Activity Report 2013

Project-Team IPSO

Invariant Preserving SOlvers

Table of contents

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

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1. Members

Research Scientists

Philippe Chartier [Team leader, Inria, Senior Researcher, HdR]
Nicolas Crouseilles [Inria, Researcher, HdR]
Erwan Faou [Inria, Senior Researcher, HdR]
Mohammed Lemou [CNRS, Senior Researcher, HdR]

Faculty Members

François Castella [Univ. Rennes I, Professor, HdR]
Arnaud Debussche [ENS Cachan, Professor, HdR]
Florian Méhats [Univ. Rennes I, Professor, HdR]
Gilles Vilmart [ENS Cachan, Assistant Professor, HdR]

External Collaborator

Michel Crouzeix [Univ. Rennes I, until Jun 2013]

Engineer

Alexandre Boritchev [Inria, granted by FP7 ERC GEOPARDI project, from May 2013 until Jun 2013]

PhD Students

Helene Hivert [Univ. Rennes I, from Sep 2013]
Marie Kopec [Inria, granted by FP7 ERC GEOPARDI project]
Guillaume Leboucher [Univ. Rennes I]
Julie Sauzeau [Univ. Rennes I, from Sep 2013]
Maxime Tusseau [ENS Cachan, from Sep 2013]

Post-Doctoral Fellows

Tiphaine Jezequel [Inria, granted by FP7 ERC GEOPARDI project]
Loïc Letreust [LODIQUAS-IRMAR, from Sep 2013]
Katharina Schratz [Inria, granted by FP7 ERC GEOPARDI project, until Aug 2013]

Administrative Assistant

Cécile Bouton [Inria]

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 [67], [64], [63] and led to many significant theoretical achievements (symplectic and symmetric methods, volume-preserving integrators, Lie-group methods, ...). In practice, a few simple schemes such as the Verlet method or the Störmer method have been used for years with great success in molecular dynamics or astronomy. However, they now need to be further improved in order to fit the tremendous increase of complexity and size of the models.

2.2. Overall objectives

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

- systems of differential equations posed on a manifold.

- systems of differential-algebraic equations of index 2 or 3, where the constraints are part of the equations.

- Hamiltonian systems and constrained Hamiltonian systems (which are special cases of the first two items though with some additional structure).

- highly-oscillatory systems (with a special focus of those resulting from the Schrödinger equation).

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

- There is a large demand in biomolecular modeling for models that integrate microscopic molecular dynamics simulation into statistical macroscopic quantities. These simulations involve huge systems of ordinary differential equations over very long time intervals. This is a typical situation where the determination of accurate trajectories is out of reach and where one has to rely on the good qualitative behavior of structure-preserving integrators. Due to the complexity of the problem, more efficient numerical schemes need to be developed.

- The demand for new models and/or new structure-preserving schemes is also quite large in laser simulations. The propagation of lasers induces, in most practical cases, several well-separated scales: the intrinsically highly-oscillatory *waves* travel over long distances. In this situation, filtering the oscillations in order to capture the long-term trend is what is required by physicists and engineers.

2.3. Highlights of the Year

- A. Debussche was the main organizer of the thematic semester "Perspectives in Analysis and Probability" organized by the Lebesgue Center in Nantes and Rennes from april to september 2013 (see: http://www.lebesgue.fr/content/sem2013-perspectives-analysis-and-probability).
- E. Faou received the Blaise Pascal prize (GAMNI/SMAI and French Academy of Sciences).
- G. Vilmart defended his Habilitation to supervise research (HDR) in Mathematics, [12], July.
- G. Vilmart receives the "Prix Bretagne Jeune Chercheur 2013" from the Region Bretagne, December.

3. Research Program

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

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

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

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

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

For a given y_0, the solution $y(t)$ at time t is denoted $\varphi_t(y_0)$. For fixed t, 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 [62] 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:

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

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

$$J = \left[\begin{array}{cc} 0 & I_d \\ -I_d & 0 \end{array} \right].$$

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

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

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

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

and of the so-called hidden manifold

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

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

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

3.2. Highly-oscillatory systems

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

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

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

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

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

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, Gilles Vilmart.

Schrödinger equation, variational splitting, energy conservation.

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

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

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

where $\psi = \psi(x, t)$ is the wave function depending on the spatial variables $x = (x_1, \cdots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, 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 [66], [65] 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. Application Domains

4.1. Laser physics

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

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

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

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

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

4.2. Molecular Dynamics

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

4.3. Plasma physics

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

5. New Results

5.1. Multi-revolution composition methods for highly oscillatory differential equations

In [45], we introduce a new class of multi-revolution composition methods (MRCM) for the approximation of the Nth-iterate of a given near-identity map. When applied to the numerical integration of highly oscillatory systems of differential equations, the technique benefits from the properties of standard composition methods: it is intrinsically geometric and well-suited for Hamiltonian or divergence-free equations for instance. We prove error estimates with error constants that are independent of the oscillatory frequency. Numerical experiments, in particular for the nonlinear Schrödinger equation, illustrate the theoretical results, as well as the efficiency and versatility of the methods.

5.2. Weak second order multi-revolution composition methods for highly oscillatory stochastic differential equations with additive or multiplicative noise

In [61], we introduce a class of numerical methods for highly oscillatory systems of stochastic differential equations with general noncommutative noise. We prove global weak error bounds of order two uniformly with respect to the stiffness of the oscillations, which permits to use large time steps. The approach is based on the micro-macro framework of multi-revolution composition methods recently introduced for deterministic problems and inherits its geometric features, in particular to design integrators preserving exactly quadratic first integral. Numerical experiments, including the stochastic nonlinear Schrödinger equation with space-time multiplicative noise, illustrate the performance and versatility of the approach.

5.3. High order numerical approximation of the invariant measure of ergodic SDEs

In [41], we introduce new sufficient conditions for a numerical method to approximate with high order of accuracy the invariant measure of an ergodic system of stochastic differential equations, independently of the weak order of accuracy of the method. We then present a systematic procedure based on the framework of modified differential equations for the construction of stochastic integrators that capture the invariant measure of a wide class of ergodic SDEs (Brownian and Langevin dynamics) with an accuracy independent of the weak order of the underlying method. Numerical experiments confirm our theoretical findings.

5.4. PIROCK: a swiss-knife partitioned implicit-explicit orthogonal Runge-Kutta Chebyshev integrator for stiff diffusion-advection-reaction problems with or without noise

In [13], a partitioned implicit-explicit orthogonal Runge-Kutta method (PIROCK) is proposed for the time integration of diffusion-advection-reaction problems with possibly severely stiff reaction terms and stiff stochastic terms. The diffusion terms are solved by the explicit second order orthogonal Chebyshev method (ROCK2), while the stiff reaction terms (solved implicitly) and the advection and noise terms (solved explicitly) are integrated in the algorithm as finishing procedures. It is shown that the various coupling (between diffusion, reaction, advection and noise) can be stabilized in the PIROCK method. The method, implemented in a single black-box code that is fully adaptive, provides error estimators for the various terms present in the problem, and requires from the user solely the right-hand side of the differential equation. Numerical experiments and comparisons with existing Chebyshev methods, IMEX methods and partitioned methods show the efficiency and flexibility of our new algorithm.

5.5. An offline-online homogenization strategy to solve quasilinear two-scale problems at the cost of one-scale problems

In [39], inspired by recent analyses of the finite element heterogeneous multiscale method and the reduced basis technique for nonlinear problems, we present a simple and concise finite element algorithm for the reliable and efficient resolution of elliptic or parabolic multiscale problems of nonmonotone type. Solutions of appropriate cell problems on sampling domains are selected by a greedy algorithm in an offline stage and assembled in a reduced basis (RB). This RB is then used in an online stage to solve two-scale problems at a computational cost comparable to the single-scale case. Both the offline and the online cost are independent of the smallest scale in the physical problem. The performance and accuracy of the algorithm are illustrated on 2D and 3D stationary and evolutionary nonlinear multiscale problems.

5.6. Reduced basis finite element heterogeneous multiscale method for quasilinear elliptic homogenization problems

In [40], a reduced basis nite element heterogeneous multiscale method (RB-FE-HMM) for a class of nonlinear homogenization elliptic problems of nonmonotone type is introduced. In this approach, the solutions of the micro problems needed to estimate the macroscopic data of the homogenized problem are selected by a Greedy algorithm and computed in an online stage. It is shown that the use of reduced basis (RB) for nonlinear numerical homogenization reduces considerably the computational cost of the nite element heterogeneous multiscale method (FE-HMM). As the precomputed microscopic functions depend nonlinearly on the macroscopic solution, we introduce a new a posteriori error estimator for the Greedy algorithm that guarantees the convergence of the online Newton method. A priori error estimates and uniqueness of the numerical solution are also established. Numerical experiments illustrate the e ciency of the proposed method.

5.7. Weak second order explicit stabilized methods for stiff stochastic differential equations

In [16], we introduce a new family of explicit integrators for stiff Itô stochastic differential equations (SDEs) of weak order two. These numerical methods belong to the class of one-step stabilized methods with extended stability domains and do not suffer from the stepsize reduction faced by standard explicit methods. The family is based on the standard second order orthogonal Runge-Kutta Chebyshev methods (ROCK2) for deterministic problems. The convergence, and the mean-square and asymptotic stability properties of the methods are analyzed. Numerical experiments, including applications to nonlinear SDEs and parabolic stochastic partial differential equations are presented and confirm the theoretical results.

5.8. Mean-square A-stable diagonally drift-implicit integrators of weak second order for stiff Itô stochastic differential equations

In [15], we introduce two drift-diagonally-implicit and derivative-free integrators for stiff systems of Itô stochastic differential equations with general non-commutative noise which have weak order 2 and deterministic order 2, 3, respectively. The methods are shown to be mean-square A-stable for the usual complex scalar linear test problem with multiplicative noise and improve significantly the stability properties of the drift-diagonally-implicit methods previously introduced [K. Debrabant and A. Rößler, Appl. Num. Math., 59, 2009].

5.9. Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field

In [25], we build a Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field. This consists in writing the solution of this equation as a sum of two oscillating functions with circonscribed oscillations. The first of these functions has a shape which is close to the shape of the Two-Scale limit of the solution and the second one is a correction built to offset this imposed shape. The aim of such a decomposition is to be the starting point for the construction of Two-Scale Asymptotic-Preserving Schemes.

5.10. A dynamic multi-scale model for transient radiative transfer calculations

In [33], a dynamic multi-scale model which couples the transient radiative transfer equation (RTE) and the diffusion equation (DE) is proposed and validated. It is based on a domain decomposition method where the system is divided into a mesoscopic subdomain, where the RTE is solved, and a macroscopic subdomain where the DE is solved. A buffer zone is introduced between the mesoscopic and the macroscopic subdomains, as proposed by Degond and Jin, who solve a coupled system of two equations, one at the mesoscopic and the other at the macroscopic scale. The DE and the RTE are coupled through the equations inside the buffer zone, instead of being coupled through a geometric interface like in standard domain decomposition methods. One main advantage is that no boundary or interface conditions are needed for the DE. The model is compared to Monte Carlo, finite volume and P1 solutions in one dimensional stationary and transient test cases, and presents promising results in terms of trade-off between accuracy and computational requirements.

5.11. Quasi-periodic solutions of the 2D Euler equation

In [24], we consider the two-dimensional Euler equation with periodic boundary conditions. We construct time quasi-periodic solutions of this equation made of localized travelling profiles with compact support propagating over a stationary state depending on only one variable. The direction of propagation is orthogonal to this variable, and the support is concentrated on flat strips of the stationary state. The frequencies of the solution are given by the locally constant velocities associated with the stationary state.

5.12. Optimization and parallelization of Emedge3D on shared memory architecture

In [38], a study of techniques used to speedup a scientific simulation code is presented. The techniques include sequential optimizations as well as the parallelization with OpenMP. This work is carried out on two different multicore shared memory architectures, namely a cutting edge 8x8 core CPU and a more common 2x6 core board. Our target application is representative of many memory bound codes, and the techniques we present show how to overcome the burden of the memory bandwidth limit, which is quickly reached on multi-core or many-core with shared memory architectures. To achieve efficient speedups, strategies are applied to lower the computation costs, and to maximize the use of processors caches. Optimizations are: minimizing memory accesses, simplifying and reordering computations, and tiling loops. On 12 cores processor Intel X5675, aggregation of these optimizations results in an execution time 21.6 faster, compared to the original version on one core.

5.13. Vlasov on GPU (VOG Project)

In [58], we are concerned with the numerical simulation of the Vlasov-Poisson set of equations using semi- Lagrangian methods on Graphical Processing Units (GPU). To accomplish this goal, modifications to traditional methods had to be implemented. First and foremost, a reformulation of semi-Lagrangian methods is performed, which enables us to rewrite the governing equations as a circulant matrix operating on the vector of unknowns. This product calculation can be performed efficiently using FFT routines. Second, to overcome the limitation of single precision inherent in GPU, a δf type method is adopted which only needs refinement in specialized areas of phase space but not throughout. Thus, a GPU Vlasov-Poisson solver can indeed perform high precision simulations (since it uses very high order reconstruction methods and a large number of grid points in phase space). We show results for rather academic test cases on Landau damping and also for physically relevant phenomena such as the bump on tail instability and the simulation of Kinetic Electrostatic Electron Nonlinear (KEEN) waves.

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

In [37], we are interested in the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called "Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. The method is based on two main ingredients. First, we embed our problem in a suitable "two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

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

In [26], we focus on the numerical simulation of the Wigner-Poisson-BGK equation in the diffusion asymptotics. Our strategy is based on a "micro-macro" decomposition, which leads to a system of equations that couple the macroscopic evolution (diffusion) to a microscopic kinetic contribution for the fluctuations. A semi-implicit discretization provides a numerical scheme which is stable with respect to the small parameter ε

(mean free path) and which possesses the following properties: (i) it enjoys the asymptotic preserving property in the diffusive limit; (ii) it recovers a standard discretization of the Wigner-Poisson equation in the collision-less regime. Numerical experiments confirm the good behaviour of the numerical scheme in both regimes. The case of a spatially dependent $\varepsilon(x)$ is also investigated.

5.16. Existence and stability of solitons for fully discrete approximations of the nonlinear Schrödinger equation

In [19], we study the long time behavior of a discrete approximation in time and space of the cubic nonlinear Schrödinger equation on the real line. More precisely, we consider a symplectic time splitting integrator applied to a discrete nonlinear Schrödinger equation with additional Dirichlet boundary conditions on a large interval. We give conditions ensuring the existence of a numerical soliton which is close in energy norm to the continuous soliton. Such result is valid under a CFL condition between the time and space stepsizes. Furthermore we prove that if the initial datum is symmetric and close to the continuous soliton, then the associated numerical solution remains close to the orbit of the continuous soliton for very long times.

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

In [32], we consider the Klein-Gordon equation in the non-relativistic limit regime, i.e. the speed of light c tending to infinity. We construct an asymptotic expansion for the solution with respect to the small parameter depending on the inverse of the square of the speed of light. As the first terms of this asymptotic can easily be simulated our approach allows us to construct numerical algorithms that are robust with respect to the large parameter c producing high oscillations in the exact solution.

5.18. Sobolev stability of plane wave solutions to the cubic nonlinear Schrödinger equation on a torus

In [31], it is shown that plane wave solutions to the cubic nonlinear Schrödinger equation on a torus behave orbitally stable under generic perturbations of the initial data that are small in a high-order Sobolev norm, over long times that extend to arbitrary negative powers of the smallness parameter. The perturbation stays small in the same Sobolev norm over such long times. The proof uses a Hamiltonian reduction and transformation and, alternatively, Birkhoff normal forms or modulated Fourier expansions in time.

5.19. Weak backward error analysis for overdamped Langevin equation

In [57], we consider an overdamped Langevin stochastic differential equation and show a weak backward error analysis result for its numerical approximations defined by implicit methods. In particular, we prove that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the implicit scheme considered is exponentially mixing.

5.20. Weak backward error analysis for Langevin equation

In [56], We consider numerical approximations of stochastic Langevin equations by implicit methods. We show a weak backward error analysis result in the sense that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the implicit scheme considered is exponentially mixing.

5.21. Approximation of the invariant law of SPDEs: error analysis using a Poisson equation for a full-discretization scheme

In [44], we study the long-time behavior of fully discretized semilinear SPDEs with additive space-time white noise, which admit a unique invariant probability measure μ. We show that the average of regular enough test functions with respect to the (possibly non unique) invariant laws of the approximations are close to the corresponding quantity for μ.

More precisely, we analyze the rate of the convergence with respect to the different discretization parameters. Here we focus on the discretization in time thanks to a scheme of Euler type, and on a Finite Element discretization in space.

The results rely on the use of a Poisson equation; we obtain that the rates of convergence for the invariant laws are given by the weak order of the discretization on finite time intervals: order $1/2$ with respect to the time-step and order 1 with respect to the mesh-size.

5.22. An asymptotic preserving scheme based on a new formulation for NLS in the semiclassical limit

In [20], we consider the semiclassical limit for the nonlinear Schrodinger equation. We introduce a phase/amplitude representation given by a system similar to the hydrodynamical formulation, whose novelty consists in including some asymptotically vanishing viscosity. We prove that the system is always locally well-posed in a class of Sobolev spaces, and globally well-posed for a fixed positive Planck constant in the one-dimensional case. We propose a second order numerical scheme which is asymptotic preserving. Before singularities appear in the limiting Euler equation, we recover the quadratic physical observables as well as the wave function with mesh size and time step independent of the Planck constant. This approach is also well suited to the linear Schrodinger equation.

5.23. Asymptotic Preserving schemes for highly oscillatory Vlasov-Poisson equations

The work [28] is devoted to the numerical simulation of a Vlasov-Poisson model describing a charged particle beam under the action of a rapidly oscillating external field. We construct an Asymptotic Preserving numerical scheme for this kinetic equation in the highly oscillatory limit. This scheme enables to simulate the problem without using any time step refinement technique. Moreover, since our numerical method is not based on the derivation of the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, and in the highly oscillatory regime as well. Our method is based on a "two scale" reformulation of the initial equation, with the introduction of an additional periodic variable.

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

The work [37] is devoted to the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called "Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. In the same spirit as in [28], the method is based on two main ingredients. First, we embed our problem in a suitable "two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of

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

5.25. On the controllability of quantum transport in an electronic nanostructure

In [59], we investigate the controllability of quantum electrons trapped in a two-dimensional device, typically a MOS field-effect transistor. The problem is modeled by the Schrödinger equation in a bounded domain coupled to the Poisson equation for the electrical potential. The controller acts on the system through the boundary condition on the potential, on a part of the boundary modeling the gate. We prove that, generically with respect to the shape of the domain and boundary conditions on the gate, the device is controllable. We also consider control properties of a more realistic nonlinear version of the device, taking into account the self-consistent electrostatic Poisson potential.

5.26. 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 involved 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 [42] 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.

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

In [46], we present the Stroboscopic Averaging Method (SAM), recently introduced in [7,8,10,12], 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).

5.28. Analysis of models for quantum transport of electrons in graphene layers

In [51], we present and analyze two mathematical models for the self consistent quantum transport of electrons in a graphene layer. We treat two situations. First, when the particles can move in all the plane R^2, the model takes the form of a system of massless Dirac equations coupled together by a selfconsistent potential, which is the trace in the plane of the graphene of the 3D Poisson potential associated to surface densities. In this case, we prove local in time existence and uniqueness of a solution in $H^s(R^2)$, for $s > 3/8$ which includes in particular the energy space $H^{1/2}(R^2)$. The main tools that enable to reach $s \in (3/8, 1/2)$ are the dispersive Strichartz estimates that we generalized here for mixed quantum states. Second, we consider a situation where the particles are constrained in a regular bounded domain Ω. In order to take into account Dirichlet boundary conditions which are not compatible with the Dirac Hamiltonian H_0, we propose a different model built on a modified Hamiltonian displaying the same energy band diagram as H_0 near the Dirac points. The well-posedness of the system in this case is proved in H^s_A, the domain of the fractional order Dirichlet Laplacian operator, for $1/2 \leq s$.

5.29. Analysis of a large number of Markov chains competing for transitions

In [18], we consider the behavior of a stochastic system composed of several identically distributed, but non independent, discrete-time absorbing Markov chains competing at each instant for a transition. The competition consists in determining at each instant, using a given probability distribution, the only Markov chain allowed to make a transition. We analyze the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyze the asymptotic behavior of the system for an arbitrary probability mass function governing the competition. We give conditions for the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed systems when the competition between the Markov chains is handled by using a geometric distribution.

5.30. Markov Chains Competing for Transitions: Application to Large-Scale Distributed Systems

In [17], we consider the behavior of a stochastic system composed of several identically distributed, but non independent, discrete-time absorbing Markov chains competing at each instant for a transition. The competition consists in determining at each instant, using a given probability distribution, the only Markov chain allowed to make a transition. We analyze the first time at which one of the Markov chains reaches its absorbing state. We obtain its distribution and its expectation and we propose an algorithm to compute these quantities. We also exhibit the asymptotic behavior of the system when the number of Markov chains goes to infinity. Actually, this problem comes from the analysis of large-scale distributed systems and we show how our results apply to this domain.

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

In [30], we prove three results on the existence of densities for the laws of finite dimensional functionals of the solutions of the stochastic Navier-Stokes equations in dimension 3. In particular, under very mild assumptions on the noise, we prove that finite dimensional projections of the solutions have densi- ties with respect to the Lebesgue measure which have some smoothness when measured in a Besov space. This is proved thanks to a new argument inspired by an idea introduced by N. Fournier and J. Printems.

5.32. Invariant measure of scalar first-order conservation laws with stochastic forcing

In [50], we assume an hypothesis of non-degeneracy of the flux and study the long-time behaviour of periodic scalar first-order conservation laws with stochastic forcing in any space dimension. For sub-cubic fluxes, we show the existence of an invariant measure. Moreover for sub-quadratic fluxes we show uniqueness and ergodicity of the invariant measure. Also, since this invariant measure is supported by L^p for some p small, we are led to generalize to the stochastic case the theory of L^1 solutions developed by Chen and Perthame.

5.33. Degenerate Parabolic Stochastic Partial Differential Equations: Quasilinear case

In [49], 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 previous works of the authors concerning stochastic hyperbolic conservation laws and semilinear degenerate parabolic SPDEs, the present result contains two new ingredients that provide simpler and more effective method of the proof: 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.

5.34. Existence of densities for stable-like driven SDE's with Hölder continuous coefficients

In [29], we consider a multidimensional stochastic differential equation driven by a stable-like Lévy process. We prove that the law of the solution immediately has a density in some Besov space, under some non-degeneracy condition on the driving Lévy process and some very light Hölder-continuity assumptions on the drift and diffusion coefficients.

5.35. Ergodicity results for the stochastic Navier-Stokes equations: an introduction

In the chapter [36], we give an overview of the results on ergodicity for the stochastic Navier-Stokes equations. We first explain the basis on SPDEs and on the concept of invariant measures and ergodicity. Then, in the 2D case, we introduce progressively the various methods, finishing with a celebrated result due to M. Hairer and J. Mattingly on ergodicity with very degenerated noises. In the 3D case, the theory is much less complete. Nonetheles, we show that it is possible to construct Markov evolutions and, under some non degenary assumptions on the noise, to obtain ergodicity.

5.36. Weak truncation error estimates for elliptic PDEs with lognormal coefficients

In [22], we are interested in the weak error committed on the solution of an elliptic partial differential equation with a lognormal coefficient, resulting from the approximation of the lognormal coefficient through a Karhunen-Loéve expansion. We improve results of a previous work, in which L^p-estimates of the weak error are provided. Only small enough values of p (the corresponding values of p depend on the space dimension) could be considered and such bounds are not sufficient to be applied to practical cases. Moreover, the optimality of this weak order (which turns out to be twice the strong order) has not been studied numerically. Therefore, the aim of this paper is double. First we improve drastically the weak error estimate by providing a bound of the C^1-norm of the weak error. This requires regularity results in Hölder spaces, with explicit bounds for the constants. We also consider much more general test functions in the definition of the weak error. Finally, we show the optimality of the weak order and illustrate this weak convergence with numerical results.

5.37. Optimized high-order splitting methods for some classes of parabolic equations

In [21], we are concerned with the numerical solution obtained by splitting methods of certain parabolic partial differential equations. Splitting schemes of order higher than two with real coefficients necessarily involve negative coefficients. It has been demonstrated that this second-order barrier can be overcome by using splitting methods with complex-valued coefficients (with positive real parts). In this way, methods of orders 3 to 14 by using the Suzuki-Yoshida triple (and quadruple) jump composition procedure have been explicitly built. Here we reconsider this technique and show that it is inherently bounded to order 14 and clearly sub-optimal with respect to error constants. As an alternative, we solve directly the algebraic equations arising from the order conditions and construct methods of orders 6 and 8 that are the most accurate ones available at present time, even when low accuracies are desired. We also show that, in the general case, 14 is not an order barrier for splitting methods with complex coefficients with positive real part by building explicitly a method of order 16 as a composition of methods of order 8.

5.38. Higher-Order Averaging, Formal Series and Numerical Integration III: Error Bounds

In earlier papers, it has been shown how formal series like those used nowadays to investigate the properties of numerical integrators may be used to construct high-order averaged systems or formal first integrals of Hamiltonian problems. With the new approach the averaged system (or the formal first integral) may be written down immediately in terms of (i) suitable basis functions and (ii) scalar coefficients that are computed via simple recursions. In [23], we show how the coefficients/basis functions approach may be used advantageously to derive exponentially small error bounds for averaged systems and approximate first integrals.

6. Partnerships and Cooperations

6.1. National Initiatives

6.1.1. ANR Programme blanc GYPSI: 2010-2014
Participant: Nicolas Crouseilles.

Leader: Ph. Gendrih.

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

6.1.2. ANR Programme blanc E2T2: 2010-2014
Participant: Nicolas Crouseilles.

Leader: P. Beyer

6.1.3. ANR Programme blanc STOSYMAP
Participant: Arnaud Debussche.

Leader: A. Shirikyan, The full description is available at http://shirikyan.u-cergy.fr/stosymap.html

6.2. European Initiatives

6.2.1. FP7 Projects

6.2.1.1. Geopardi

Title: Geometric Partial Differential Equations

Type: IDEAS ()

Instrument: ERC Starting Grant (Starting)

Duration: September 2011 - August 2016

Coordinator: Inria (France)

See also: http://www.irisa.fr/ipso/perso/faou/geopardi.html

Abstract: The goal is to develop new numerical methods for the approximation of evolution equations possessing strong geometric properties such as Hamiltonian systems or stochastic differential equations. Use intensive numerical simulations to discover and analyze new nonlinear phenomena.

6.2.2. Collaborations in European Programs, except FP7

ANR Programme blanc international (BLAN)

LODIQUAS 2012-2015

Low DImensional QUANtum Systems

Leaders: N. Mauser (Univ. Vienna) and F. Castella (IPSO).

Participants: François Castella, Philippe Chartier, Florian Me´hats, Mohammed Lemou.

Fundings for 4 postdocs (48 months) and one pre-doc (36 months).

The whole project involves the following researchers : Norbert Mauser (Vienna), Erich Gornik (Vienna), Mechthild Thalhammer (Innsbruck), Christoph Naegerl (Innsbruck), Jörg Schmiedmayer (Vienna), Hans-Peter Stimming (Vienna). François Castella (IPSO), Florian Méhats (IPSO), Francis Nier (Rennes), Raymond El Hajj (Rennes), Mohammed Lemou (IPSO), Claudia Negulsecu (Toulouse), Fanny Delebecque (Toulouse), Stéphane Descombes (Nice), Philippe Chartier (IPSO), Christophe Besse (Lille).

Abstract: Quantum technology as the application of quantum effects in macroscopic devices has an increasing importance, not only for far future goals like the quantum computer, but already now or in the near future. The present project is mainly concerned with the mathematical and numerical analysis of these objects, in conjunction with experimental physicists. On the side of fermions quantum electronic structures like resonant tunnelling diodes show well studied non classical effects like a negative differential resistance that are exploited for novel devices. On the side of bosons the creation and manipulation of Bose Einstein Condensates (the first creation of BECs by Ketterle et al merited a Nobel prize) has become a standard technique that allows to study fundamental quantum concepts like matter-wave duality with increasingly large objects and advanced quantum effects like decoherence, thermalization, quantum chaos. In state-of-the-art experiments e.g. with ultracold atoms in optical lattices the bosonic or fermionic nature of quantum objects can change and it makes a lot of sense to treat the models in parallel in the development of mathematical methods. The experimental progress in these fields is spectacular, but the mathematical modelling and analysis as well as the numerical simulation are lagging behind. Low dimensional models are mostly introduced in a heuristic way and there is also a need for systematic derivations and comparison with the 3-d models. To close the gap is a main goal of this project that aims to deliver reliable tools and programme packages for the numerical simulation of different classes of quantum systems modelled by partial differential equation of NLS type. Virtually all participants have a strong track record of international collaboration, they grew up with the concept of the European Research Area where science knows no boundaries and scientists used to work in different countries, as it was the case in a pronounced way in mathematics and in quantum physics in the thirties of the last century. The Pre- and Post-Docs to be funded by this project will be trained in this spirit of mobility between scientific fields and between places.

6.3. International Initiatives

6.3.1. Participation In other International Programs

- PTDC/EMS-ENE FCT (Fundação para a Ciência e a Tecnologia, Portugal): 2013-2014;
  Participant: N. Crouseilles;
  Leader: M. Roger
- IFCAM (Institute France-India for Applied Mathematics, India): 2013;
  Participant: N. Crouseilles and M. Lemou;
  Leaders: R. Raghurama, M. Lemou

6.4. International Research Visitors

6.4.1. Visits of International Scientists

- A. Debussche invited Y. Bakhtin (Georgia Tech., USA) and F. Baudoin (Purdue, USA) for a one month visit.
- L. Einkemmer, University of Innsbrück, one week, july 2013.
- A. Ruhi, Indian Institute of Sciences, 2 months, september-october 2013.

- R. Raghurama, Indian Institute of Sciences, two weeks, october 2013.
- Yong Zhang, under contract in Vienna, has been invited for several periods in Rennes (4 months altogether).

6.4.2. *Visits to International Teams*

- G. Vilmart: EPF Lausanne (Switzerland), invitation by Assyr Abdulle in the chair of numerical analysis and computational mathematics, several 1-2 weeks visits (totalizing 2 months).
- G. Vilmart: Invited research and teaching position at the University of Geneva, Section of Mathematics, for the period 09/2013-08/2014.
- N. Crouseilles visited the group of E. Sonnendrücker (IPP Garching, Germany), one week (december 2012).
- N. Crouseilles and E. Faou visited the group of A. Ostermann (University of Innsbrück, Austria), one week (march 2013).
- N. Crouseilles visited the group of P. Coelho (Universitad tecnico de Lisboa, Portugal), one week (july 2013).
- N. Crouseilles and M. Lemou visited the group of R. Raghurama (Indian Institute of Sciences, Bangalore (India)), 2 weeks (december 2013).

7. Dissemination

7.1. Scientific Animation

7.1.1. *Editorial activities*

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

7.1.2. *Conference and workshop organization*

- P. Chartier was a member of the scientific committees of SciCADE 2013 and ENUMATH 2013.
- A. Debussche was the main organizer of the thematic semester *Perspectives in Analysis and Probability* organized by the Lebesgue Center in Nantes and Rennes from april to september (see: http://www.lebesgue.fr/content/sem2013-perspectives-analysis-and-probability).
- A. Debussche was in the scientific committee of the conference *Probability and PDEs*, Centro de Giorgi, Pisa, may 20-24, 2013.

- E. Faou organized with J. Erhel (Rennes) and T. Lelièvre (CERMICS) the conference NASDPE13, *Numerical analysis of stochastic Partial Differential equations*, September 10-11, Rennes, France.
- N. Crouseilles co-organized the workshop on AP scheme (with C. Negulescu, F. Deluzet, C. Besse), Porquerolles, France (9-15 june, 2013).
- P. Chartier and M. Lemou organized a minisymposium on "Numerical schemes for highly oscillatory problems". ENUMATH, Lausanne, 25-30 august.
- M. Lemou organized a minisymposium on "Asymptotic preserving schemes for kinetic and related models". Hong-Kong, 07-11 January 2013.
- M. Lemou and F. Méhats were scientific advisors in the IHP semester *Gravasco* "N-body gravitational dynamical systems from N=2 to infinity" and were co-organizers of the workshop "Dynamics & Kinetic theory of self-gravitating systems" in this semester.
- F. Méhats was co-organizer of the workshop "Confined Quantum Systems: Modeling, Analysis and Computation" in Vienna.

7.1.3. *Administrative activities*

- P. Chartier is member of the bureau of the Comité des Projets at Inria-Rennes.
- A. Debussche leads the Lebesgue Center with San Vu Ngoc (coordinator) and L. Guillopé.
- A. Debussche is a member of the administrative board of the ENS Cachan.
- M. Lemou is partly in charge of the Master 2
- M. Lemou is member of the scientific committee of the Lebesgue Center (Labex)
- F. Méhats is member of the CNU, Section 26.
- F. Méhats is the head of the numerical analysis department of IRMAR.
- G. Vilmart was partly in charge of the weekly numerical analysis seminar at ENS Rennes "Groupe de travail: application des mathématiques".
- N. Crouseilles was partly in charge of the weekly numerical analysis seminar at ENS Rennes "Groupe de travail : application des mathématiques".

7.1.4. *Talks in seminars and conferences, mini-courses*

- E. Faou was invited at the Séminaire de Mathématiques Appliquées du Collège de France.
- A. Debussche gave a mini-course on *Stochastic equations and control theory*, in the conference *Mathematical Control in Trieste*, SISSA, Trieste, Dec. 2nd-6th, 2013.
- A. Debussche gave a mini-course on *Introduction aux EDPS* in the school *École Interdisciplinaire à Rennes*, Rennes, oct. 8-10, 2013.
- A. Debussche was gave a plenary talk in the conference Theory and Applications of Stochastic PDEs, IMA, Minneapolis, Jan. 14-18, 2013.
- F. Méhats and M. Lemou were invited to give a course on stability problems in gravitational models in the IHP Gravasco semester.
- G. Vilmart was keynote speaker in NASPDE workshop (Numerical Analysis of Stochastic PDEs), Rennes, 10-11 Sept., 2013.
- G. Vilmart was keynote speaker in the workshop on Multiscale methods and Asymptotic-Preserving schemes, Porquerolles island, June 09-15, 2013.

7.2. Teaching - Supervision - Juries

7.2.1. *Teaching*

Licence 3: P. Chartier, "Equations différentielles", 36, L3, ENS Cachan-Bruz

Master 2 : P. Chartier, "Intégration numérique géométrique" , 12H, M2, University of Rennes 1

Master 2: N. Crouseilles, "Numerical methods for kinetic equations", 18H, M2, University of Rennes 1

Master 2: E. Faou, "Modélisation et analyse numérique des EDPs", ENS Paris, in collaboration with D. Lannes

Master 2: M. Lemou, "Equations hyperboliques et lois de conservation", and "Méthodes numériques pour les modèles cinétiques".

Master 1: M. Lemou, "Theory of distributions" and "Equations elliptiques".

7.2.2. *Supervision*

- N. Crouseilles: co-advising (with M. Mehrenberger) of Christophe Steiner PhD (second year in Strasbourg University), ministry grant.
- N. Crouseilles: co-advising (with S. Genaud) of Matthieu Kuhn PhD (second year in Strasbourg University), ANR "E2T2" grant.
- N. Crouseilles: co-advising (with M. Mehrenberger) of Pierre Glanc PhD (third year in Strasbourg University), Inria-Cordi grant.
- N. Crouseilles: co-advising (with M. Lemou) of H. Hivert PhD (first year in Rennes university), ENS grant.
- N. Crouseilles: co-advising (with R. Raghurama and M. Lemou) of A. Ruhi PhD (second year in IISc), Indian grant.
- F. Méhats is co-supervisor of the PhD thesis of G. Leboucher (with P. Chartier).
- F. Méhats is co-supervisor of the PhD thesis of M. Tusseau (with A. Debussche).
- A. Debussche supervizes the Phd theses of: M. Hofmanova (defended in july 2013), M. Kopec (defense scheduled on june 2014), S. De Moor (defense scheduled on june 2014).

7.2.3. *Juries*

- P. Chartier was referee of the thesis of C. Zbinden (Geneva, supervised by E. Hairer), november.
- P. Chartier was referee of the thesis of H. Xue (Bergen, Supervised by A. Zanna), november.
- P. Chartier was member of the HDR jury of G. Vilmart, july.
- N. Crouseilles: member of the PHD jury of C. Caldini-Queiros, 15 november 2013.
- F. Méhats was referee of the thesis of M. Lutz (Strasbourg, supervised by E. Frenod and E. Sonnendrücker).
- F. Méhats was referee of the thesis of J. Sabin (Cergy, supervised by M. Lewin).
- M. Lemou was referee of the PhD thesis of F. Doisneau: Ecole Centrale de Paris, april 2013.
- M. Lemou was member of the Jury for the PhD thesis of E. Franck: Univesity Paris 6, october 2013.

7.3. Popularization

- Web interview of E. Faou: A l'occasion de la remise de la médaille Blaise Pascal (2013), Inria website.
- In http://interstices.info/planetes (2013), popularization article on the field of geometric numerical integration, published in "Interstices". Theme "Mathématiques de la planète Terre 2013" and Theme 2012-2013 "Invariants et similitudes" of TIPE in preparatory classes.
- Interview (June 2012) of M. Lemou for the journal "Science de l'Ouest" on the stability of galactic models. and publication of a popularized article: "Les mathématiciens déchiffrent l'univers" in the the journal "Espace des sciences", Nov 2012.
- M. Lemou and F. Méhats wrote a popularized scientific text in a CNRS letter "Lettre de l'INSMI", june 25th, 2012.

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Major publications by the team in recent years

[1] G. ANDREOIU, E. FAOU. *Complete asymptotics for shallow shells*, in "Asymptotic analysis", 2001, vol. 25, pp. 239-270

[2] F. CASTELLA. *From the von Neumann equation to the Quantum Boltzmann equation in a deterministic framework*, in "J. Stat. Phys.", 2001, vol. 104–1/2, pp. 387–447

[3] F. CASTELLA. *Propagation of space moments in the Vlasov-Poisson Equation and further results*, in "Ann. I.H.P., Anal. NonLin.", 1999, vol. 16–4, pp. 503–533

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Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] M. HOFMANOVÁ. , *Degenerate parabolic stochastic partial differential equations*, École normale supérieure de Cachan - ENS Cachan and Charles University. Faculty of mathematics and physics. Department of metal physics (Prague), July 2013, http://hal.inria.fr/tel-00916580

[12] G. VILMART. , *Méthodes numériques géométriques et multi-échelles pour les équations différentielles (in English)*, École normale supérieure de Cachan - ENS Cachan, July 2013, Habilitation (HDR) soutenue le 2 juillet 2013 à l'Ecole Normale Supérieure de Cachan, antenne de Bretagne (ENS Rennes), http://hal.inria.fr/tel-00840733

Articles in International Peer-Reviewed Journals

[13] A. ABDULLE, G. VILMART. *PIROCK: a swiss-knife partitioned implicit-explicit orthogonal Runge-Kutta Chebyshev integrator for stiff diffusion-advection-reaction problems with or without noise*, in "Journal of Computational Physics", June 2013, vol. 242, pp. 869-888 [*DOI :* 10.1016/J.JCP.2013.02.009], http://hal.inria.fr/hal-00739757

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