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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

Table of contents

Project-Team IPSO

Keywords: Scientific Computation, Geometric Integration

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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 [57], [52], [51] 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

- ERC Grant awarded to Erwan Faou for his project GEOPARDI
- Nicolas Crouseilles has defended his 'Habilitation à diriger les recherches' in january (14th january 2011).

3. Scientific Foundations

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

Participants: François Castella, Philippe Chartier, Erwan Faou.

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 [50] 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:

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

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, Erwan Faou.

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

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

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

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

$$h\omega < C,$$

where C is a constant depending on the numerical method and where 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.

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 [55], [54] 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.

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.

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.

3.6. Spatial approximation for solving ODEs

Participants: Philippe Chartier, Erwan Faou.

The technique consists in solving an approximate initial value problem on an approximate invariant manifold for which an atlas consisting of *easily computable* charts exists. The numerical solution obtained is this way never drifts off the exact manifold considerably even for long-time integration.

Instead of solving the initial Cauchy problem, the technique consists in solving an approximate initial value problem of the form:

$$\begin{aligned} \widetilde{y}'(t) &= \widetilde{f}(\widetilde{y}(t)), \\ \widetilde{y}(0) &= \widetilde{y}_0, \end{aligned} \tag{13}$$

on an invariant manifold $\widetilde{\mathcal{M}} = \{y \in \mathbb{R}^n; \widetilde{g}(y) = 0\}$, where $\widetilde{f}$ and $\widetilde{g}$ approximate f and g in a sense that remains to be defined. The idea behind this approximation is to replace the differential manifold $\mathcal{M}$ by a suitable approximation $\widetilde{\mathcal{M}}$ for which an atlas consisting of *easily computable* charts exists. If this is the case, one can reformulate the vector field $\widetilde{f}$ on each domain of the atlas in an *easy* way. The main obstacle of *parametrization* methods [56] or of *Lie-methods* [53] is then overcome.

The numerical solution obtained is this way obviously does not lie on the exact manifold: it lives on the approximate manifold $\widetilde{\mathcal{M}}$. Nevertheless, it never drifts off the exact manifold considerably, if $\mathcal{M}$ and $\widetilde{\mathcal{M}}$ are chosen appropriately *close* to each other.

An obvious prerequisite for this idea to make sense is the existence of a neighborhood $\mathcal{V}$ of $\mathcal{M}$ containing the approximate manifold $\widetilde{\mathcal{M}}$ and on which the vector field f is well-defined. In contrast, if this assumption is fulfilled, then it is possible to construct a new admissible vector field $\widetilde{f}$ given $\widetilde{g}$. By admissible, we mean tangent to the manifold $\widetilde{\mathcal{M}}$, i.e. such that

$$\forall\, y \in \widetilde{\mathcal{M}},\ \widetilde{G}(y)\widetilde{f}(y) = 0,$$

where, for convenience, we have denoted $\widetilde{G}(y) = \widetilde{g}'(y)$. For any $y \in \widetilde{\mathcal{M}}$, we can indeed define

$$\widetilde{f}(y) = (I - P(y))f(y), \tag{14}$$

where $P(y) = \widetilde{G}^T(y)(\widetilde{G}(y)\widetilde{G}^T(y))^{-1}\widetilde{G}(y)$ is the projection along $\widetilde{\mathcal{M}}$.

4. Application Domains

4.1. Laser physics

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

This task has been partially performed in the context of a contract with Alcatel, in that we developed a new numerical scheme to discretize directly the high-frequency model derived from physical laws.

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 bewteeen 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).

5. New Results

5.1. Asymptotic preserving schemes

Participant: Nicolas Crouseilles.

In [18], we extend the micro-macro decomposition based numerical schemes developed previously to the collisional Vlasov-Poisson model in the diffusion and high-field asymptotics. In doing so, we first write the Vlasov-Poisson model as a system that couples the macroscopic (equilibrium) part with the remainder part. A suitable discretization of this micro-macro model enables to derive an asymptotic preserving scheme in the diffusion and high-field asymptotics. In addition, two main improvements are presented: On the one hand a self-consistent electric field is introduced, which induces a specific discretization in the velocity direction, and represents a wide range of applications in plasma physics. On the other hand, as suggested in a previous reference, we introduce a suitable reformulation of the micro-macro scheme which leads to an asymptotic preserving property with the following property: It degenerates into an implicit scheme for the diffusion limit model when $\varepsilon \to 0$, which makes it free from the usual diffusion constraint $\Delta t = \mathcal{O}(\Delta x^2)$ in all regimes. Numerical examples are used to demonstrate the efficiency and the applicability of the schemes for both regimes.

In [45], a Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field is derived. 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.

5.2. Resolution of the quasi-neutrality equation

Participant: Nicolas Crouseilles.

In reference [39], different parallel algorithms are proposed for the numerical resolution of the quasi-neutrality equation in the GYSELA code. A set of benchmarks on a parallel machine has permitted to evaluate the performance of the different versions of the quasi-neutrality solver. In particular, in [40], these improvements are combined with memory optimization which enable a scalability of the GYSELA code up to $64k$ cores.

In [20], 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.

5.3. High order schemes for Vlasov-Poisson system

Participant: Nicolas Crouseilles.

In [44], 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.

In [19], we present a discontinuous Galerkin scheme for the numerical approximation of the one- dimensional periodic Vlasov-Poisson equation. The scheme is based on a Galerkin-characteristics method in which the distribution function is projected onto a space of discontinuous functions. We present comparisons with a semi-Lagrangian method to emphasize the good behavior of this scheme when applied to Vlasov-Poisson test cases.

The CEMRACS is an annual summer research session promoted by the SMAI. The 15th edition of 2010 has been organized by N. Crouseilles, H. Guillard, B. Nkonga and E. Sonnendrücker around "Numerical modeling of fusion plasmas". The volume [38] gathers artless resulting from research projects initiated during the CEMRACS 2010.

5.4. Second order averaging for the nonlinear Schrödinger equation with strong anisotropic potential

Participants: Florian Méhats, François Castella.

In [10], we consider the three dimensional Gross-Pitaevskii equation (GPE) describing a Bose- Einstein Condensate (BEC) which is highly confined in vertical z direction. The confining potential induces high oscillations in time. If the confinement in the z direction is a harmonic trap – an approximation which is widely used in physical experiments – the very special structure of the spectrum of the confinement operator implies that the oscillations are periodic in time. Based on this observation, it can be proved that the GPE can be averaged out with an error of order of ϵ, which is the typical period of the oscillations. In this article, we construct a more accurate averaged model, which approximates the GPE up to errors of order $\mathcal{O}(\epsilon^2)$. Then, expansions of this model over the eigenfunctions (modes) of the confining operator H_z in the z-direction are given in view of numerical applications. Efficient numerical methods are constructed to solve the GPE with cylindrical symmetry in 3D and the approximation model with radial symmetry in 2D, and numerical results are presented for various kinds of initial data.

5.5. A problem of moment realizability in quantum statistical physics

Participant: Florian Méhats.

This work [34] is a generalization of the results previously obtained by F. MÉHATS AND O. PINAUD, in J. Stat. Phys. (2010), in a one-dimensional setting: we revisit the problem of the minimization of the quantum free energy (entropy + energy) under local constraints (moments) and prove the existence of minimizers in various configurations. While the above quoted article addressed the 1D case on bounded domains, we treat in the present paper the multi-dimensional case as well as unbounded domains and non-linear interactions as Hartree/Hartree-Fock. Moreover, whereas this article dealt with the first moment only, namely the charge density, we extend the results to the second moment, the current density.

5.6. Orbital stability of spherical galactic models

Participant: Florian Méhats.

In [33] 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 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 in 1961. In a previous work, 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. 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.

5.7. The Schrödinger Poisson system on the sphere

Participant: Florian Méhats.

In [31] we study the Schrödinger-Poisson system on the unit sphere S^2 of $\mathbb{R}^3$, modeling the quantum transport of charged particles confined on a sphere by an external potential. Our first results concern the Cauchy problem for this system. We prove that this problem is regularly well-posed on every $H^s(S^2)$ with $s > 0$, and not uniformly well-posed on $L^2(S^2)$. The proof of well-posedness relies on multilinear Strichartz estimates, the proof of ill-posedness relies on the construction of a counterexample which concentrates exponentially on a closed geodesic. In a second part of the paper, we prove that this model can be obtained as the limit of the three dimensional Schrödinger-Poisson system, singularly perturbed by an external potential that confines the particles in the vicinity of the sphere.

5.8. A boundary matching micro-macro decomposition for kinetic equations

Participant: Florian Méhats.

In [32], we introduce a new micro-macro decomposition of collisional kinetic equations which naturally incorporates the exact space boundary conditions. The idea is to write the distribution fonction f in all its domain as the sum of a Maxwellian adapted to the boundary (which is not the usual Maxwellian associated with f) and a reminder kinetic part. This Maxwellian is defined such that its 'incoming' velocity moments coincide with the 'incoming' velocity moments of the distribution function. Important consequences of this strategy are the following. i) No artificial boundary condition is needed in the micro/macro models and the exact boundary condition on f is naturally transposed to the macro part of the model. ii) It provides a new class of the so-called 'Asymptotic preserving' (AP) numerical schemes: such schemes are consistent with the original kinetic equation for all fixed positive value of the Knudsen number ϵ, and if $\epsilon \longleftarrow 0$ with fixed numerical parameters then these schemes degenerate into consistent numerical schemes for the various corresponding asymptotic fluid or diffusive models. Here, the strategy provides AP schemes not only inside the physical domain but also in the space boundary layers. We provide a numerical test in the case of a diffusion limit of the one-group transport equation, and show that our AP scheme recovers the boundary layer and a good approximation of the theoretical boundary value, which is usually computed from the so-called Chandrasekhar function.

5.9. 1D quintic nonlinear equation with white noise dispersion

Participant: Arnaud Debussche.

Under certain scaling the nonlinear Schrödinger equation with random dispersion converges to the nonlinear Schrödinger equation with white noise dispersion. The aim of these works is to prove that this latter equation is globally well posed in L^2 or H^1. In [28], we improve the Strichartz estimates obtained previously for the Schrödinger equation with white noise dispersion in one dimension. This allows us to prove global well posedness when a quintic critical nonlinearity is added to the equation. We finally show that the white noise dispersion is the limit of smooth random dispersion

5.10. Weak approximation of stochastic partial differential equations: the nonlinear case

Participant: Arnaud Debussche.

In [22] we study the error of the Euler scheme applied to a stochastic partial differential equation. We prove that as it is often the case, the weak order of convergence is twice the strong order. A key ingredient in our proof is Malliavin calculus which enables us to get rid of the irregular terms of the error. We apply our method to the case a semilinear stochastic heat equation driven by a space-time white noise.

5.11. Ergodic BSDEs under weak dissipative assumptions

Participant: Arnaud Debussche.

In [27] we study ergodic backward stochastic differential equations (EBSDEs) dropping the strong dissipativity assumption needed previously. In other words we do not need to require the uniform exponential decay of the difference of two solutions of the underlying forward equation, which, on the contrary, is assumed to be non degenerate. We show existence of solutions by use of coupling estimates for a non-degenerate forward stochastic differential equations with bounded measurable non-linearity. Moreover we prove uniqueness of "Markovian" solutions exploiting the recurrence of the same class of forward equations. Applications are then given to the optimal ergodic control of stochastic partial differential equations and to the associated ergodic Hamilton-Jacobi-Bellman equations.

5.12. Asymptotic first exit times of the Chafee-Infante equation with small heavy tailed noise

Participant: Arnaud Debussche.

Motivated by paleoclimatological issues, we determine in [26] asymptotic

first exit times for the Chafee-Infante equation forced by heavy-tailed Levy diffusions from reduced domains of attraction in the limit of small intensity. We show that in contrast to the case of Gaussian diffusion the expected first exit times are polynomial in terms of the intensity.

5.13. Stochastic Cahn-Hilliard equation with double singular nonlinearities and two reflections

Participant: Arnaud Debussche.

In [25] we consider a stochastic partial differential equation with two logarithmic nonlinearities, two reflections at 1 and -1, and a constraint of conservation of the space average. The equation, driven by the derivative in space of a space-time white noise, contains a bi-Laplacian in the drift. The lack of a maximum principle for the bi-Laplacian generates difficulties for the classical penalization method, which uses a crucial monotonicity property. Being inspired by the works of Debussche, Goudenège, and Zambotti, we obtain existence and uniqueness of a solution for initial conditions in the interval $(-1, 1)$. Finally, we prove that the unique invariant measure is ergodic, and we give a result of exponential mixing.

5.14. Diffusion limit for a stochastic kinetic problem

Participants: Arnaud Debussche, Erwan Faou.

In [29] we consider numerical approximations of stochastic differential equations by the Euler method. In the case where the SDE is elliptic or hypo-elliptic, 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.

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

Participant: Arnaud Debussche.

In [47] we consider numerical approximations of stochastic differential equations by the Euler method. In the case where the SDE is elliptic or hypo-elliptic, 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 step-size. 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.

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

Participant: Arnaud Debussche.

In [11] 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.

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

Participant: Arnaud Debussche.

In thus survey article [46], we review recent progresses in the study of ergodicity for the stochastic Navier-Stokes equations. The first part introduces general concept, the second deals with the 2D case and the 3D case is treated in the third part.

5.18. Local Martingale and Pathwise Solutions for an Abstract Fluids Model

Participant: Arnaud Debussche.

In the first article [23], we establish the existence and uniqueness of both local martingale and local pathwise solutions of an abstract nonlinear stochastic evolution system. The primary application of this abstract framework is to infer the local existence of strong, pathwise solutions to the 3D primitive equations of the oceans and atmosphere forced by a nonlinear multiplicative white noise. In the second article [24] global existence is obtained.

5.19. Geometric numerical integration and Schrödinger equations

Participant: Erwan Faou.

The goal of geometric numerical integration is the simulation of evolution equations by preserving their geometric properties over long times. This question is of particular importance in the case of Hamiltonian partial differential equations typically arising in many application fields such as quantum mechanics or wave propagations phenomena. This implies many important dynamical features such as energy preservation and conservation of adiabatic invariants over long times. In this setting, a natural question is to know how and to which extent the reproduction of such long time qualitative behavior is ensured by numerical schemes.

Starting from numerical examples, these notes [37] try to provide a detailed analysis in the case of the Schrödinger equation in a simple setting (periodic boundary conditions, polynomial nonlinearities) approximated by symplectic splitting methods. This text analyzes the possible stability and instability phenomena induced by space and time discretization, and provides rigorous mathematical explanations for them.

5.20. On the influence of the geometry on skin effect in electromagnetism

Participant: Erwan Faou.

In [14], we consider the equations of electromagnetism set on a domain made of a dielectric and a conductor subdomain in a regime where the conductivity is large. Assuming smoothness for the dielectric-conductor interface, relying on recent works we prove that the solution of the Maxwell equations admits a multiscale asymptotic expansion with profile terms rapidly decaying inside the conductor. This skin effect is measured by introducing a skin depth function that turns out to depend on the mean curvature of the boundary of the conductor. We then confirm these asymptotic results by numerical experiments in various axisymmetric configurations. We also investigate numerically the case of a nonsmooth interface, namely a cylindrical conductor.

5.21. Reconciling alternate methods for the determination of charge distributions: A probabilistic approach to high-dimensional least-squares approximations

Participant: Erwan Faou.

In [17], we propose extensions and improvements of the statistical analysis of distributed multipoles (SADM) algorithm put forth by CHIPOT in 1998 for the derivation of distributed atomic multipoles from the quantum-mechanical electrostatic potential. The method is mathematically extended to general least-squares problems and provides an alternative approximation method in cases where the original least-squares problem is computationally not tractable, either because of its ill-posedness or its high-dimensionality. The solution is approximated employing a Monte Carlo method that takes the average of a random variable defined as the solutions of random small least-squares problems drawn as subsystems of the original problem. The conditions that ensure convergence and consistency of the method are discussed, along with an analysis of the computational cost in specific instances.

5.22. Hamiltonian interpolation of splitting approximations for nonlinear PDEs

Participant: Erwan Faou.

In [30], we consider a wide class of semi linear Hamiltonian partial differential equations and their approximation by time splitting methods. We assume that the nonlinearity is polynomial, and that the numerical trajectory remains at least uniformly integrable with respect to an eigenbasis of the linear operator (typically the Fourier basis). We show the existence of a modified interpolated Hamiltonian equation whose exact solution coincides with the discrete flow at each time step over a long time. While for standard splitting or implicit-explicit schemes, this long time depends on a cut-off condition in the high frequencies (CFL condition), we show that it can be made exponentially large with respect to the step size for a class of modified splitting schemes.

5.23. Energy cascades for NLS on the torus

Participant: Erwan Faou.

In the work [16], we consider the nonlinear Schrödinger equation with cubic (focusing or defocusing) nonlinearity on the multidimensional torus. For special small initial data containing only five modes, we exhibit a countable set of time layers in which arbitrarily large modes are created. The proof relies on a reduction to multiphase weakly nonlinear geometric optics, and on the study of a particular two-dimensional discrete dynamical system.

5.24. A Nekhoroshev type theorem for the nonlinear Schrödinger equation on the d-dimensional torus

Participant: Erwan Faou.

In [49] we prove a Nekhoroshev type theorem for the nonlinear Schrödinger equation

$$iu_t = -\Delta u + V \bar{\star} u + \partial_{\overline{u}} g(u, \overline{u}) \ , \quad x \in T^d,$$

where V is a typical smooth Fourier multiplier and g is analytic in both variables. More precisely we prove that if the initial datum is analytic in a strip of width $\rho > 0$ whose norm on this strip is equal to ϵ then, if ϵ is small enough, the solution of the nonlinear Schrödinger equation above remains analytic in a strip of width $\rho/2$, with norm bounded on this strip by $C\epsilon$ over a very long time interval of order $\epsilon^{-\alpha|\ln \epsilon|^\beta}$, where $0 < \beta < 1$ is arbitrary and $C > 0$ and $\alpha > 0$ are positive constants depending on β and ρ.

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

Participant: Erwan Faou.

In [48], 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.

5.26. Approximate travelling wave solutions to the 2D Euler equation on the torus

Participants: Erwan Faou, Nicolas Crouseilles.

In [43], we consider the two-dimensional Euler equation with periodic boundary conditions. We construct approximate solutions of this equation made of localized travelling profiles with compact support propagating over a stationary state depending on only one variable. The direction or propagation is orthogonal to this variable, and the support is concentrated around flat points of the stationary state. Under regularity assumptions, we prove that the approximation error can be made exponentially small with respect to the width of the support of the travelling wave. We illustrate this result by numerical simulations.

5.27. Markov chains competing for transitions : applications to large-scale distributed systems

Participant: François Castella.

We consider in [12] 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.

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

Participant: François Castella.

This text [41] generalizes the previous one [12] in the following sense.

In the situation on the previous article, 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 storage when the competition is handled using a geometric distribution.

5.29. Splitting methods with complex coefficients for some classes of evolution equations

Participant: Philippe Chartier.

We are concerned in [13] 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. In a previous paper, Castella et al. demonstrated the possibility to overcome this second-order barrier by considering splitting methods with complex-valued coefficients and built up methods of orders 3 to 14 . In this paper, we reconsider the technique employed therein and show that it is inherently bound to order 14 and largely sub-optimal with respect to error constants. As an alternative, we solve directly the algebraic equations arising from the order conditions and construct several methods of orders 4 , 6 , 8 and 16 that are the most accurate ones available at present time.

5.30. Higher-order averaging, formal series and numerical integration

Participant: Philippe Chartier.

The paper [42] 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 coupled harmonic oscillators with one slow frequency and four resonant fast frequencies.

The stroboscopic averaging method (SAM) is a technique for the integration of highly oscillatory differential systems $\dot{y} = f(y,t)$ with a single high frequency. The method may be seen as a purely numerical way of implementing the analytical technique of stroboscopic averaging which constructs an averaged differential system $\dot{Y} = F(Y)$ whose solutions Y interpolate the sought highly oscillatory solutions y. SAM integrates numerically the averaged system without using the analytic expression of F; all information on F required by the algorithm is gathered on the fly by numerically integrating the originally given system in small time windows. SAM may be easily implemented in combination with standard software and may be applied with variable step sizes. Furthermore it may also be used successfully to integrate oscillatory DAEs. The paper [15] provides an analytic and experimental study of SAM and two related techniques: the LISP algorithms of Kirchgraber and multirevolution methods.

6. Contracts and Grants with Industry

6.1. Contracts with Industry

6.1.1. Contract with CEA Bruyères-Le-Châtel: Determination of the numerical diffusion in a Lagrange-Projection type scheme with a slope limiter, using the associated equivalent equation

Participant: Nicolas Crouseilles.

Other participants (outside IPSO) are D. Bouche, J.P. Braeunig, Ch. Steiner, M. Mehrenberger. The main goal of this contract is to determine equivalent equations for standard numerical schemes dedicated to advection equations. In particular, the first term arising in these equivalent equation concerns the numerical diffusion. These computations enable to quantify in a analytical way the numerical diffusion.

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. 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 is financed for 3 years, coordinated by Tony Lelièvre and gathers 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 is the coordinator for IPSO.

7.1.2. ANR GYPSI (leader P. Beyer)

Participant: Nicolas Crouseilles.

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

7.1.3. INRIA Large scale initiative FUSION

Participant: Nicolas Crouseilles.

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

7.2. European Initiatives

7.2.1. FP7 Projet

7.2.1.1. Geopardi

Title: Geometric Partial Differential Equations

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.

7.3. International Initiatives

8. Dissemination

8.1. Animation of the scientific community

8.1.1. Editorial activities

- P. Chartier is member of the editorial board of M2AN.
- P. Chartier is member of the editorial board of ESAIM Proceedings.
- 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 Director of the mathematics department of the antenne de Bretagne ENS Cachan.

8.1.2. Conference and workshop organisation

- The team organized a workshop on numerical methods for stiff problems, Saint-Malo (January).
- F. Méhats and F. Castella were members of the organization and scientific committees of the Conference in honor of N. Ben Abdallah, Toulouse.
- P. Chartier was member of the scientific committee of SciCADE11, Toronto, Canada, July 11-15, 2011.

8.1.3. Administrative activities

- P. Chartier was member of the Commission d'Evaluation at INRIA until june.
- P. Chartier is member of the bureau of the Comité des Projets at INRIA-Rennes.
- A. Debussche is member of the CNU, Section 26.

8.1.4. Talks in seminars and conferences, mini-courses

- P. Chartier: Seminar INRIA Pau, December 12, 2011.
- P. Chartier: Seminar University of Geneva, November 2, 2011.
- P. Chartier: FOCM'11, Budapest, Hungary, July 4-6, 2011 (Invited Speaker)

- P. Chartier: Meeting on Geometric Numerical Integration, Oberwolfach, Germany, March 20-26, 2011 (Invited Speaker)
- P. Chartier: Real Matematica Sociedad Espagnola 2011 conference, special session on “Numerical integrators for Hamiltonian systems and related problem”, Avila, February 1-5, 2011 (Invited Speaker)
- E. Faou: June 2011, Workshop : *KAM theory and geometric integrators*, BIRS, Banff, Canada. Organized with W. Craig and B. Grébert.
- E. Faou: January 2011, Workshop : *Advanced Numerical Studies in Nonlinear Partial Differential Equations*, University of Edinburgh, UK. Organized with S. Kuksin, B. Leimkuhler and C. Sulem.
- E. Faou: November 2011: Seminar at the CNR, Pavia
- E. Faou: October 2011: Séminaire du laboratoire Jacques-Louis Lions, University of Paris 6.
- E. Faou: September 2011: Colloque “Rencontre Mathématiques-Mécanique, hommage à Paul Germain”, Congrès français de mécanique, Besançon.
- E. Faou: June 2011: Conference: *Nonlinear Dispersive Partial Differential Equations and Related Topics*, Institut Henri Poincaré, Paris.
- E. Faou: June 2011: Seminar at Fields Institute, Toronto (Canada)
- E. Faou: March 2011: Workshop on Geometric Numerical Integration, Oberwolfach (Germany)
- E. Faou: February 2011: Invitation to the university of Tokyo (Japan).
- E. Faou: February 2011: Séminaire *systèmes dynamiques*, Univ. Paris 7.
- F. Castella: talk at the conference in honnor of N. Ben Abdallah, Toulouse.
- Arnaud Debussche: September 6-11, mini course on “Stochastic Navier-Stokes equations: well posedness and ergodic properties" in the CIME summer school "Topics in mathematical fluid-mechanics” at Cetraro, Italy.
- Arnaud Debussche: july 6 - 8 2011, Workshop: *FoCM 2011, Conference on the Foundations of Computational Mathematics*, Budapest. Organisation de la session *Stochastic Computations* avec T. Mueller-Gronbach et B. Baxter.
- Arnaud Debussche: january 19 - 21 2011, Workshop: *Maximum principles, fractional diffusion and differential or integral inequalities for deterministic and stochastic partial differential equations*, Université d’Evry-Val d’Essone. Organised by L. Denis, P.G. Lemarie-Rieusset and J. Matos.
- Arnaud Debussche: January 25 2011: Exposé à la journée de l’ANR HANDDY, université de Nantes.
- Arnaud Debussche: February 1-5 2011, *Congreso de la real Sociedad Matematica Espanola 2011, centenaraio de la RSME*, Avila. Mini course (3h)..
- Arnaud Debussche: March 25 2011: *One day on SPDE and applications*, université du Mans, organisez by A. Matoussi.
- Arnaud Debussche: April 28-30: *Stochastics and Dynamics*, Brown Lefschetz Center for Dynamic Systems, organised by K. Ramanan and B. Rozovsky.
- Arnaud Debussche: June 2011: Séminaire EDP, IECN, université de Nancy.
- Arnaud Debussche: November 2011: Colloquium de Mathématiques, université de Pau.
- Arnaud Debussche: December 2011 : *Workshop: The stochastic Schrödinger equations in selected physics problems*, ENST, CEA, Gif-sur-Yvette.
- Nicolas Crouseilles: Numerical methods for stiff problems in Hamiltonian systems and kinetic equations, at Saint-Malo. http://anum-maths.univ-rennes1.fr/quatrain/saintmalo/saintmalo.html
- Nicolas Crouseilles: : talk at the meeting of ANR E2T2

- Florian Méhats: Colloque "Asymptotic dynamics driven by solitons and traveling fronts in nonlinear PDE", Santiago (Chili).
- Florian Méhats: Workshop "Asymptotic Regimes for Schrodinger equation", Vienna (Autriche).
- Florian Méhats: Workshop "KAM theory and Geometric Integration", Banff (Canada).
- Florian Méhats: Workshop du GdR CHANT "Transport et Nanostructures", Grenoble.
- Florian Méhats: Seminar MODANT Grenoble.
- Florian Méhats: Colloque "Kinetic models of classical and quantum particle systems", Toulouse.
- Florian Méhats: Seminars IHP, Orsay, Rennes.

8.2. Teaching

HdR : Nicolas Crouseilles, “Contributions à la simulation numérique des modèles de Vlasov en physique des plasmas”, Université de Strasbourg [9]

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Major publications by the team in recent years

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Publications of the year

Doctoral Dissertations and Habilitation Theses

[9] N. CROUSEILLES. *Contributions à la simulation numérique des modèles de Vlasov en physique des plasmas*, Université de Strasbourg, January 2011, HDR, http://tel.archives-ouvertes.fr/tel-00529809/en/.

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