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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

# *Project-Team ipso*

# *Invariant Preserving SOlvers*

*Rennes - Bretagne-Atlantique*

Theme : Computational models and simulation

# Table of contents

# 1. Team

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# 2. Overall Objectives

## 2.1. An overview of geometric numerical integration

A fundamental and enduring challenge in science and technology is the quantitative prediction of time-dependent nonlinear phenomena. While dynamical simulation (for ballistic trajectories) was one of the first applications of the digital computer, the problems treated, the methods used, and their implementation have all changed a great deal over the years. Astronomers use simulation to study long term evolution of the solar system. Molecular simulations are essential for the design of new materials and for drug discovery. Simulation can replace or guide experiment, which often is difficult or even impossible to carry out as our ability to fabricate the necessary devices is limited.

During the last decades, we have seen dramatic increases in computing power, bringing to the fore an ever widening spectrum of applications for dynamical simulation. At the boundaries of different modeling regimes, it is found that computations based on the fundamental laws of physics are under-resolved in the textbook sense of numerical methods. Because of the vast range of scales involved in modeling even relatively simple biological or material functions, this limitation will not be overcome by simply requiring more computing power within any realistic time. One therefore has to develop numerical methods which capture crucial structures even if the method is far from “converging" in the mathematical sense. In this context, we are forced increasingly to think of the numerical algorithm as a part of the modeling process itself. A major step forward in this area has been the development of structure-preserving or “geometric" integrators which maintain conservation laws, dissipation rates, or other key features of the continuous dynamical model. Conservation of energy and momentum are fundamental for many physical models; more complicated invariants are maintained in applications such as molecular dynamics and play a key role in determining the long term stability of methods. In mechanical models (biodynamics, vehicle simulation, astrodynamics) the available structure may include constraint dynamics, actuator or thruster geometry, dissipation rates and properties determined by nonlinear forms of damping.

In recent years the growth of geometric integration has been very noticeable. Features such as *symplecticity* or *time-reversibility* are now widely recognized as essential properties to preserve, owing to their physical significance. This has motivated a lot of research [42], [37], [35] 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.

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# 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 $t$, $\varphi_t$ 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 $\Phi_h$ of $\varphi_h$. One of the main questions of *geometric integration* is whether *intrinsic* properties of $\varphi_t$ may be passed on to $\Phi_h$.

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

### *3.1.1. Reversible ODEs*

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

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

It is then natural to require that $\Phi_h$ satisfies the same relation. If this is so, $\Phi_h$ 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 $\varphi_t$. 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 [34] 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:

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

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 $\omega$, 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

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

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 $\omega$ 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 $\varepsilon$ 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 $\varepsilon$. 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, $\varepsilon$ 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 $\Delta_{x_k}$ the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential $V$ acts as a multiplication operator on $\psi$.

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 [40], [39] 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 $\delta t$ 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, $\varepsilon$ 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 $\varepsilon$) 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 [41] or of *Lie-methods* [38] 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. Quasi invariant modified Sobolev norms for semi linear reversible PDEs

**Participant:** Erwan Faou.

This is a joint work with B. Grébert, from the University of Nantes.

We consider a general class of infinite dimensional reversible differential systems. In [22] we assume a non resonance condition on the linear frequencies, and we construct for such systems almost invariant pseudo norms that are closed to Sobolev-like norms. This allows us to prove that if the Sobolev norm of index $s$ of the initial data $z_0$ is sufficiently small (of order $\epsilon$) then the Sobolev norm of the solution is bounded by $2\epsilon$ during very long time (of order $\epsilon^{-r}$ with $r$ arbitrary). It turns out that this theorem applies to a large class of reversible semi linear PDEs including the non linear Schrödinger equation on the d-dimensional torus. We also apply our method to a system of coupled NLS equations which is reversible but not Hamiltonian. We also notice that for the same class of reversible systems we can prove a Birkhoff normal form theorem that in turn implies the same bounds on the Sobolev norms. Nevertheless the technics that we use to prove the existence of quasi invariant pseudo norms is much more simple and direct.

## 5.2. Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs

**Participant:** Erwan Faou.

This is a joint work with B. Grébert and E. Paturel, from the University of Nantes.

We consider here Hamiltonian PDEs associated with a Hamiltonian function that can be split into a linear unbounded operator and a regular nonlinear part. We consider splitting methods associated with this decomposition. Using a finite dimensional Birkhoff normal form result, we show the almost preservation of the *actions* of the numerical solution associated with the splitting method over arbitrary long time and for asymptotically large level of space approximation, provided the Sobolev norm of the initial data is small enough. This result holds under *generic* Ênon-resonance conditions on the frequencies of the linear operator and on the step size. We apply these results to nonlinear Schrödinger equations as well as the nonlinear wave equation. In [23] we consider the case of fully discrete Hamiltonian PDEs, and in [24] we consider abstract splitting methods associated with this decomposition where no discretization in space is made. In this latter situation, the results hold for *rounded* numerical schemes avoiding at each step possible high frequency energy drift.

## 5.3. Koiter Estimate Revisited

**Participant:** Erwan Faou.

This is a joint work with M. Dauge, from the University of Rennes I.

The goal of the work [13] is to prove a universal energy estimate between the solution of the three-dimensional Lamé system on a thin *clamped* shell and a displacement reconstructed from the solution of the classical Koiter model. The mid-surface $S$ of the shell is an arbitrary smooth manifold with boundary. The bound of our energy estimate only involves the thickness parameter $\varepsilon$, constants attached to $S$, the loading, the two-dimensional energy of the solution of the Koiter model and "wave-lengths" associated with this latter solution. This result is in the same spirit as Koiter's who gave a heuristic estimate in the end of the sixties. Taking boundary layers into account, we obtain rigorous estimates, which prove to be sharp in the cases of plates and elliptic shells.

## 5.4. Comportement asymptotique à haute conductivité de l'épaisseur de peau en électromagnétisme

**Participant:** Erwan Faou.

This is a joint work with V. Péron and M. Dauge, from the University of Rennes I.

In [28], [14], [26], [25], 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 dielectricÐconductor 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.

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

**Participant:** Erwan Faou.

This is a joint work with N. Champagnat, from INRIA (TOSCA).

In [31], 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.

## 5.6. Hamiltonian interpolation of splitting approximations for nonlinear PDEs

**Participant:** Erwan Faou.

This is a joint work with B. Grébert, from the University of Nantes.

In [21], 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.

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

**Participant:** Erwan Faou.

This is a joint work with B. Grébert, from the University of Nantes.

In [32] 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 $\epsilon$ then, if $\epsilon$ 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 $\beta$ and $\rho$.

## 5.8. Energy cascades for NLS on the torus

**Participant:** Erwan Faou.

This is a joint work with R. Carles, from CNRS.

In the work [29], 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.

## 5.9. Composing B-series of integrators and vector fields

**Participant:** Philippe Chartier.

This is a joint work with E. Hairer, from the University of Geneva and G. Vilmart from EPFL.

Hairer and Wanner [36] introduced the concept of B-series. B-series and extensions thereof are now exposed in various textbooks and lie at the core of several recent theoretical developments. B-Series owe their success to their ability to represent most numerical integrators, e.g. Runge-Kutta methods, splitting and composition methods, underlying one-step method of linear multistep formulae, as well as *modified* vector fields, i.e. vector fields built on derivatives of a given function. In some applications, B-series naturally combine with each other, according to two different laws. The composition law of Butcher and the substitution law of Chartier, Hairer and Vilmart.

The aim of the paper [10] is to explain the fundamental role in numerical analysis of these two laws and to explore their common algebraic structure and relationships. It complements, from a numerical analyst perspective, the work of Calaque, Ebraihimi-Fard & Manchon [33], where more sophisticated algebra is used. We introduce into details the composition and substitution laws, as considered in the context of numerical analysis and relate each law to a Hopf algebra. Then we explore various relations between the two laws and consider a specific map related to the logarithm. Eventually, we mention the extension of the substitution law to P-series, which are of great use for partitionned or split systems of ordinary differential equations.

## 5.10. Higher-order averaging, formal series and numerical integration

**Participant:** Philippe Chartier.

This is a joint work with A. Murua, from the University of the Basque Country (Spain) and J.M. Sanz-Serna and M.P. Calvo, from the University of Valladolid (Spain).

In [11], we show how B-series may be used to derive in a systematic way the analytical expressions of the high-order stroboscopic averaged equations that approximate the slow dynamics of highly oscillatory systems. For first order systems we give explicitly the form of the averaged systems with $\mathcal{O}(\epsilon^j)$-errors, $j = 1, 2, 3$ ($2\pi\epsilon$ denotes the period of the fast oscillations). For second order systems with large forces, we also give the explicit form of the averaged systems. The Fermi-Pasta-Ulam model and the inverted Kapitsa pendulum are used as illustrations. For the former it is shown that our approach establishes the adiabatic invariance of the oscillatory energy. Finally we use B-series to analyze multiscale numerical integrators that implement the method of averaging. We construct integrators that are able to approximate not only the simplest, lowest order averaged equation but also its high-order counterparts.

## 5.11. A Fast Multipole Method for Geometric Numerical Integrations of Hamiltonian Systems

**Participants:** Philippe Chartier, Erwan Faou.

This is joint work with E. Darrigrand from the University of Rennes I.

The Fast Multipole Method (FMM) has been widely developed and studied for the evaluation of Coulomb energy and Coulomb forces. A major problem occurs when the FMM is applied to approximate the Coulomb energy and Coulomb energy gradient within geometric numerical integrations of Hamiltonian systems considered for solving astronomy or molecular-dynamics problems: The FMM approximation involves an approximated potential which is not regular. Its lack of regularity implies a loss of the preservation of the Hamiltonian of the system. In [9], we contributed to a significant improvement of the FMM with regard to this problem : we investigated a regularization of the Fast Multipole Method in order to recover Hamiltonian preservation. Numerical results obtained on a toy problem confirm the gain of such a regularization of the fast method.

## 5.12. High frequency behaviour of the Maxwell-Bloch model with relaxations: convergence to the Schrödinger-Boltzmann system

**Participant:** François Castella.

In [30], with E. Dumas, we analyze the high-frequency behaviour of a physically natural model for the propagation of electromagnetic waves in a cristal.

Our starting point is a Maxwell equation for the wave, coupled with a Schrödinger-like equation for the atoms in the cristal, known as the Bloch model. The coupling term is quadratic. It describes, at a quantum level, the interaction between the wave and the atoms, like photon exchange, excitation of the atom, frequency conversion through nonlinear interaction, or so. The context makes it natural to cpnsider a high-frequency situation, since we aim at deriving a macroscopic model, valid at the macro scale, to modelize the interaction between the atom and the actual waves, which naturally have a short wavelength, hence a large frequency. The initial system is thus stiff (due to the high-frequency situation), and it involves a large number of nknowns: 6 unknowns for the wave (electric field + magnetic field), and $N^2$ unknowns for the cristal, where $N$ is the number of energy levels of each individual atom.

We show that this system is asymptotically well described by a simpler, non-stiff equation, involving $1 + N$ unknowns only. The asymptotic model involves one Schrödinger-like equation for the wave, and one Boltzmann-like equation for the atoms to describe the evolution of the occupation rate of the atoms' $N$ energy levels. The coupling between both equations is cubic. The Schrödinger equation for the wave describes the slow evolution of the waves' envelope. The Boltzmann equation for the atoms describes the transitions between the various energy levels of the atom, under the action of the electromagnetic wave.

We recover here in a rigorous fashion the physically relevant asymptotic model, and we point out the very value of the transition rates between the various energy levels of the atom, a new result.

## 5.13. Scalar conservation laws with stochastic forcing

**Participant:** Arnaud Debussche.

In [20], we show that the Cauchy Problem for a randomly forced, periodic multi-dimensional scalar first-order conservation law with additive or multiplicative noise is well-posed: it admits a unique solution, characterized by a kinetic formulation of the problem, which is the limit of the solution of the stochastic parabolic approximation.

## 5.14. Asymptotic behavior of stochastic PDEs with random coefficients

**Participant:** Arnaud Debussche.

In [12], we study the long time behavior of the solution of a stochastic PDEs with random coefficients assuming that randomness arises in a different independent scale. We apply the obtained results to $2D$- Navier–Stokes equations.

## 5.15. The nonlinear Schrödinger equation with white noise dispersion

**Participant:** Arnaud Debussche.

In [15], we prove that 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 $H^1$. The main ingredient is the generalization of the classical Strichartz estimates. Additionally, we justify rigorously the formal limit described above.

In the second article [19], 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.

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

**Participant:** Arnaud Debussche.

In [16], 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.

## 5.17. Ergodic BSDEs under weak dissipative assumptions

**Participant:** Arnaud Debussche.

In this paper [18] 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.

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

**Participant:** Arnaud Debussche.

Motivated by paleoclimatological issues, in [17] we determine 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.

# 6. Other Grants and Activities

## 6.1. National Initiatives

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

### *6.1.1. ARC grant HYBRID 2009-2010*

The Hybrid ARC project has been granted by the INRIA and group members of

- The IPSO project and the ENS Cachan Bretagne
- The TOSCA Project (head: D. Talay)
- The MICMAC project (head: E. Cancès)
- The SIMPAF Project (head: T. Goudon)
- The eDAM laboratory (head: C. Chipot)

The main aim of this project is to derive and analyze numerical methods for the simulation of complex systems arising in molecular dynamics. It turns out that these systems are in essence hybrid, and include in their definition deterministic and stochastic terms. Our goal is to group and mix technics that are a priori disjoint: use of symplectic integrator to handle Hamiltonian ordinary differential over long time and probabilistic methods to sample the invariant law of a stochastic differential equation.

### *6.1.2. Programme INRIA "Equipes Associées": MIMOL*

This is an exchange program between the IPSO team and the numerical analysis groups in Tübingen, headed by C. Lubich and in the University of the Basque Country headed by A. Murua. E. Faou is the coordinator of the french part of this project.

This program was valid for three years (2008-2009-2010).

### *6.1.3. Programme Hubert Curien Picasso*

This is an exchange program between the IPSO team and the numerical analysis groups in San Sebastian (Ander Murua), Valladolid (Jesus-Maria Sanz-Serna and Maripaz Calvo), Valencia (Sergio Blanes) and Castellon (Fernando Casas). This program was valid for two years (2009 and 2010). P. Chartier is the coodinator for the french side.

### *6.1.4. ANR Programme blanc (BLAN) MEGAS: 2009-2012*

Title: 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. Dissemination

## 7.1. Program committees, editorial Boards and organization of conferences

- P. Chartier is member of the editorial board of M2AN.
- P. Chartier is member of the editorial board of ESAIM Proceedings.
- P. Chartier organised a workshop on Numerical methods for Highly-oscillatory ODEs and PDEs, Dinard, January 27-29.
- E. Faou is the leader of the INRIA associated team MIMOL (2008–2010)
- 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.
- A. Debussche co-organised with M. Hairer the workshop: *Stochastic Partial Differential Equations: Approximation, Asymptotics and Computation*, Isaac Newton Institute, Cambridge, June 28 - july.

## 7.2. INRIA and University committees

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

## 7.3. Teaching

- E. Faou was oral examiner at ENS Cachan Bruz ("agrégation").
- P. Chartier was lecturer at the Ecole Normale Supérieure de Cachan Bretagne. Course: *Ordinary differential equations.*
- E. Faou was Visiting Professor, FIM, ETH Zürich during the spring trimester.
- A. Debussche gave a 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.

## 7.4. Participation in conferences

Concerning P. Chartier:

- JEAN, IRMAR, Rennes, November 25, 2010 (Invited Speaker).
- Workshop DANCE on Dynamics, Attractors and Nonlinearities, Calatayud, November 04-06, 2010 (Invited Speaker)
- Seminar University of Nice, October 12, 2010.
- Simulation of hybrid dynamical systems and applications to molecular dynamics, IHP-Paris, 27-30 september, 2010 (Invited Speaker)
- IMAC Workshop on Splitting methods for differential equations, Castellon, 6-8 september, 2010 (Invited Speaker)
- Workshop on Combinatorics and Control, Madrid (CSIC), April 6-9, 2010 (Invited Plenary Speaker).
- Seminar Ecole Polytechnique Fédérale de Lausanne, February 17, 2010.

Concerning E. Faou:

- December 2010: Séminaire EDP et applications, ENS Lyon & Univ. Lyon 1.
- October 2010: Workshop on time integration, Innsbruck (Austria).
- September 2010: Workshop on *Asymptotic Regimes for Schrödinger equations*, CIRM, Marseille.
- September 2010: Workshop on *splitting methods for differential equations*, Castellon (Spain).
- July 2010: Seminar at the Basque center for applied mathematics, Bilbao (Spain).
- June 2010: Invitation to the workshop on *Stochastic Partial Differential Equations: Approximation, Asymptotics and Computation*, Newton Institute, Cambridge (UK).
- May 2010: Séminaire d'analyse numérique, Université de Genève (Switzerland).
- April 2010: Journée *Dynamiques des équations Hamiltoniennes*, Nantes (France).
- April 2010: Seminar in the University of Strasbourg (France).
- March 2010: Seminar of Numerical analysis, University of Tübingen (Germany).
- March 2010: Analysis Seminar, University of Zürich (Switzerland).
- March 2010: Seminar at the CMAP, Ecole Polytechnique (France).
- February 2010: Seminar in the University of Karlsruhe (Germany)

Concerning A. Debussche:

- February 2010: Séminaire MOX, Politecnico di Milano.
- April 2010: Séminaire Probabiltés, ENS Lyon & Univ. Lyon 1.
- April 2010: Séminaire Physique Mathématiques, Institut Fourier, Grenoble.
- June 2010: International Conference on Advances in PDE and their applications, Fudan Univ., Shangai.
- June 2010: Mathematical problems in Hydrodynamics, Univ. Cergy-Pontoise.
- December 2010: Berliner Kolloquium Wahrscheinlichkeitstheorie, T.U. Berlin.

## 7.5. International exchanges

- P. Chartier visited the University of the Basque Country for two weeks.
- Arnaud Debussche visited the Isaac Newton Institute, Cambridge, for one month.

# 8. Bibliography

## 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.

[2] A. AUBRY, P. CHARTIER. *On improving the convergence of Radau IIA methods when applied to index-2 DAEs*, in "SIAM Journal on Numerical Analysis", 1998, vol. 35, n$^{o}$ 4, p. 1347-1367.

[3] A. AUBRY, P. CHARTIER. *Pseudo-symplectic Runge-Kutta methods*, in "BIT", 1998, vol. 38, p. 439–461.

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

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

[6] R. CHAN, P. CHARTIER, A. MURUA. *Post-projected Runge-Kutta methods for index-2 differential-algebraic equations*, in "Applied Numerical Mathematics", 2002, vol. 42, n° 1-3, p. 77-94.

[7] M. DAUGE, I. DJURDJEVIC, E. FAOU, A. ROESSLE. *Eigenmode asymptotics in thin elastic plates*, in "J. Math. Pures Appl.", 1999, vol. 78, p. 925-954.

[8] E. FAOU. *Elasticity on a thin shell: Formal series solution*, in "Asymptotic analysis", 2002, vol. 31, p. 317-361.

## Publications of the year

### Articles in International Peer-Reviewed Journal

[9] P. CHARTIER, E. DARRIGRAND, E. FAOU. *A regular fast multipole method for geometric numerical integrations of Hamiltonian systems*, in "BIT Numerical Mathematics", 2010, vol. 50, n° 1, p. 23-40 [*DOI :* 10.1007/s10543-010-0248-6], http://hal.inria.fr/hal-00536695/en.

[10] P. CHARTIER, E. HAIRER, G. VILMART. *Algebraic structures of B-series*, in "Found. Comput. Math.", 2010, vol. 10, n° 4, p. 407–427, http://dx.doi.org/10.1007/s10208-010-9065-1.

[11] P. CHARTIER, A. MURUA, J. M. SANZ-SERNA. *Higher-Order Averaging, Formal Series and Numerical Integration I: B-series*, in "Foundations of Computational Mathematics", 2010, vol. 10, p. 695-727, 10.1007/s10208-010-9074-0, http://dx.doi.org/10.1007/s10208-010-9074-0.

[12] G. DA PRATO, A. DEBUSSCHE. *Asymptotic behavior of stochastic PDEs with random coefficients*, in "DCDS A", 2010, vol. 27, n° 4, p. 1553–1570.

[13] M. DAUGE, E. FAOU. *Koiter Estimate Revisited*, in "Mathematical Models and Methods in Applied Sciences", 2010, vol. 20, n° 1, p. pp. 1-42 [*DOI :* 10.1142/S0218202510004131], http://hal.inria.fr/hal-00202628/en.

[14] M. DAUGE, E. FAOU, V. PÉRON. *Comportement asymptotique à haute conductivité de l'épaisseur de peau en électromagnétisme*, in "C. R. Acad. Sci. Paris, Sér. I.", 2010, vol. 348, p. 385–390.

[15] A. DE BOUARD, A. DEBUSSCHE. *The nonlinear Schrodinger equation with white noise dispersion*, in "Journal of Funct. Anal.", 2010, vol. 259, n° 1, p. pp. 1300-1321.

[16] A. DEBUSSCHE. *Weak approximation of stochastic partial differential equations: the nonlinear case*, in "Math. of Comp.", 2010, To appear.

[17] A. DEBUSSCHE, M. HOGELE, P. IMKELLER. *Asymptotic first exit times of the Chafee-Infante equation with small heavy tailed noise*, in "Elect. Comm. Prob.", 2010, To appear.

[18] A. DEBUSSCHE, Y. HU, G. TESSITORE. *Ergodic BSDEs under weak dissipative assumptions*, in "Stoch. Proc; Appl.", 2010, To appear.

[19] A. DEBUSSCHE, Y. TSUSTUMI. *1D quintic nonlinear equation with white noise dispersion*, in "Journal de Math. Pures et Appl.", 2010, To appear.

[20] A. DEBUSSCHE, J. VOVELLE. *Scalar conservation laws with stochastic forcing*, in "Journal of Funct. Anal.", 2010, vol. 259, p. 1014–1042.

[21] E. FAOU, B. GRÉBERT. *Hamiltonian interpolation of splitting approximations for nonlinear PDEs*, in "Found. Comput. Math.", 2010, In revision.

[22] E. FAOU, B. GRÉBERT. *Quasi invariant modified Sobolev norms for semi linear reversible PDEs*, in "Nonlinearity", 2010, vol. 23, p. 429–443.

[23] E. FAOU, B. GRÉBERT, E. PATUREL. *Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs. Part I: Finite dimensional discretization.*, in "Numer. Math.", 2010, vol. 114, p. 429–458.

[24] E. FAOU, B. GRÉBERT, E. PATUREL. *Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs. Part II: Abstract splitting.*, in "Numer. Math.", 2010, vol. 114, p. 459–490.

### Invited Conferences

[25] G. CALOZ, M. DAUGE, E. FAOU, V. PÉRON, C. POIGNARD. *A Transmission Problem in Electromagnetism with a Singular Interface*, in "6th Singular Days on Asymptotic Methods for PDEs", Allemagne Berlin, May 2010, http://hal.inria.fr/inria-00528523/en.

[26] V. PÉRON, G. CALOZ, M. DAUGE, E. FAOU. *Skin Effect in Electromagnetism and Asymptotic Behaviour of Skin Depth for High Conductivity*, in "WONAPDE 2010 Third Chilean Workshop on Numerical Analysis of Partial Differential Equations", Chili Concepcion, Jan 2010, http://hal.inria.fr/inria-00528519/en.

### Research Reports

[27] E. ANCEAUME, F. CASTELLA, R. LUDINARD, B. SERICOLA. *Markov Chains Competing for Transitions: Application to Large-Scale Distributed Systems*, INRIA, May 2010, http://hal.inria.fr/inria-00485667/en.

### Other Publications

[28] G. CALOZ, M. DAUGE, E. FAOU, V. PÉRON. *On the influence of the geometry on skin effect in electromagnetism*, 2010, unpublished, http://hal.inria.fr/hal-00503170/en.

[29] R. CARLES, E. FAOU. *Energy cascades for NLS on $T^d$*, 2010, unpublished, http://hal.inria.fr/hal-00528792/en.

[30] F. CASTELLA, E. DUMAS. *High frequency behaviour of the Maxwell-Bloch model with relaxations: convergence to the Schrödinger-Boltzmann system*, 2010, unpublished, http://hal.inria.fr/hal-00505587/en.

[31] N. CHAMPAGNAT, C. CHIPOT, E. FAOU. *Reconciling alternate methods for the determination of charge distributions: A probabilistic approach to high-dimensional least-squares approximations*, 2010, unpublished, http://hal.inria.fr/inria-00345411/en.

[32] E. FAOU, B. GRÉBERT. *A Nekhoroshev type theorem for the nonlinear Schrödinger equation on the d-dimensional torus.*, 2010, unpublished, http://hal.inria.fr/hal-00466803/en.

## References in notes

[33] D. CALAQUE, K. EBRAHIMI-FARD, D. MANCHON. *Two Hopf algebras of trees interacting*, 2008, http://www.citebase.org/abstract?id=oai:arXiv.org:0806.2238.

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

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

[36] E. HAIRER, G. WANNER. *On the Butcher group and general multi-value methods*, in "Computing", 1974, vol. 13, p. 1–15.

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

[38] A. ISERLES, H. Z. MUNTHE-KAAS, S. P. NØRSETT, A. ZANNA. *Lie-group methods*, in "Acta Numerica", 2000, p. 215–365.

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

[40] C. LUBICH. *On variational approximations in quantum molecular dynamics*, in "Math. Comp.", 2009, to appear.

[41] F. A. POTRA, W. C. RHEINBOLDT. *On the numerical solution of Euler-Lagrange equations*, in "Mech. Struct. & Mech.", 1991, vol. 19, p. 1–18.

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