential-type integrators converge to the classical Lie, respectively, Strang splitting in the nonlinear Schrödinger limit.

4.1.10. Convergence of a normalized gradient algorithm for computing ground states

In [45], we consider the approximation of the ground state of the one-dimensional cubic nonlinear Schrödinger equation by a normalized gradient algorithm combined with linearly implicit time integrator, and finite difference space approximation. We show that this method, also called *imaginary time evolution method* in the physics literature, is locally convergent, and we provide error estimates: for an initial data in a neighborhood of the ground state, the algorithm converges exponentially towards a modified soliton that is a space discretization of the exact soliton, with error estimates depending on the discretization parameters.

4.1.11. Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations

In [8], we analyse the error behavior of operator splitting methods for highly-oscillatory differential equations. The scope of applications includes time-dependent nonlinear Schrödinger equations, where the evolution operator associated with the principal linear part is highly-oscillatory and periodic in time. In a first step, a known convergence result for the second-order Strang splitting method applied to the cubic Schrödinger equation is adapted to a wider class of nonlinearities. In a second step, the dependence of the global error on the decisive parameter $0 < \varepsilon < 1$, defining the length of the period, is examined. The main result states that, compared to established error estimates, the Strang splitting method is more accurate by a factor ε, provided that the time stepsize is chosen as an integer fraction of the period. This improved error behavior over a time interval of fixed length, which is independent of the period, is due to an averaging effect. The extension of the convergence result to higher-order splitting methods and numerical illustrations complement the investigations.

4.1.12. Solving highly-oscillatory NLS with SAM: numerical efficiency and geometric properties

In [7], we present the Stroboscopic Averaging Method (SAM), which aims at numerically solving highly-oscillatory differential equations. More specifically, we first apply SAM to the Schrödinger equation on the 1-dimensional torus and on the real line with harmonic potential, with the aim of assessing its efficiency: as compared to the well-established standard splitting schemes, the stiffer the problem is, the larger the speed-up grows (up to a factor 100 in our tests). The geometric properties of SAM are also explored: on very long time intervals, symmetric implementations of the method show a very good preservation of the mass invariant and of the energy. In a second series of experiments on 2-dimensional equations, we demonstrate the ability of SAM to capture qualitatively the long-time evolution of the solution (without spurring high oscillations).

4.1.13. Highly-oscillatory evolution equations with non-resonant frequencies: averaging and numerics

In [40], 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.

4.1.14. A formal series approach to the Center Manifold theorem

In [35], 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.

4.1.15. Uniformly accurate time-splitting methods for the semi-classical Schrödinger equation, Part II: Numerical analysis

This article [39] is second part of a twofold paper devoted to the construction of numerical methods which remain insensitive to the smallness of the semiclassical parameter for the Schrödinger equation in the semiclassical limit. Here, we specifically analyse the convergence behavior of the first-order splitting introduced in Part I, for a linear equation with smooth potential. Our main result is a proof of uniform accuracy.

4.1.16. Averaging of highly-oscillatory transport equations

In [38], we develop a new strategy aimed at obtaining high-order asymptotic models for transport equations with highly-oscillatory solutions. The technique relies upon recent developments averaging theory for ordinary differential equations, in particular normal form expansions in the vanishing parameter. Noteworthy, the result we state here also allows for the complete recovery of the exact solution from the asymptotic model. This is done by solving a companion transport equation that stems naturally from the change of variables underlying high-order averaging. Eventually, we apply our technique to the Vlasov equation with external electric and magnetic fields. Both constant and non-constant magnetic fields are envisaged, and asymptotic models already documented in the literature and re-derived using our methodology. In addition, it is shown how to obtain new high-order asymptotic models.

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

In [11], 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 asymptotically stable 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.

4.1.18. Asymptotic Preserving scheme for a kinetic model describing incompressible fluids

The kinetic theory of fluid turbulence modeling developed by Degond and Lemou (2002) 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 in this work [17] 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.

4.1.19. Numerical schemes for kinetic equations in the diffusion and anomalous diffusion limits. Part I: the case of heavy-tailed equilibrium

In [15], we propose some numerical schemes for linear kinetic equations in the diffusion and anomalous diffusion limit. When the equilibrium distribution function is a Maxwellian distribution, it is well known that for an appropriate time scale, the small mean free path limit gives rise to a diffusion type equation. However, when a heavy-tailed distribution is considered, another time scale is required and the small mean free path limit leads to a fractional anomalous diffusion equation. Our aim is to develop numerical schemes for the original kinetic model which works for the different regimes, without being restricted by stability conditions of standard explicit time integrators. First, we propose some numerical schemes for the diffusion asymptotics; then, their extension to the anomalous diffusion limit is studied. In this case, it is crucial to capture the effect of the large velocities of the heavy-tailed equilibrium, so that some important transformations of the schemes derived for the diffusion asymptotics are needed. As a result, we obtain numerical schemes which enjoy the Asymptotic Preserving property in the anomalous diffusion limit, that is: they do not suffer from the restriction on the time step and they degenerate towards the fractional diffusion limit when the mean free path goes to zero. We also numerically investigate the uniform accuracy and construct a class of numerical schemes satisfying this property. Finally, the efficiency of the different numerical schemes is shown through numerical experiments.

4.1.20. Numerical schemes for kinetic equations in the anomalous diffusion limit. Part II: degenerate collision frequency

In [14], which is the continuation of [15], we propose numerical schemes for linear kinetic equation which are able to deal with the fractional diffusion limit. When the collision frequency degenerates for small velocities it is known that for an appropriate time scale, the small mean free path limit leads to an anomalous diffusion equation. From a numerical point of view, this degeneracy gives rise to an additional stiffness that must be treated in a suitable way to avoid a prohibitive computational cost. Our aim is therefore to construct a class of numerical schemes which are able to undertake these stiffness. This means that the numerical schemes are able to capture the effect of small velocities in the small mean free path limit with a fixed set of numerical parameters. Various numerical tests are performed to illustrate the efficiency of our methods in this context.

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

In [12], 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.

4.1.22. Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equations.

In [16], we deal with 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.

4.1.23. Multi-scale methods for the solution of the radiative transfer equation

Various methods have been developed and tested over the years to solve the radiative transfer equation (RTE) with different results and trade-offs. Although the RTE is extensively used, the approximate diffusion equation is sometimes preferred, particularly in optically thick media, due to the lower computational requirements. Recently, multi-scale models, namely the domain decomposition methods, the micro-macro model and the hybrid transport- diffusion model, have been proposed as an alternative to the RTE. In domain decomposition methods, the domain is split into two subdomains, namely a mesoscopic subdomain where the RTE is solved and a macroscopic subdomain where the diffusion equation is solved. In the micro-macro and hybrid transport-diffusion models, the radiation intensity is decomposed into a macroscopic component and a mesoscopic one. In both cases, the aim is to reduce the computational requirements, while maintaining the accuracy, or to improve the accuracy for similar computational requirements. In [10], these multi-scale methods are described, and the application of the micro-macro and hybrid transport-diffusion models to a three- dimensional transient problem is reported. It is shown that when the diffusion approximation is accurate, but not over the entire domain, the multi-scale methods may improve the solution accuracy in comparison with the solution of the RTE. The order of accuracy of the numerical schemes and the radiative properties of the medium play a key role in the performance of the multi-scale methods.

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

In [42], 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.

4.1.25. Asymptotic Preserving numerical schemes for multiscale parabolic problems

In [18], we consider a class of multiscale parabolic problems with diffusion coefficients oscillating in space at a possibly small scale ε. Numerical homogenization methods are popular for such problems, because they capture efficiently the asymptotic behaviour as ε goes to 0, without using a dramatically fine spatial discretization at the scale of the fast oscillations. However, known such homogenization schemes are in general not accurate for both the highly oscillatory regime ($\varepsilon << 1$) and the non oscillatory regime ($\varepsilon \approx 1$). In this paper, we introduce an Asymptotic Preserving method based on an exact micro-macro decomposition of the solution which remains consistent for both regimes.

4.1.26. Uniformly accurate numerical schemes for the nonlinear dirac equation in the nonrelativistic limit regime

In [47], 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 $\varepsilon \to 0$ in the nonrelativistic limit regime. The small parameter causes high oscillations in time which bring severe numerical burden for classical numerical methods. We present a suitable two-scale formulation as a general strategy to tackle a class of highly oscillatory problems involving the two small scales ε and ε^2. A numerical scheme with uniform (with respect to $\varepsilon \in [0, 1]$) second order accuracy in time and a spectral accuracy in space are proposed. Numerical experiments are done to confirm the UA property.

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

In [26], we deal with 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.

4.1.28. On the MIT bag model: self-adjointness and non-relativistic limit

This paper [32] is devoted to the mathematical investigation of the MIT bag model, that is the Dirac operator on a smooth and bounded domain with certain boundary conditions. We prove that the operator is self-adjoint and, when the mass goes to infinity, we provide spectral asymptotic results.

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

It is known that the competitive exclusion principle holds for a large kind of models involving several species competing for a single resource in an homogeneous environment. Various works indicate that the coexistence is possible in an heterogeneous environment. We propose in [6] a spatially heterogeneous system modeling the competition of several species for a single resource. If spatial movements are fast enough, we show that our system can be well approximated by a spatially homogeneous system, called aggregated model, which can be explicitly computed. Moreover, we show that if the competitive exclusion principle holds for the aggregated model, it holds for the spatially heterogeneous model too.

4.1.30. Extended Rearrangement inequalities and applications to some quantitative stability results

In [28], we prove a new functional inequality of Hardy-Littlewood type for generalized rearrangements of functions. We then show how this inequality provides *quantitative* stability results of steady states to evolution systems that essentially preserve the rearrangements and some suitable energy functional, under minimal regularity assumptions on the perturbations. In particular, this inequality yields a *quantitative* stability result of a large class of steady state solutions to the Vlasov-Poisson systems, and more precisely we derive a quantitative control of the L^1 norm of the perturbation by the relative Hamiltonian (the energy functional) and rearrangements. A general non linear stability result has been obtained recently by Lemou, Méhats and Raphaël (2012) in the gravitational context, however the proof relied in a crucial way on compactness arguments which by construction provides no quantitative control of the perturbation. Our functional inequality is also applied to the context of 2D-Euler system and also provides quantitative stability results of a large class of steady-states to this system in a natural energy space.

4.1.31. Mate Finding, Sexual Spore Production, and the Spread of Fungal Plant Parasites

Sexual reproduction and dispersal are often coupled in organisms mixing sexual and asexual reproduction, such as fungi. The aim of this study [27] is to evaluate the impact of mate limitation on the spreading speed of fungal plant parasites. Starting from a simple model with two coupled partial differential equations, we take

advantage of the fact that we are interested in the dynamics over large spatial and temporal scales to reduce the model to a single equation. We obtain a simple expression for speed of spread, accounting for both sexual and asexual reproduction. Taking Black Sigatoka disease of banana plants as a case study, the model prediction is in close agreement with the actual spreading speed (100 km per year), whereas a similar model without mate limitation predicts a wave speed one order of magnitude greater. We discuss the implications of these results to control parasites in which sexual reproduction and dispersal are intrinsically coupled.

4.1.32. Dimension reduction for rotating Bose-Einstein condensates with anisotropic confinement

In [29], we consider the three-dimensional time-dependent Gross-Pitaevskii equation arising in the description of rotating Bose-Einstein condensates and study the corresponding scaling limit of strongly anisotropic confinement potentials. The resulting effective equations in one or two spatial dimensions, respectively, are rigorously obtained as special cases of an averaged three dimensional limit model. In the particular case where the rotation axis is not parallel to the strongly confining direction the resulting limiting model(s) include a negative, and thus, purely repulsive quadratic potential, which is not present in the original equation and which can be seen as an effective centrifugal force counteracting the confinement.

4.1.33. Averaging of nonlinear Schrödinger equations with strong magnetic confinement

In [46], 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.

4.1.34. The Interaction Picture method for solving the generalized nonlinear Schrödinger equation in optics

The interaction picture (IP) method is a very promising alternative to Split-Step methods for solving certain type of partial differential equations such as the nonlinear Schrödinger equation used in the simulation of wave propagation in optical fibers. The method exhibits interesting convergence properties and is likely to provide more accurate numerical results than cost comparable Split-Step methods such as the Symmetric Split-Step method. In [1] we investigate in detail the numerical properties of the IP method and carry out a precise comparison between the IP method and the Symmetric Split-Step method.

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

In [21], 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.

4.1.36. Estimate for P_tD for the stochastic Burgers equation

In [20], we consider the Burgers equation on $H = L^2(0,1)$ perturbed by white noise and the corresponding transition semigroup P_t. We prove a new formula for $P_tD\phi$ (where $\phi : H \to \mathbb{R}$ is bounded and Borel) which depends on ϕ but not on its derivative. Then we deduce some new consequences for the invariant measure ν of P_t as its Fomin differentiability and an integration by parts formula which generalises the classical one for gaussian measures.

4.1.37. Degenerate Parabolic Stochastic Partial Differential Equations: Quasilinear case

In [22], we study the Cauchy problem for a quasilinear degenerate parabolic stochastic partial differential equation driven by a cylindrical Wiener process. In particular, we adapt the notion of kinetic formulation and kinetic solution and develop a well-posedness theory that includes also an L^1-contraction property. In comparison to the first-order case (Debussche and Vovelle, 2010) and to the semilinear degenerate parabolic

case (Hofmanová, 2013), the present result contains two new ingredients: a generalized Itô formula that permits a rigorous derivation of the kinetic formulation even in the case of weak solutions of certain nondegenerate approximations and a direct proof of strong convergence of these approximations to the desired kinetic solution of the degenerate problem.

4.1.38. An integral inequality for the invariant measure of a stochastic reaction-diffusion equation

In [19], 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 H.

4.1.39. Large deviations for the two-dimensional stochastic Navier-Stokes equation with vanishing noise correlation

In [36], we are dealing with the validity of a large deviation principle for the two-dimensional Navier-Stokes equation, with periodic boundary conditions, 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 ε and $\delta(\varepsilon)$, respectively, with $0 < \varepsilon, \delta(\varepsilon) << 1$. Depending on the relationship between ε and $\delta(\varepsilon)$ we will prove the validity of the large deviation principle in different functional spaces.

4.1.40. Quasilinear generalized parabolic Anderson model

In [33], we provide a local in time well-posedness result for a quasilinear generalized parabolic Anderson model in dimension two $\partial_t u = a(u)\Delta u + g(u)\xi$. The key idea of our approach is a simple transformation of the equation which allows to treat the problem as a semilinear problem. The analysis is done within the setting of paracontrolled calculus.

4.1.41. The Schrödinger equation with spatial white noise potential

In [44], we consider the linear and nonlinear Schrödinger equation with a spatial white noise as a potential in dimension 2. We prove existence and uniqueness of solutions thanks to a change of unknown used by Hairer and Labbé (2015) and conserved quantities.

5. Partnerships and Cooperations

5.1. National Initiatives

5.1.1. ANR MOONRISE: 2015-2019

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

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.

5.1.2. 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.

5.1.3. 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 2015 and will end in august 2016.

5.2. European Initiatives

5.2.1. FP7 & H2020 Projects

Project acronym: GEOPARDI

Program: FP7

Project title: Numerical integration of Geometric Partial Differential Equations

Duration: September 2011 - August 2016

Coordinator: Erwan Faou, Inria

Abstract: The goal of this project is to develop new numerical methods for the approximation of evolution equations possessing strong geometric properties such as Hamiltonian systems or stochastic differential equations. In such situations the exact solutions endow with many physical properties that are consequences of the geometric structure: Preservation of the total energy, momentum conservation or existence of ergodic invariant measures. However the preservation of such qualitative properties of the original system by numerical methods at a reasonable cost is not guaranteed at all, even for very precise (high order) methods. The principal aim of geometric numerical integration is the understanding and analysis of such problems: How (and to which extend) reproduce qualitative behavior of differential equations over long time? The extension of this theory to partial differential equations is a fundamental ongoing challenge, which require the invention of a new mathematical framework bridging the most recent techniques used in the theory of nonlinear PDEs and stochastic ordinary and partial differential equations. The development of new efficient numerical schemes for geometric PDEs has to go together with the most recent progress in analysis (stability phenomena, energy transfers, multiscale problems, etc..) The major challenges of the project are to derive new schemes by bridging the world of numerical simulation and the analysis community, and to consider deterministic and stochastic equations, with a general aim at deriving hybrid methods. We also aim to create a research platform devoted to extensive numerical simulations of difficult academic PDEs in order to highlight new nonlinear phenomena and test numerical methods.

Erwan Faou was the principal investigator of the ERC Starting Grant Project Geopardi (2011-2016).

Between 2011 and 2016, Erwan Faou was the principal investigator of this ERC Starting grant project. This research project is centered on the numerical simulation of geometric evolution partial differential equations (PDEs). Typical examples are given by Hamiltonian Partial Differential Equations (PDE) such as wave equations in nonlinear propagations problems, Schrödinger equations in quantum mechanics, or Vlasov equations in plasma physics. The main goals of the project can be summarized as follows:

- Analyze numerical schemes for Hamiltonian PDEs and stochastic differential equations as mathematical objects in their own right, and study their global behavior (invariant preservation, ergodicity with respect to some invariant measure, averaging properties, scattering, etc...)
- Develop new numerical methods in connection with the most recent advances in the theoretical studies, and devoted to specific situations (high frequency computations, stochastic and hybrid methods, Vlasov and Euler equations). In particular, an important objective is the analysis of the long time behavior of these equations.

The main originality of the Geopardi project is the combination of rigorous nonlinear analysis, numerical analysis and numerical simulations, as well as its hybrid nature mixing deterministic and stochastic problems. The project has an excellent international visibility. The participants have been invited in many conferences to present their works in the last year (Scicade 13 & 15, Numdiff 13, workhops in Toronto, Harvard, IHES, Oberwolfach or Luminy, etc..). The research outcomes are published in high level international journals such as J. Amer. Math. Soc., Numer. Math., SIAM J. Numer. Anal. or Math. Comp. The project has also been used to invite collaborators and researcher to visit Inria. In particular, E. Faou organized with T. Lelièvre and J. Erhel in september 2013 the NASPDE conference whose main topic is the numerical simulation of stochastic PDEs, and that was mainly funded by the Geopardi project.

5.2.2. Collaborations in European Programs, Except FP7 & H2020

Project acronym: WPENR

Program: EUROFusion Enabling Research project ER15-IPP-01

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

Duration: January 2015 - December 2018

Coordinator: Eric Sonnenndrücker (Max-Planck-Institut für Plasmaphysik (IPP), Germany)

Other partners: IPP (Germany), EPFL (Switzerland), CEA-Cadarache (France), university of Strasbourg, Toulouse, Marseille, Paris 6 (France).

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.

5.3. International Research Visitors

5.3.1. Visits of International Scientists

- Philippe Chartier and Nicolas Crouseilles invited Eric Sonnendrücker (IPP Max Planck) for one week in june 2016.
- Nicolas Crouseilles and Mohammed Lemou invited Shi Jin and Liu Liu (university of Wisconsin) for two weeks in june 2016.
- Arnaud Debussche invited Martina Hofmanova (TU Berlin) for one week in november 2016.
- Erwan Faou invited Chuchu Chen (Michigan state university) for two weeks in november 2016.

5.3.2. Visits to International Teams

5.3.2.1. Research Stays Abroad

- Philippe Chartier was invited for a one-week working visit by Gilles Vilmart, university of Geneva (Switzerland).
- Nicolas Crouseilles was invited for a one-week working visit by Gilles Vilmart, university of Geneva (Switzerland).
- Arnaud Debussche was invited at SNS Pisa (Italy) for two periods of one week in april and november 2016.
- Erwan Faou was invited in the university of Trondheim (Norway) in october 2016.

6. Dissemination

6.1. Promoting Scientific Activities

6.1.1. Scientific Events Organisation

6.1.1.1. Member of the Organizing Committees

- François Castella and Philippe Chartier organized the workshop "Multiscale methods for Schödinger and kinetic equations", Saint-Malo (France), december 12-14, 2016.
- Arnaud Debussche organized the conference "Stochastic Partial Differential Equations and Applications-X, Levico Terme (Italy), may 30-june 4, 2016.
- Erwan Faou organized the workshop "Geometric Numerical Integration", Oberwolfach (Germany), march 20-26, 2016. Co-organized with E. Hairer, M. Hochbruck and C. Lubich.

6.1.2. Journal

6.1.2.1. Member of the Editorial Boards

- Philippe Chartier is member of the editorial board of "Mathematical Modelling and Numerical Analysis" (2007-).
- Arnaud Debussche is editor in chief of the journal "Stochastics and Partial Differential Equations: analysis and computations".
- Arnaud Debussche is member of the editorial board of Potential Analysis (2011-).
- Arnaud Debussche is member of the editorial board of Differential and Integral Equations (2002-).
- Arnaud Debussche is member of the editorial board of ESAIM:PROC (2012-).
- Arnaud Debussche is member of the editorial board of Journal of Evolution Equation (2014-).
- Arnaud Debussche is member of the editorial board of Applied Mathematics & Optimization (2014-).
- Arnaud Debussche is member of the editorial board of the collection : "Mathématiques & Applications" (Springer).
- Erwan Faou was editor of the Oberwolfach reports [31] (2016).

6.1.2.2. Reviewer - Reviewing Activities

Members of IPSO are reviewers for almost the journals in which they publish.

6.1.3. Invited Talks

- Philippe Chartier was invited speaker at the workshop "Mould calculus, from multiple zeta values to B-series", Pau (France), december 1-2, 2016.
- Philippe Chartier was plenary speaker at the international conference ICNAAM, Rhodes (Greece), september 2016.
- Philippe Chartier was invited speaker at the workshop "GAMPP", IPP Garching (Germany), september 12-16, 2016.
- Philippe Chartier was invited speaker at the workshop "Stability and discretization issues in differential equations", Trieste (Italy), june 2016.
- Philippe Chartier gave a seminar at the university of Lille (France), june 9, 2016.
- Philippe Chartier was invited speaker at Meeting ANR Moonrise, Toulouse (France), june 2-3, 2016.
- Philippe Chartier gave a seminar at the university of Geneva (Switzerland), may 26-june 1, 2016.
- Philippe Chartier was invited at the workshop "Geometric Numerical Integration", Oberwolfach (Germany), march 20-26, 2016.
- Nicolas Crouseilles was invited at the workshop "Geometric Numerical Integration", Oberwolfach (Germany), march 20-26, 2016.
- Nicolas Crouseilles gave a seminar at the university of Geneva (Switzerland), may 13, 2016.
- Nicolas Crouseilles gave a seminar at the university of Paris Sud, Orsay (France), november 17, 2016.
- Nicolas Crouseilles was invited speaker at the workshop "NumKin", Strasbourg (France), october 17-21, 2016.
- Nicolas Crouseilles was invited speaker at the workshop "Kinet", Madison (US), april 21-25, 2016.
- Arnaud Debussche was invited speaker at the workshop "Probabilistic models-from discrete to continuous", university of Warwick (UK), march 29-april 2, 2016.
- Arnaud Debussche was invited speaker at the workshop "Stochastic Analysis and Related Fields", Humboldt university Berlin (Germany), july 28-30, 2016.

- Arnaud Debussche was invited speaker at the workshop "Nonlinear Wave and Dispersive Equations", Kyoto university (Japan), september 6-8, 2016.
- Arnaud Debussche was invited speaker at the workshop "Nonlinear Stochastic Evolution Equations: Analysis and Numerics", TU Berlin (Germany), november 3-5, 2016.
- Erwan Faou gave a seminar at the CERMICS, Marne-La-Vallée (France), december 2016.
- Erwan Faou was invited at the workshop "Structure and scaling in computational field theories", Oslo (Norway), november 2016.
- Erwan Faou was invited at the conference "Nonlinear waves", IHES (France), may 2016.
- Erwan Faou was invited at the workshop "Nonlinear Evolution Problems", Oberwolfach (Germany), march 2016.
- Erwan Faou was invited at the workshop "Recent trends in nonlinear evolution equations", CIRM-Luminy (France), april 4-8, 2016.
- Mohammed Lemou was plenary speaker at the workshop "Asymptotic behavior of systems of PDE arising in physics and biology: theoretical and numerical points of view", Lille (France), june 2016.
- Mohammed Lemou was invited speaker at the workshop "NumKin", Strasbourg (France), october 17-21, 2016.
- Mohammed Lemou was invited speaker at the workshop "Kinet", Madison (US), april 21-25, 2016.
- Mohammed Lemou was invited speaker at the ANR Moonrise Meeting, Toulouse (France), june 2016.
- Florian Méhats was plenary speaker at the workshop "Journée des jeunes EDPistes français", Bordeaux (France).
- Florian Méhats gave a seminar of the university of Paris Sud, Orsay (France).
- Florian Méhats gave a seminar of the university of Nice (France).
- Florian Méhats gave a seminar of the university of Lille (France).

6.1.4. Scientific Expertise

- Philippe Chartier was member of the hiring committee of an associate professor, university of Trondheim (Norway).
- Philippe Chartier was member of the hiring committee CR2-Inria (Bordeaux).
- Nicolas Crouseilles was member of the CORDI-S committee at Inria-Rennes.
- Arnaud Debussche was a member of the hiring committee of a professor, university of Rennes 1
- Arnaud Debussche was a member of the hiring committee of a "Maître de conférence", university of Orléans.
- Mohammed Lemou was member of the hiring committee of a professor, university of Rennes 1.
- Mohammed Lemou was was a member of the hiring committee of a "Maître de conférence", university of Nantes.

6.1.5. Research Administration

- François Castella is member of the IRMAR laboratory council.
- Philippe Chartier is the vice-head of science (DSA) of the Rennes Inria-Center.
- Philippe Chartier is member of the direction committee (ED) of the Rennes Inria-Center.
- Philippe Chartier is member of the national evaluation committee (CE) of Inria.
- Nicolas Crouseilles is member of the Scientific Council of the ENS Rennes.
- Nicolas Crouseilles is member of the committee of the Fédération de Fusion".
- Arnaud Debussche is vice president in charge of research and international relations of the Ecole Normale Supérieure de Rennes.

- Arnaud Debussche is member of the executive board of the Lebesgue Center.
- Arnaud Debussche is director of the "Agence Lebesgue de Mathématiques pour l'Innovation".
- Erwan Faou was member of the COST-GTRI (Comité d'orientation scientifique et technologique, groupe de travail pour les relations internationales) at Inria.
- Erwan Faou is member of the Scientific Council of the Pôle Universitaire Léonard de Vinci.
- Erwan Faou is member of the CNU 26.
- Mohammed Lemou is member of the Scientific Council of the ENS Rennes.
- Mohammed Lemou is member of the Scientific Council of the Lebesgue Center.
- Mohammed Lemou is head of the team "analyse numérique" of IRMAR laboratory.
- Florian Méhats is head of the IRMAR laboratory.

6.2. Teaching - Supervision - Juries

6.2.1. Teaching

- François Castella gave a course in M1 on kinetic equations, university of Rennes 1 (60 hours).
- Philippe Chartier gave a course in L3 on ordinary differential equations, Ecole Normale Supérieure de Rennes (24 hours).
- Philippe Chartier gave a course in M2 on geometric numerical integration and averaging methods, university of Rennes 1 (24 hours).
- Nicolas Crouseilles gave a course in M2 on numerical methods for kinetic equations, university of Rennes 1 (12 hours).
- Arnaud Debussche gave a course in M2 on stochastic partial differential equations, university of Rennes 1 (24 hours).
- Erwan Faou gave a course in M1 on modelisation and numerical analysis of PDEs, ENS Paris, in collaboration with E. Dormy.
- Mohammed Lemou gave a course in M2 on partial differential equations, university of Rennes 1 (24 hours).
- Mohammed Lemou is head of the M2 "Analyse et Applications".

6.2.2. Supervision

- François Castella supervises the PhD thesis of Valentin Doli, *Mathematical and ecological study of the propagation of a specific virus attacking plants*, (2014-). Co-advisor: Frédéric Hamelin (Agro-Rennes).
- François Castella and Philippe Chartier supervised the PhD thesis of Julie Sauzeau, *Highly-oscillatory central manifold and application to ecology* (2013-2016). Julie Sauzeau is now teacher.
- Nicolas Crouseilles and Erwan Faou supervise the PhD thesis of Joackim Bernier, *Mathematical and numerical anaysis of nonlinear transport equations*, (2016-).
- Nicolas Crouseilles and Mohammed Lemou supervised the PhD thesis of Hélène Hivert *Mathematical and numerical study of kinetic model and their asymptotics: diffusion and anomalous diffusion limit*, (2013-2016). Hélène Hivert is now post-doc at ENS Lyon.
- Erwan Faou supervises the PhD thesis of Romain Horsin, *Mathematical and numerical analysis of the Vlasov-HMF model*, (2014-). Co-advisor: Frédéric Rousset (university Paris Sud Orsay).
- Arnaud Debussche supervizes the PhD thesis of Mac Jugal Nankep *PDMP with spatial dependency for the dynamics of gene networks*, (2014-).
- Arnaud Debussche and Florian Méhats are supervisors of the PhD thesis of Maxime Tusseau. *Highly oscillatory nonlinear Schrödinger equation with stochastic potential*, (2013-).

- Mohammed Lemou and Florian Méhats are supervisors of the PhD thesis of Marine Malo *Collisionless kinetic equations: stability, oscillations*, (2015-).

6.2.3. Juries

- Erwan Faou was referee of the PhD thesis of Ahmed-Amine Homman (CEA and ENPC), june 2016.
- Nicolas Crouseilles was referee of the PhD thesis of Mehdi Badsi (university Paris 6), october 2016.
- Nicolas Crouseilles was referee of the PhD thesis of Nhung Pham (university of Strasbourg), december 2016.
- Nicolas Crouseilles was member of the jury of the PhD thesis of Julie Sauzeau (university of Rennes 1), june 2016.
- Arnaud Debussche was referee of the PhD thesis of Nathalie Ayi (university of Nice), june 2016.
- Arnaud Debussche was member of jury of the PhD thesis of Vincent Renault (university of Paris 6), september 2016.
- Mohammed Lemou was referee of the PhD thesis of Thomas Le Roy (university Paris 6), january 2016.
- Mohammed Lemou was referee of the PhD thesis of Ankit Ruhi (IIS, Bangalore, India), december 2016.
- Mohammed Lemou was member of the jury of the PhD thesis of Sébastien Guisset (university of Bordeaux 1), september 2016.

7. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

[1] S. BALAC, A. FERNANDEZ, F. MAHÉ, F. MÉHATS, R. TEXIER-PICARD. *The Interaction Picture method for solving the generalized nonlinear Schrödinger equation in optics*, in "ESAIM: Mathematical Modelling and Numerical Analysis", June 2016, vol. 50, n^{o} 4, pp. 945-964 [*DOI :* 10.1051/M2AN/2015060], https://hal.archives-ouvertes.fr/hal-00850518

[2] V. BANICA, E. FAOU, E. MIOT. *Collision of almost parallel vortex filaments*, in "Communications on Pure and Applied Mathematics", 2017, vol. 70, n^{o} 2, pp. 378-405 [*DOI :* 10.1002/CPA.21637], https://hal.archives-ouvertes.fr/hal-01170929

[3] W. BAO, L. LE TREUST, F. MÉHATS. *Dimension reduction for dipolar Bose-Einstein condensates in the strong interaction regime*, in "Kinetic and Related Models ", September 2017, https://hal.archives-ouvertes.fr/hal-01101793

[4] A. BOUILLARD, E. FAOU, M. ZAVIDOVIQUE. *Fast Weak-Kam Integrators for separable Hamiltonian systems*, in "Mathematics of Computation", 2016, vol. 85, n^{o} 297, pp. 85-117, https://hal.archives-ouvertes.fr/hal-00743462

[5] F. CASAS, N. CROUSEILLES, E. FAOU, M. MEHRENBERGER. *High-order Hamiltonian splitting for Vlasov-Poisson equations*, in "Numerische Mathematik", 2016, https://hal.inria.fr/hal-01206164

[6] F. CASTELLA, S. MADEC, Y. LAGADEUC. *Global behavior of N competing species with strong diffusion: diffusion leads to exclusion*, in "Applicable Analysis", 2016, vol. 95, n^{o} 2, pp. 341-372 [*DOI :* 10.1080/00036811.2015.1004320], https://hal.archives-ouvertes.fr/hal-01026195

[7] P. CHARTIER, N. J. MAUSER, F. MÉHATS, Y. ZHANG. *Solving highly-oscillatory NLS with SAM: numerical efficiency and geometric properties*, in "Discrete and Continuous Dynamical Systems - Series S", October 2016, vol. 9, n^{o} 5, pp. 1327-1349 [*DOI :* 10.3934/DCDSS.2016053], https://hal.archives-ouvertes.fr/hal-00850513

[8] P. CHARTIER, F. MÉHATS, M. THALHAMMER, Y. ZHANG. *Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations*, in "Mathematics of Computation", 2016, vol. 85, n^{o} 302, pp. 2863-2885 [*DOI :* 10.1090/MCOM/3088], https://hal.archives-ouvertes.fr/hal-01373280

[9] A. CHERNOV, A. DEBUSSCHE, F. NOBILE. *Numerical methods for random and stochastic partial differential equations*, in "Stochastics and Partial Differential Equations Analysis and Computations", March 2016, vol. 4, n^{o} 1, pp. 1-2 [*DOI :* 10.1007/s40072-016-0073-2], https://hal.archives-ouvertes.fr/hal-01297401

[10] P. J. COELHO, N. CROUSEILLES, P. PEREIRA, M. ROGER. *Multi-scale methods for the solution of the radiative transfer equation*, in "Journal of Quantitative Spectroscopy and Radiative Transfer", March 2016, vol. 172, pp. 36-49 [*DOI :* 10.1016/J.JQSRT.2015.10.001], https://hal.archives-ouvertes.fr/hal-01274991

[11] N. CROUSEILLES, G. DIMARCO, M. LEMOU. *Asymptotic preserving and time diminishing schemes for rarefied gas dynamic*, in "Kinetic and Related Models ", 2016, https://hal.inria.fr/hal-01392412

[12] N. CROUSEILLES, G. DIMARCO, M.-H. VIGNAL. *Multiscale schemes for the BGK-Vlasov-Poisson system in the quasi-neutral and fluid limits. Stability analysis and first order schemes*, in "Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal", 2016, vol. 14, n^{o} 1, pp. 65-95 [*DOI :* 10.1137/140991558], https://hal.inria.fr/hal-01090676

[13] N. CROUSEILLES, L. EINKEMMER, E. FAOU. *An asymptotic preserving scheme for the relativistic Vlasov–Maxwell equations in the classical limit*, in "Computer Physics Communications", December 2016, vol. 209, https://hal.inria.fr/hal-01283779

[14] N. CROUSEILLES, H. HIVERT, M. LEMOU. *Numerical schemes for kinetic equations in the anomalous diffusion limit. Part II: degenerate collision frequency.* , in "SIAM Journal on Scientific Computing", 2016, vol. 38, n^{o} 4, https://hal.inria.fr/hal-01245312

[15] N. CROUSEILLES, H. HIVERT, M. LEMOU. *Numerical schemes for kinetic equations in the diffusion and anomalous diffusion limits. Part I: the case of heavy-tailed equilibrium*, in "SIAM J. Sci. Comput.", 2016, vol. 38, n^{o} 2, pp. 737-764, https://hal.inria.fr/hal-01130002

[16] N. CROUSEILLES, M. LEMOU, F. MÉHATS, X. ZHAO. *Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equations*, in "Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal", 2017, https://hal.inria.fr/hal-01286947

[17] N. CROUSEILLES, M. LEMOU, S. RAGHURAMA RAO, A. RUHI, M. SEKHAR. *Asymptotic Preserving scheme for a kinetic model describing incompressible fluids*, in "Kinetic and Related Models ", 2016, vol. 9, pp. 51-74, https://hal.inria.fr/hal-01090677

[18] N. CROUSEILLES, M. LEMOU, G. VILMART. *Asymptotic Preserving numerical schemes for multiscale parabolic problems*, in "Comptes Rendus Mathématique", 2016, vol. 354, n^{o} 3, pp. 271-276, 7 pages [*DOI :* 10.1016/J.CRMA.2015.11.010], https://hal.archives-ouvertes.fr/hal-01187092

[19] G. DA PRATO, A. DEBUSSCHE. *An integral inequality for the invariant measure of a stochastic reaction–diffusion equation*, in "Journal of Evolution Equations", 2016, pp. 1-18 [*DOI :* 10.1007/s00028-016-0349-z], https://hal.archives-ouvertes.fr/hal-01235038

[20] G. DA PRATO, A. DEBUSSCHE. *Estimate for P_tD for the stochastic Burgers equation*, in "Annales de l'Institut Henri Poincaré (B) Probabilités et Statistiques", 2016, vol. 52, n° 3, pp. 1248-1258 [*DOI :* 10.1214/15-AIHP685], https://hal.archives-ouvertes.fr/hal-01110454

[21] A. DEBUSSCHE, S. DE MOOR, J. VOVELLE. *Diffusion limit for the radiative transfer equation perturbed by a Markovian process*, in "Asymptotic Analysis", 2016, vol. 98, n° 1-2, pp. 31-58, 24 pages. arXiv admin note: text overlap with arXiv:1311.4743 [*DOI :* 10.3233/ASY-161360], https://hal.archives-ouvertes.fr/hal-01044426

[22] A. DEBUSSCHE, M. HOFMANOVÁ, J. VOVELLE. *Degenerate Parabolic Stochastic Partial Differential Equations: Quasilinear case*, in "The Annals of Probability", 2016, vol. 44, n° 3, pp. 1916-1955 [*DOI :* 10.1214/15-AOP1013], https://hal.archives-ouvertes.fr/hal-00863829

[23] E. FAOU, P. GERMAIN, Z. HANI. *The weakly nonlinear large-box limit of the 2D cubic nonlinear Schrödinger equation*, in "Journal of the American Mathematical Society", 2016, vol. 29, n° 4, pp. 915-982, 68 pages, 1 figure [*DOI :* 10.1090/JAMS/845], https://hal.archives-ouvertes.fr/hal-00905851

[24] E. FAOU, R. HORSIN, F. ROUSSET. *On numerical Landau damping for splitting methods applied to the Vlasov-HMF model*, in "Foundations of Computational Mathematics", 2016, 38 p. [*DOI :* 10.1007/s10208-016-9333-9], https://hal.archives-ouvertes.fr/hal-01219115

[25] E. FAOU, F. ROUSSET. *Landau damping in Sobolev spaces for the Vlasov-HMF model*, in "Archive for Rational Mechanics and Analysis", 2016, vol. 219, n° 2, pp. 887-902 [*DOI :* 10.1007/s00205-015-0911-9], https://hal.archives-ouvertes.fr/hal-00956595

[26] S. FOURNAIS, L. LE TREUST, N. RAYMOND, J. VAN SCHAFTINGEN. *Semiclassical Sobolev constants for the electro-magnetic Robin Laplacian*, in "Journal of the Mathematical Society of Japan", 2017, https://hal.archives-ouvertes.fr/hal-01285311

[27] F. M. HAMELIN, F. CASTELLA, V. DOLI, B. MARÇAIS, V. RAVIGNÉ, M. A. LEWIS. *Mate Finding, Sexual Spore Production, and the Spread of Fungal Plant Parasites*, in "Bulletin of Mathematical Biology", April 2016, vol. 78, n° 4, pp. 695-712 [*DOI :* 10.1007/s11538-016-0157-1], https://hal.archives-ouvertes.fr/hal-01313012

[28] M. LEMOU. *Extended Rearrangement inequalities and applications to some quantitative stability results*, in "Communications in Mathematical Physics", 2016, vol. 348, n° 2, pp. 695-727 [*DOI :* 10.1007/s00220-016-2750-4], https://hal.archives-ouvertes.fr/hal-01207621

[29] F. MÉHATS, C. SPARBER. *Dimension reduction for rotating Bose-Einstein condensates with anisotropic confinement*, in "Discrete and Continuous Dynamical Systems - Series A", 2016, vol. 36, n° 9, pp. 5097-5118, 22 pages [*DOI :* 10.3934/DCDS.2016021], https://hal.archives-ouvertes.fr/hal-01178431

Scientific Books (or Scientific Book chapters)

[30] M. CHAUSSADE-BEAUDOUIN, M. DAUGE, E. FAOU, Z. YOSIBASH. *High frequency oscillations of first eigenmodes in axisymmetric shells as the thickness tends to zero*, in "Operator Theory Advances and Application", Recent Trends in Operator Theory and Partial Differential Equations - The Roland Duduchava Anniversary Volume, Birkhäuser/Springer, 2017, vol. 258, pp. 89-110, https://hal.archives-ouvertes.fr/hal-01278861

Research Reports

[31] E. FAOU, E. HAIRER, M. HOCHBRUCK, C. LUBICH. *Geometric Numerical Integration*, Mathematisches Forschungsinstitut Oberwolfach, 2016, n^{o} 18/2016, pp. 869 - 948, Oberwolfach Reports, vol. 13 n° 1 (2016) [*DOI :* 10.4171/OWR/2016/18], https://hal.archives-ouvertes.fr/hal-01403326

Other Publications

[32] N. ARRIZABALAGA, L. LE TREUST, N. RAYMOND. *On the MIT bag model: self-adjointness and non-relativistic limit*, July 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01343717

[33] I. BAILLEUL, A. DEBUSSCHE, M. HOFMANOVA. *Quasilinear generalized parabolic Anderson model*, 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01389489

[34] S. BAUMSTARK, E. FAOU, K. SCHRATZ. *Uniformly accurate exponential-type integrators for klein-gordon equations with asymptotic convergence to classical splitting schemes in the nonlinear schroedinger limit*, June 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01331949

[35] F. CASTELLA, P. CHARTIER, J. SAUZEAU. *A formal series approach to the center manifold theorem*, April 2016, working paper or preprint, https://hal.inria.fr/hal-01279715

[36] S. CERRAI, A. DEBUSSCHE. *Large deviations for the two-dimensional stochastic Navier-Stokes equation with vanishing noise correlation*, 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01287049

[37] P. CHARTIER, N. CROUSEILLES, M. LEMOU. *An averaging technique for transport equations*, September 2016, working paper or preprint, https://hal.inria.fr/hal-01374655

[38] P. CHARTIER, N. CROUSEILLES, M. LEMOU. *Averaging of highly-oscillatory transport equations*, November 2016, working paper or preprint, https://hal.inria.fr/hal-01396685

[39] P. CHARTIER, L. LE TREUST, F. MÉHATS. *Uniformly accurate time-splitting methods for the semiclassical Schrödinger equationPart 2 : Numerical analysis of the linear case*, January 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01257753

[40] P. CHARTIER, M. LEMOU, F. MÉHATS. *Highly-oscillatory evolution equations with multiple frequencies: averaging and numerics*, October 2016, working paper or preprint, https://hal.inria.fr/hal-01281950

[41] M. CHAUSSADE-BEAUDOUIN, M. DAUGE, E. FAOU, Z. YOSIBASH. *Free Vibrations of Axisymmetric Shells: Parabolic and Elliptic cases*, January 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01264125

[42] N. CROUSEILLES, S. JIN, M. LEMOU. *Nonlinear Geometric Optics method based multi-scale numerical schemes for highly-oscillatory transport equations*, May 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01323721

[43] N. CROUSEILLES, M. LEMOU, F. MÉHATS, X. ZHAO. *Uniformly accurate Particle-In-Cell method for the long time two-dimensional Vlasov-Poisson equation with strong magnetic field*, December 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01418976

[44] A. DEBUSSCHE, H. WEBER. *The Schrödinger equation with spatial white noise potential*, 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01411205

[45] E. FAOU, T. JÉZÉQUEL. *Convergence of a normalized gradient algorithm for computing ground states*, March 2016, working paper or preprint, https://hal.inria.fr/hal-01284679

[46] R. L. FRANK, F. MÉHATS, C. SPARBER. *Averaging of nonlinear Schrödinger equations with strong magnetic confinement*, 2016, 12 pages, https://hal.archives-ouvertes.fr/hal-01397325

[47] M. LEMOU, F. MÉHATS, X. ZHAO. *Uniformly accurate numerical schemes for the nonlinear dirac equation in the nonrelativistic limit regime*, May 2016, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01313976

References in notes

[48] E. HAIRER. *Geometric integration of ordinary differential equations on manifolds*, in "BIT", 2001, vol. 41, pp. 996–1007

[49] E. HAIRER, C. LUBICH, G. WANNER. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, Second edition*, Springer Series in Computational Mathematics 31, Springer, Berlin, 2006

[50] E. HAIRER, G. WANNER. *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, Springer Series in Computational Mathematics 14, 2, Springer-Verlag, Berlin, 1996

[51] C. LUBICH. *A variational splitting integrator for quantum molecular dynamics*, in "Appl. Numer. Math.", 2004, vol. 48, pp. 355–368

[52] C. LUBICH. *On variational approximations in quantum molecular dynamics*, in "Mathematics of Computation", 2009

[53] J. M. SANZ-SERNA, M. P. CALVO. *Numerical Hamiltonian Problems*, Chapman & Hall, London, 1994