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Activity Report 2012

Project-Team IPSO

Invariant Preserving SOlvers

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

RESEARCH CENTER
Rennes - Bretagne-Atlantique

THEME
Computational models and simulation

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Project-Team IPSO

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

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

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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 [61], [58], [57] 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.

2.3. Highlights of the Year

- The team is part of the newly accepted Labex “Lebesgues Center" (see http://www.lebesgue.fr/).

  The Lebesgue Center (Foundations, Interactions, Application and Training) has been selected as an excellence cluster in February 2012. The Center proposes to build a highly attractive and efficient Research Center and Graduate School in Western France that will coordinate the research in geometry, analysis, statistics and probabilities with strong interdisciplinary links to the socio-economic environment and its applications.

  Coordinators : Vũ Ngọc San (Irmar, Rennes 1) together with Arnaud Debussche (Irmar, ENS Cachan, IPSO), Christoph Sorger and Laurent Guillopé (LMJL, Nantes).
- Two members of the team, Florian Méhats and Mohammed Lemou, published a paper in “Inventiones Mathematicae” (see [31])
- Erwan Faou published the book [34] in the series “Zurich Lectures in Advanced Mathematics. Zürich: European Mathematical Society (EMS)".
- Arnaud Debussche has launched with Boris Rozovskii a new journal entitled "Stochastic Partial Differential Equations: Analysis and Computations", edited by Springer.

3. Scientific Foundations

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 [56] 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, 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 [60], [59] 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. PIROCK: a swiss-knife partitioned implicit-explicit orthogonal Runge-Kutta Chebyshev integrator for stiff diffusion-advection-reaction problems with or without noise

In [37], 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.

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

In [38], 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. Röß ler, Appl. Num. Math., 59, 2009].

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

In [39], 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.

5.4. High weak order methods for stochastic differential equations based on modified equations

Inspired by recent advances in the theory of modified differential equations, we propose in [11], a new methodology for constructing numerical integrators with high weak order for the time integration of stochastic differential equations. This approach is illustrated with the constructions of new methods of weak order two, in particular, semi-implicit integrators well suited for stiff (mean-square stable) stochastic problems, and implicit integrators that exactly conserve all quadratic first integrals of a stochastic dynamical system. Numerical examples confirm the theoretical results and show the versatility of our methodology.

5.5. Analysis of the finite element heterogeneous multiscale method for nonmonotone elliptic homogenization problems

In [13], an analysis of the finite element heterogeneous multiscale method for a class of quasilinear elliptic homogenization problems of nonmonotone type is proposed. We obtain optimal convergence results for dimension $d \leq 3$. Our results, which also take into account the microscale discretization, are valid for both simplicial and quadrilateral finite elements. Optimal a-priori error estimates are obtained for the H^1 and L^2 norms, error bounds similar as for linear elliptic problems are derived for the resonance error. Uniqueness of a numerical solution is proved. Moreover, the Newton method used to compute the solution is shown to converge. Numerical experiments confirm the theoretical convergence rates and illustrate the behavior of the numerical method for various nonlinear problems.

5.6. Coupling heterogeneous multiscale FEM with Runge-Kutta methods for parabolic homogenization problems: a fully discrete space-time analysis

Numerical methods for parabolic homogenization problems combining finite element methods (FEMs) in space with Runge-Kutta methods in time are proposed in [14]. The space discretization is based on the coupling of macro and micro finite element methods following the framework of the Heterogeneous Multiscale Method (HMM). We present a fully-discrete analysis in both space and time. Our analysis relies on new (optimal) error bounds in the norms $L^2(H^1)$, $C^0(L^2)$, and $C^0(H^1)$ for the fully discrete analysis in space. These bounds can then be used to derive fully discrete space-time error estimates for a variety of Runge-Kutta methods, including implicit methods (e.g., Radau methods) and explicit stabilized method (e.g., Chebyshev methods). Numerical experiments confirm our theoretical convergence rates and illustrate the performance of the methods.

5.7. A priori error estimates for finite element methods with numerical quadrature for nonmonotone nonlinear elliptic problems

The effect of numerical quadrature in finite element methods for solving quasilinear elliptic problems of nonmonotone type is studied in [12]. Under similar assumption on the quadrature formula as for linear problems, optimal error estimates in the L^2 and the H^1 norms are proved. The numerical solution obtained from the finite element method with quadrature formula is shown to be unique for a sufficiently fine mesh. The analysis is valid for both simplicial and rectangular finite elements of arbitrary order. Numerical experiments corroborate the theoretical convergence rates.

5.8. An Isogeometric Analysis Approach for the study of the gyrokinetic quasi-neutrality equation

In [25], a new discretization scheme of the gyrokinetic quasi-neutrality equation is proposed. It is based on Isogeometric Analysis; the IGA which relies on NURBS functions, seems to accommodate arbitrary coordinates and the use of complicated computation domains. Moreover, arbitrary high order degree of basis functions can be used. Here, this approach is successfully tested on elliptic problems like the quasi-neutrality equation.

5.9. Guiding-center simulations on curvilinear meshes using semi-Lagrangian conservative methods

The purpose of this work [32] is to design simulation tools for magnetised plasmas in the ITER project framework. The specic issue we consider is the simulation of turbulent transport in the core of a Tokamak plasma, for which a 5D gyrokinetic model is generally used, where the fast gyromotion of the particles in the strong magnetic field is averaged in order to remove the associated fast time-scale and to reduce the dimension of 6D phase space involved in the full Vlasov model. Very accurate schemes and efficient parallel algorithms are required to cope with these still very costly simulations. The presence of a strong magnetic field constrains the time scales of the particle motion along and accross the magnetic field line, the latter being at least an order of magnitude slower. This also has an impact on the spatial variations of the observables. Therefore, the efficiency of the algorithm can be improved considerably by aligning the mesh with the magnetic field lines. For this reason, we study the behavior of semi-Lagrangian solvers in curvilinear coordinates. Before tackling the full gyrokinetic model in a future work, we consider here the reduced 2D Guiding-Center model. We introduce our numerical algorithm and provide some numerical results showing its good properties.

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

In [45], 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.

5.11. Kinetic/fluid micro-macro numerical schemes for Vlasov-Poisson-BGK equation using particles

This work [24] is devoted to the numerical simulation of the Vlasov equation in the fluid limit using particles. To that purpose, we first perform a micro-macro decomposition as in [Benoune, Lemou, Mieussens, JCP 08] where asymptotic preserving schemes have been derived in the fluid limit. In [Benoune, Lemou, Mieussens, JCP 08] , a uniform grid was used to approximate both the micro and the macro part of the full distribution function. Here, we modify this approach by using a particle approximation for the kinetic (micro) part, the fluid (macro) part being always discretized by standard finite volume schemes. There are many advantages

in doing so: (i) the so-obtained scheme presents a much less level of noise compared to the standard particle method; (ii) the computational cost of the micro-macro model is reduced in the fluid regime since a small number of particles is needed for the micro part; (iii) the scheme is asymptotic preserving in the sense that it is consistent with the kinetic equation in the rarefied regime and it degenerates into a uniformly (with respect to the Knudsen number) consistent (and deterministic) approximation of the limiting equation in the fluid regime.

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

In this paper [26], 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.

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

In [55], 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, Jin, SIAM J. Num. Anal. 05], where a coupled system of two equations, one at the mesoscopic and the other at the macroscopic scale, is solved. 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.

5.14. Accuracy of unperturbed motion of particles in a gyrokinetic semi-Lagrangian code

Inaccurate description of the equilibrium can yield to spurious effects in gyrokinetic turbulence simulations. Also, the Vlasov solver and time integration schemes impact the conservation of physical quantities, especially in long-term simulations. Equilibrium and Vlasov solver have to be tuned in order to preserve constant states (equilibrium) and to provide good conservation property along time (mass to begin with). Several illustrative simple test cases are given in [36] to show typical spurious effects that one can observes for poor settings. We explain why Forward Semi-Lagrangian scheme bring us some benefits. Some toroidal and cylindrical GYSELA runs are shown that use FSL.

5.15. High order Runge-Kutta-Nyström splitting methods for the Vlasov-Poisson equation

In this work [46], we derive the order conditions for fourth order time splitting schemes in the case of the $1D$ Vlasov-Poisson system. Computations to obtain such conditions are motivated by the specific Poisson structure of the Vlasov-Poisson system : this structure is similar to Runge-Kutta-Nyström systems. The obtained conditions are proved to be the same as RKN conditions derived for ODE up to the fourth order. Numerical results are performed and show the benefit of using high order splitting schemes in that context.

5.16. A Discontinuous Galerkin semi-Lagrangian solver for the guiding-center problem

In this paper [49], we test an innovative numerical scheme for the simulation of the guiding-center model, of interest in the domain of plasma physics, namely for fusion devices. We propose a 1D Discontinuous Galerkin (DG) discretization, whose basis are the Lagrange polynomials interpolating the Gauss points inside each cell, coupled to a conservative semi-Lagrangian (SL) strategy. Then, we pass to the 2D setting by means of a second-order Strangsplitting strategy. In order to solve the 2D Poisson equation on the DG discretization, we adapt the spectral strategy used for equally-spaced meshes to our Gauss-point-based basis. The 1D solver is validated on a standard benchmark for the nonlinear advection; then, the 2D solver is tested against the swirling deformation ow test case; nally, we pass to the simulation of the guiding-center model, and compare our numerical results to those given by the Backward Semi-Lagrangian method.

5.17. Asymptotic preserving schemes for highly oscillatory kinetic equation

This work [48] is devoted to the numerical simulation of a Vlasov-Poisson model describing a charged particle beam under the action of a rapidly oscillating external electric 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 "double-scale" reformulation of the initial equation, with the introduction of an additional periodic variable.

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

This work [47] focusses 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 collisionless regime. Numerical experiments confirm the good behaviour of the numerical scheme in both regimes. The case of a spatially dependent $\varepsilon(x)$ is also investigated.

5.19. Orbital stability of spherical galactic models

In [31], we consider the three dimensional gravitational Vlasov Poisson system which is a canonical model in astrophysics to describe the dynamics of galactic clusters. A well known conjecture (Binney, Tremaine in Galactic Dynamics, Princeton University Press, Princeton, 1987) is the stability of spherical models which are nonincreasing radially symmetric steady states solutions. This conjecture was proved at the linear level by several authors in the continuation of the breakthrough work by Antonov (Sov. Astron. 4:859-867, 1961). In the previous work (Lemou et al. in A new variational approach to the stability of gravitational systems, submitted, 2011), we derived the stability of anisotropic models under spherically symmetric perturbations using fundamental monotonicity properties of the Hamiltonian under suitable generalized symmetric rearrangements first observed in the physics literature (Lynden-Bell in Mon. Not. R. Astron. Soc. 144:189-217, 1969; Gardner in Phys. Fluids 6:839-840, 1963; Wiechen et al. in Mon. Not. R. Astron. Soc. 223:623-646, 1988; Aly in Mon. Not. R. Astron. Soc. 241:15, 1989). In this work, we show how this approach combined with a new generalized Antonov type coercivity property implies the orbital stability of spherical models under general perturbations.

5.20. Stable ground states and self-similar blow-up solutions for the gravitational Vlasov-Manev system

In this work [54], we study the orbital stability of steady states and the existence of blow-up self-similar solutions to the so-called Vlasov-Manev (VM) system. This system is a kinetic model which has a similar Vlasov structure as the classical Vlasov-Poisson system, but is coupled to a potential in $-1/r - 1/r^2$ (Manev potential) instead of the usual gravitational potential in -1/r, and in particular the potential field does not satisfy a Poisson equation but a fractional- Laplacian equation. We first prove the orbital stability of the ground states type solutions which are constructed as minimizers of the Hamiltonian, following the classical strategy: compactness of the minimizing sequences and the rigidity of the flow. However, in driving this analysis, there are two mathematical obstacles: the first one is related to the possible blow-up of solutions to the VM system, which we overcome by imposing a sub-critical condition on the constraints of the variational problem. The second difficulty (and the most important) is related to the nature of the Euleri-Lagrange equations (fractional-Laplacian equations) to which classical results for the Poisson equation do not extend. We overcome this difficulty by proving the uniqueness of the minimizer under equimeasurabilty constraints, using only the regularity of the potential and not the fractional- Laplacian Euler-Lagrange equations itself. In the second part of this work, we prove the existence of exact self-similar blow-up solutions to the Vlasov-Manev equation, with initial data arbitrarily close to ground states. This construction is based on a suitable variational problem with equimeasurability constraint.

5.21. Micro-macro schemes for kinetic equations including boundary layers

In this paper [53], we introduce a new micro-macro decomposition of collisional kinetic equations in the specific case of the diffusion limit, which naturally incorporates the incoming boundary conditions. The idea is to write the distribution function f in all its domain as the sum of an equilibrium adapted to the boundary (which is not the usual equilibrium associated with f) and a remaining kinetic part. This equilibrium is defined such that its incoming velocity moments coincide with the incoming velocity moments of the distribution function. A consequence of this strategy is that no artificial boundary condition is needed in the micromacro models and the exact boundary condition on f is naturally transposed to the macro part of the model. This method provides an “Asymptotic preserving" numerical scheme which generates a very good approximation of the space boundary values at the diffusive limit, without any mesh refinement in the boundary layers. Our numerical results are in very good agreement with the exact so-called Chandrasekhar value, which is explicitely known in some simple cases.

5.22. Stroboscopic averaging for the nonlinear Schrödinger equation

In this paper [35], we are concerned with an averaging procedure, -namely Stroboscopic averaging-, for highly-oscillatory evolution equations posed in a (possibly infinite dimensional) Banach space, typically partial differential equations (PDEs) in a high-frequency regime where only one frequency is present. We construct a high order averaged system whose solution remains exponentially close to the exact one over long time intervals, possesses the same geometric properties (structure, invariants, . . .) as compared to the original system, and is non-oscillatory. We then apply our results to the nonlinear Schrödinger equation on the d-dimensional torus T^d, or in R^d with a harmonic oscillator, for which we obtain a hierarchy of Hamiltonian averaged models. Our results are illustrated numerically on several examples borrowed from the recent literature.

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

In [41], we consider the semiclassical limit for the nonlinear Schrödinger 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 Schrödinger equation.

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

In [17], we consider the behaviour 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 analyse the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyse the asymptotic behaviour of the system for an arbitrary probability mass function governing the competition. We give conditions that ensure the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed storage when the competition is handled using a geometric distribution.

5.25. High frequency behavior of the Maxwell-Bloch mdel with relaxations: convergence to the Schrödinger-rate system

We study in [20] the Maxwell-Bloch model, which describes the propagation of a laser through a material and the associated interaction between laser and matter (polarization of the atoms through light propagation, photon emission and absorption, etc.). The laser field is described through Maxwell's equations, a classical equation, while matter is represented at a quantum level and satisfies a quantum Liouville equation known as the Bloch model. Coupling between laser and matter is described through a quadratic source term in both equations. The model also takes into account partial relaxation effects, namely the trend of matter to return to its natural thermodynamic equilibrium. The whole system involves 6+$N\,(N+1)/2$ unknowns, the six-dimensional electromagnetic field plus the $N\,(N+1)/2$ unknowns describing the state of matter, where N is the number of atomic energy levels of the considered material. We consider at once a high-frequency and weak coupling situation, in the general case of anisotropic electromagnetic fields that are subject to diffraction. Degenerate energy levels are allowed. The whole system is stiff and involves strong nonlinearities. We show the convergence to a nonstiff, nonlinear, coupled Schrödinger-Boltzmann model, involving 3+N unknowns. The electromagnetic field is eventually described through its envelope, one unknown vector in C^3. It satisfies a Schrödinger equation that takes into account propagation and diffraction of light inside the material. Matter on the other hand is described through a N-dimensional vector describing the occupation numbers of each atomic level. It satisfies a Boltzmann equation that describes the jumps of the electrons between the various atomic energy levels, as induced by the interaction with light. The rate of exchange between the atomic levels is proportional to the intensity of the laser field. The whole system is the physically natural nonlinear model. In order to provide an important and explicit example, we completely analyze the specific (two dimensional) Transverse Magnetic case, for which formulae turn out to be simpler. Technically speaking, our analysis does not enter the usual mathematical framework of geometric optics: it is more singular, and requires an *ad hoc* Ansatz.

5.26. Radiation condition at infinity for the high-frequency Helmholtz equation: optimality of a non-refocusing criterion

In [43], we consider the high frequency Helmholtz equation with a variable refraction index $n^2(x)$ ($x \in \mathbb{R}^d$), supplemented with a given high frequency source term supported near the origin $x = 0$. A small absorption parameter $\alpha_\varepsilon > 0$ is added, which prescribes a radiation condition at infinity for the considered Helmholtz equation. The semi-classical parameter is $\varepsilon > 0$. We let ε and α_ε go to zero *simultaneously*. We study the question whether the prescribed radiation condition at infinity is satisfied *uniformly* along the asymptotic process $\varepsilon \to 0$. This question has been previously studied by the first author, who has proved that the radiation

condition is indeed satisfied uniformly in ε, provided the refraction index satisfies a specific *non-refocusing condition*. The non-refocusing condition requires, in essence, that the rays of geometric optics naturally associated with the high-frequency Helmholtz operator, and that are sent from the origin $x = 0$ at time $t = 0$, should not refocus at some later time $t > 0$ near the origin again. In the present text we show the *optimality* of the above mentioned non-refocusing condition. We exhibit a refraction index which *does* refocus the rays of geometric optics sent from the origin near the origin again, and we show that the limiting solution *does not* satisfy the natural radiation condition at infinity in that case.

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

We study in [44] the competition of two species for a single resource in a chemostat. In the simplest space-homogeneous situation, it is known that only one species survives, namely the best competitor. In order to exhibit *coexistence* phenomena, where the two competitors are able to survive, we consider a space dependent situation: we assume that the two species and the resource follow a diffusion process in space, on top of the competition process. Besides, and in order to consider the most general case, we assume each population is associated with a *distinct* diffusion constant. This is a key difficulty in our analysis: the specific (and classical) case where all diffusion constants are equal, leads to a particular conservation law, which in turn allows to eliminate the resource in the equations, a fact that considerably simplifies the analysis and the qualitative phenomena. Using the global bifurcation theory, we prove that the underlying 2-species, stationary, diffusive, chemostat-like model, does possess *coexistence solutions*, where both species survive. On top of that, we identify the domain, in the space of the identified bifurcation parameters, for which the system does have coexistence solutions.

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

In [16], we consider the behaviour 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 analyse the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyse the asymptotic behaviour of the system for an arbitrary probability mass function governing the competition. We give conditions that ensure the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed storage when the competition is handled using a geometric distribution.

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

In this paper [21], we are concernedwith 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.

5.30. A formal series approach to averaging: exponentially small error estimates

The techniques, based on formal series and combinatorics, used nowadays to analyze numerical integrators may be applied to perform high-order averaging in oscillatory periodic or quasi-periodic dynamical systems. When this approach is employed, the averaged system may be written in terms of (i) scalar coefficients that are universal, i.e. independent of the system under consideration and (ii) basis functions that may be written in an explicit, systematic way in terms of the derivatives of the Fourier coefficients of the vector field being averaged. The coefficients may be recursively computed in a simple fashion. We show in [22] that this approach may be used to obtain exponentially small error estimates, as those first derived by Neishtadt. All the constants that feature in the estimates have a simple explicit expression.

5.31. Higher-order averaging, formal series and numerical integration II: the quasi-periodic case

The paper [23] considers non-autonomous oscillatory systems of ordinary differential equations with d>1 non-resonant constant frequencies. Formal series like those used nowadays to analyze the properties of numerical integrators are employed to construct higher-order averaged systems and the required changes of variables. With the new approach, the averaged system and the change of variables consist of vector-valued functions that may be written down immediately and scalar coefficients that are universal in the sense that they do not depend on the specific system being averaged and may therefore be computed once and for all. The new method may be applied to obtain a variety of averaged systems. In particular we study the quasi-stroboscopic averaged system characterized by the property that the true oscillatory solution and the averaged solution coincide at the initial time. We show that quasi- stroboscopic averaging is a geometric procedure because it is independent of the particular choice of co-ordinates used to write the given system. As a consequence, quasi-stroboscopic averaging of a canonical Hamiltonian (resp. of a divergence-free) system results in a canonical (resp. in a divergence-free) averaged system. We also study the averaging of a family of near-integrable systems where our approach may be used to construct explicitly d formal first integrals for both the given system and its quasi-stroboscopic averaged version. As an application we construct three first integrals of a system that arises as a nonlinear perturbation of five coupled harmonic oscillators with one slow frequency and four resonant fast frequencies.

5.32. Existence of densities for the 3D Navier-Stokes equations driven by Gaussian noise

We prove in [50] three results on the existence of densities for the laws of finite dimensional functionals of the solutions of the stochastic Navier-Stokes equations in dimension 3. In particular, under very mild assumptions on the noise, we prove that finite dimensional projections of the solutions have densities with respect to the Lebesgue measure which have some smoothness when measured in a Besov space. This is proved thanks to a new argument inspired by an idea introduced in Fournier and Printems (2010).

5.33. Diffusion limit for a stochastic kinetic problem

We study in [30] the limit of a kinetic evolution equation involving a small parameter and perturbed by a smooth random term which also involves the small parameter. Generalizing the classical method of perturbed test functions, we show the convergence to the solution of a stochastic diffusion equation.

5.34. Global Existence and Regularity for the 3D Stochastic Primitive Equations of the Ocean and Atmosphere with Multiplicative White Noise

The Primitive Equations are a basic model in the study of large scale Oceanic and Atmospheric dynamics. These systems form the analytical core of the most advanced General Circulation Models. For this reason and

due to their challenging nonlinear and anisotropic structure the Primitive Equations have recently received considerable attention from the mathematical community. In view of the complex multi-scale nature of the earth's climate system, many uncertainties appear that should be accounted for in the basic dynamical models of atmospheric and oceanic processes. In the climate community stochastic methods have come into extensive use in this connection. For this reason there has appeared a need to further develop the foundations of nonlinear stochastic partial differential equations in connection with the Primitive Equations and more generally. In this work [29] we study a stochastic version of the Primitive Equations. We establish the global existence of strong, pathwise solutions for these equations in dimension 3 for the case of a nonlinear multiplicative noise. The proof makes use of anisotropic estimates, $L^p\_tL^q\_x$ estimates on the pressure and stopping time arguments.

5.35. Weak backward error analysis for SDEs

We consider in [28] numerical approximations of stochastic differential equations by the Euler method. In the case where the SDE is elliptic or hypoelliptic, 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 invariant 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 Euler scheme is exponentially mixing.

5.36. Convergence of stochastic gene networks to hybrid piecewise deterministic processes

In [27], we study the asymptotic behavior of multiscale stochastic gene networks using weak limits of Markov jump processes. Depending on the time and concentration scales of the system we distinguish four types of limits: continuous piecewise deterministic processes (PDP) with switching, PDP with jumps in the continuous variables, averaged PDP, and PDP with singular switching. We justify rigorously the convergence for the four types of limits. The convergence results can be used to simplify the stochastic dynamics of gene network models arising in molecular biology.

5.37. Exponential mixing of the 3D stochastic Navier-Stokes equations driven by mildly degenerate noises

In [15], we prove the strong Feller property and exponential mixing for 3D stochastic Navier-Stokes equation driven by mildly degenerate noises (i.e. all but finitely many Fourier modes are forced) via Kolmogorov equation approach.

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

In [40] 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.

5.39. Fast Weak-Kam Integrators

We consider in [42] a numerical scheme for Hamilton-Jacobi equations based on a direct discretization of the Lax-Oleinik semi-group. We 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, we 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, we show that the numerical scheme can be implemented in a very efficient way.

5.40. Sparse spectral approximations for computing polynomial functionals

In [51], we give a new fast method for evaluating spectral approximations of nonlinear polynomial functionals. We prove that the new algorithm is convergent if the functions considered are smooth enough, under a general assumption on the spectral eigenfunctions that turns out to be satisfied in many cases, including the Fourier and Hermite basis.

6. Partnerships and Cooperations

6.1. National Initiatives

6.1.1. ANR Programme blanc (BLAN) MEGAS: 2009-2012

Participants: François Castella, Philippe Chartier, Arnaud Debussche, Erwan Faou.

Geometric methods and sampling: application to molecular simulation. The project was financed for 3 years, coordinated by Tony Lelièvre and has gathered the following teams and persons:

- Team of Eric Cancès at CERMICS
- Team IPSO
- Mathias Rousset from Inria Lille
- Christophe Chipot, from the CNRS in Nancy.

P. Chartier was the coordinator for IPSO.

6.1.2. ANR Programme blanc GYPSI: 2010-2014

Participant: Nicolas Crouseilles.

Leader: Ph. Gendrih.

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

6.1.3. ANR Programme blanc E2T2: 2010-2014

Participant: Nicolas Crouseilles.

Leader: P. Beyer

6.1.4. ANR Programme blanc STOSYMAP

Participant: Arnaud Debussche.

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

6.1.5. Inria Large scale initiative FUSION

Participant: Nicolas Crouseilles.

Leader: E. Sonnendrücker. The full description is available at http://www-math.u-strasbg.fr/ae_fusion

6.2. European Initiatives

6.2.1. FP7 Projects

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

6.3. International Initiatives

6.3.1. Participation In International Programs

6.3.1.1. ANR Programme blanc international (BLAN) LODIQUAS 2012-2015

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

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

The project, entitled "LODIQUAS" (for: Low DImensional QUANtum Systems), received fundings for 4 postdocs (48 months) and one pre-doc (36 months). The whole project involves the following rechearchers :

Norbert Mauser (Vienna), Erich Gornik (Vienna), Mechthild Thalhammer (Innsbruck), Christoph Naegerl (Innsbruck), Joerg Schmiedmayer (Vienna), Hans-Peter Stimming (Vienna).

Francois Castella (IPSO), Florian Mehats (IPSO), Francis Nier (Rennes), Raymond El Hajj (Rennes), Mohammed Lemou (IPSO), Claudia Negulsecu (Toulouse), Fanny Delebecque (Toulouse), Stephane Descombes (Nice), Philippe Chartier (IPSO), Christophe Besse (Lille),

The expected scientific and technological progress brought by the present project are as follows. “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.

6.4. International Research Visitors

6.4.1. Visits of International Scientists

- Mechthild Thalhammer, University of Innsbrück, one week
- Yong Zhang, University of Vienna, three weeks

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 3 months).

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 member of the editorial board of “SINUM"
- A. Debussche is member of the editorial board of “Differential and Integral Equations"
- A. Debussche is a member of the editorial board of “Potential Analysis"
- A. Debussche is a member of the editorial board of “ESAIM Proceeding"
- A. Debussche is a member of the editorial board of the collection “Mathématiques & Applications" edited by Springer
- A. Debussche is the editor in chief of “Stochastic Partial Differential Equations: Analysis and Conputations"
- M. Lemou is associate editor of “Annales de la faculté de Toulouse"

7.1.2. Conference and workshop organization

- P. Chartier, A. Debussche and E. Faou were members of the programm committee of DD21: 21th International Conference on Domain Decomposition Methods, 25-29 June 2012, Rennes, France.
- N. Crouseilles was member of the organization committee of the workshop WASPs 20-26 may 2012 http://www.math.univ-toulouse.fr/~cnegules/WAPs2012.html
- A. Debussche organizes the semester "Perspectives in Analysis and Probability" to be held in Rennes in 2013. Among others, there will be two international conferences, 3 workshops and 1 summer school.

7.1.3. Administrative activities

- P. Chartier is member of the bureau of the Comité des Projets at Inria-Rennes.
- 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.
- A. Debussche is member of the board of directors of the ENS Cachan.

- A. Debussche is member of the Executive Board of the Lebesgue Center, Labex funded by the french government.

7.1.4. Talks in seminars and conferences, mini-courses

- P. Chartier was plenary speaker at the Tenth International Conference of Numerical Analysis and Applied Mathematics (ICNAAM 2012) in honor of Gerhard Wanner, Greece, September 19-25, 2012.
- P. Chartier was plenary speaker at the Workshop INNOVATIVE TIME INTEGRATION, Innsbruck, Austria, May 13-16, 2012.
- E. Faou was plenary speaker at the conference NUMDIFF13 (september 2012), Halle, Germany.
- E. Faou gave a lecture at the Winter School “Dynamics and PDEs", Saint-Etienne de Tinée.
- G. Vilmart was keynote speaker at the Special session on "Algebraic structures in numerical analysis of differential equations", Universitad Jaume I (IMAC), Castellon (Spain), May 2012.
- A. Debussche was plenary speaker at the conference “Recent Developments in Stochastic Analysis", EPFL Lausanne, february 2012.
- A. Debussche was plenary speaker at the conference “Stochastic Analysis and Stochastic PDEs ", University of Warwick, april 2012
- A. Debussche was plenary speaker at the conference “NASPDE12 - Numerical Analysis of Stochastic PDEs", University of Warwick, june 2012
- A. Debussche was plenary speaker at the conference “Stochastic Partial Differential Equations (SPDEs) Follow-up Meeting " in Cambridge, september 2012.

7.2. Teaching - Supervision - Juries

7.2.1. Teaching

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

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

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

Master 1 and 2: M. Lemou, “Equations elliptiques" and “Equations hyperboliques"

7.2.2. Supervision

PhD : Charles-Edouard Bréhier, “Analyse numérique d’EDP stochastiques hautement oscillantes", defended the 27th of november 2012 (supervised by A. Debussche et E. Faou).

7.2.3. Juries

- Nicolas Crouseilles: member of the PhD-jury of A. Crestetto, 4 october, 2012 (Strasbourg).
- A. Debussche was member of the jury for Yohann Offret (PhD, Rennes, juin 2012), Florent Barret (Hdr, Ecole Polytechnique, juillet 2012), Maxime Gazeau (PhD, Ecole Polytechnique, octobre 2012), Bruno Saussereau (Hdr, Besancon, novembre 2012)
- M. Lemou was member of the jury for E. Franck (PhD, Paris 6) and S. Soulaiman (PhD, IRMAR).

7.3. Popularization

S. Fiorelli-Vilmart and G. Vilmart, Les planètes tournent-elles rond?, submitted for publication in “Interstices" Theme 2012-2013 “Invariants et similitudes" of TIPE in preparatory classes.

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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, p. 239-270.

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Publications of the year

Articles in International Peer-Reviewed Journals

[11] A. ABDULLE, D. COHEN, G. VILMART, K. ZYGALAKIS. *High weak order methods for stochastic differential equations based on modified equations*, in "SIAM J. Sci. Comput.", June 2012, vol. 34, n^{o} 3, p. 1800-1823 [*DOI :* 10.1137/110846609], http://hal.archives-ouvertes.fr/hal-00746563.

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