INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

# *Project-Team IPSO*

# *Invariant Preserving Solvers*

*Rennes - Bretagne-Atlantique*

Theme : Computational models and simulation

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# 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 [53], [46], [44] and led to many significant theoretical achievements (symplectic and symmetric methods, volume-preserving integrators, Lie-group methods, ...). In practice, a few simple schemes such as the Verlet method or the Störmer method have been used for years with great success in molecular dynamics or astronomy. However, they now need to be further improved in order to fit the tremendous increase of complexity and size of the models.

## 2.2. Overall objectives

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

- systems of differential equations posed on a manifold.
- systems of differential-algebraic equations of index 2 or 3, where the constraints are part of the equations.
- Hamiltonian systems and constrained Hamiltonian systems (which are special cases of the first two items though with some additional structure).
- highly-oscillatory systems (with a special focus of those resulting from the Schrödinger equation).

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

- There is a large demand in biomolecular modeling for models that integrate microscopic molecular dynamics simulation into statistical macroscopic quantities. These simulations involve huge systems of ordinary differential equations over very long time intervals. This is a typical situation where the determination of accurate trajectories is out of reach and where one has to rely on the good qualitative behavior of structure-preserving integrators. Due to the complexity of the problem, more efficient numerical schemes need to be developed.
- The demand for new models and/or new structure-preserving schemes is also quite large in laser simulations. The propagation of lasers induces, in most practical cases, several well-separated scales: the intrinsically highly-oscillatory *waves* travel over long distances. In this situation, filtering the oscillations in order to capture the long-term trend is what is required by physicists and engineers.

# 3. Scientific Foundations

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

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

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 [43] 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, Guillaume Dujardin, Erwan Faou, Gilles Vilmart.

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, Guillaume Dujardin, 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 [50], [49] 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 [51] or of *Lie-methods* [47] 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. A Fast Multipole Method for Geometric Numerical Integrations of Hamiltonian Systems

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

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 [14], 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.

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

**Participants:** Philippe Chartier, Gilles Vilmart.

This is a joint work with E. Hairer, from the University of Geneva.

Following the pioneering work of Butcher [34], [35] in the study of order conditions for Runge-Kutta methods applied to ordinary differential equations

$$\left\{ \begin{array}{rcl} \dot{y} & = & f(y) \\ y(0) & = & y_0 \end{array} \right. , \tag{15}$$

Hairer and Wanner [45] introduced the concept of B-series. A B-series $B(f,a)(y)$ is a formal expression of the form

$$B(f,a)(y) \quad = \quad y + \sum_{t \in T} \frac{h^{|t|}}{\sigma(t)} a(t)\, F(t)(y) \tag{16}$$

where the index set $T$ is a set of rooted trees, $\sigma$ and $a$ are real coefficients, and $F(t)$ a derivative of $f$ associated to $t$. 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 [15] 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 [36], 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.

## 5.3. Resonances in long time integration of semi-linear Hamiltonian PDEs.

**Participant:** Erwan Faou.

In this joint work [31] with B. Grébert (University of Nantes), we consider a class of Hamiltonian PDEs that can be split into a linear unbounded operator and a regular non linear part, and we analyze their numerical discretizations by symplectic methods when the initial value is small in Sobolev norms. The goal of this work is twofold: First we show how standard approximation methods cannot in general avoid resonances issues, and we give numerical examples of pathological behavior for the midpoint rule and implicit-explicit integrators. Such phenomena can be avoided by suitable truncations of the linear unbounded operator combined with classical splitting methods. We then give a sharp bound for the cut-off depending on the time step. Using a new normal form result, we show the long time preservation of the actions for such schemes for all values of the time step, provided the initial continuous system does not exhibit resonant frequencies. This work in is the continuation of the previous publications [24], [25].

## 5.4. Quasi invariant modified Sobolev norms for semi-linear reversible PDEs.

**Participant:** Erwan Faou.

In this joint work [30] with B. Grébert (University of Nantes), we consider a general class of infinite dimensional reversible differential systems. Assuming a non resonance condition on the linear frequencies, 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 (NLS) 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 techniques that we use to prove the existence of quasi invariant pseudo norms is much more simple and direct.

## 5.5. Modified energy for split-step methods applied to the linear Schrödinger equation.

**Participants:** Arnaud Debussche, Erwan Faou.

In this work [20] we consider the linear Schrödinger equation and its discretization by split-step methods where the part corresponding to the (unbounded) Laplace operator is approximated by the midpoint rule. We show that the numerical solution coincides with the exact solution of a modified partial differential equation at each time step. This shows the existence of a modified energy preserved by the numerical scheme over arbitrarily long time. This energy is close to the exact energy if the numerical solution is smooth. As a consequence, we give uniform regularity estimates for the numerical solution over arbitrarily long time. The analysis is valid in the case where the Schrödinger equation is set on a domain with periodic boundary condition, or on the whole space. This “backward error analysis" result is the first one given for the case of symplectic method applied to a Hamiltonian Partial differential equation (which is considered here as an infinite dimensional ordinary differential equation).

## 5.6. Birkhoff normal form for splitting methods applied semi linear Hamiltonian PDEs. Part II: Abstract splitting

**Participant:** Erwan Faou.

This work [25] extends the results of the previous paper to the case where no space discretization is made in the splitting methods applied to Hamiltonian PDEs that can be split into a linear unbounded operator and a regular non linear part. Obtaining results for the abstract splitting method is equivalent to obtaining bounds in classical Birkhoff normal form results that are independent of the dimension of the phase space. Using techniques recently developed to prove conservation results for the exact solution of Hamiltonian PDEs, we prove a normal form result for the corresponding discrete flow under generic non resonance conditions on the frequencies of the linear operator and on the step size. This result implies the conservation of the regularity of the numerical solution associated with the splitting method over arbitrary long time, provided the initial data is small enough. This result holds for numerical schemes controlling the round-off error at each step to avoid possible high frequency energy drift.

## 5.7. A probabilistic approach of high-dimensional least-squares approximations

**Participant:** Erwan Faou.

The main goal of this work is to derive and analyze new schemes for the numerical approximation of least-squares problems set on high dimensional spaces. This work [29],originates from the Statistical Analysis of Distributed Multipoles (SADM) algorithm introduced by Chipot *et al.* in 1998 for the derivation of atomic multipoles from the quantum mechanical electrostatic potential mapped on a grid of points surrounding a molecule of interest. The main idea is to draw subsystems of the original large least-square problem and compute the average of the corresponding distribution of solutions as an approximation of the original solution. Moreover, this method not only provides a numerical approximation of the solution, but a global statistical distribution reflecting the accuracy of the physical model used.

Strikingly, it turns out that this kind of approach can be extended to many situations arising in computational mathematics and physics. The principle of the SADM algorithm is in fact very general, and can be adapted to derive efficient algorithms that are robust with the dimension of the underlying space of approximation. This provides new numerical methods that are of practical interest for high dimensional least-squares problems where traditional methods are impossible to implement.

The goal of this paper is twofold:

- Give a general mathematical framework, and analyze the consistency, convergence and cost of these new algorithms in an abstract setting and in specific situations where calculations can be made explicit (Wishart or subgaussian distribution). The main outcome is that the subsystems drawn from the original system have to be chosen rectangular and not square (as initially proposed in the SADM method) to obtain convergent and efficient algorithms.
- Apply these results to revisit and improve the SADM method. This is mainly done in Section 5 by considering the three-point charge model of water.

## 5.8. Computing semi-classical quantum dynamics with Hagedorn wavepackets

**Participant:** Erwan Faou.

In Ref. [26], we consider the approximation of multi-particle quantum dynamics in the semiclassical regime by Hagedorn wavepackets, which are products of complex Gaussians with polynomials that form an orthonormal $L2$ basis and preserve their type under propagation in Schrödinger equations with quadratic potentials. We build a time-reversible, fully explicit time-stepping algorithm to approximate the solution of the Hagedorn wavepacket dynamics. The algorithm is based on a splitting between the kinetic and potential part of the Hamiltonian operator, as well as on a splitting of the potential into its local quadratic approximation and the remainder. The algorithm is robust in the semi-classical limit. It reduces to the Strang splitting of the Schrödinger equation in the limit of the full basis set, and it advances positions and momenta by the Störmer-Verlet method for the classical equations of motion. The algorithm allows for the treatment of multi-particle problems by thinning out the basis according to a hyperbolic cross approximation, and of high-dimensional problems by Hartree-type approximations in a moving coordinate frame.

## 5.9. Conservative stochastic differential equations: Mathematical and numerical analysis

**Participant:** Erwan Faou.

In Ref. [27], we consider stochastic differential equations on the whole Euclidean space possessing a scalar invariant along their solutions. The stochastic dynamics therefore evolves on a hypersurface of the ambiant space. Using orthogonal coordinate systems, we show the existence and uniqueness of smooth solutions of the Kolmogorov equation under some ellipticity conditions over the invariant hypersurfaces. If we assume moreover the existence of an invariant measure, we show the exponential convergence of the solution towards its average. In a second part, we consider numerical approximation of the stochastic differential equation, and show the convergence and numerical ergodicity of a class of projected schemes. In the context of molecular dynamics, this yields numerical schemes that are ergodic with respect to the microcanonical measure over isoenergy surfaces.

## 5.10. Analysis of splitting methods for reaction-diffusion problems using stochastic calculus

**Participant:** Erwan Faou.

In Ref. [23], we consider linear and nonlinear reaction-diffusion problems, and their time discretization by splitting methods. We give probabilistic interpretations of the splitting schemes, and show how these representations allow to give error bounds for the deterministic propagator under weak hypothesis on the reaction part. To show these results, we only use the Itô formula, and basic properties of solutions of stochastic differential equations. Eventually, we show how probabilistic representations of splitting schemes can be used to derive "hybrid" numerical schemes based on Monte Carlo approximations of the splitting method itself.

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

**Participant:** Arnaud Debussche.

In this work [19], 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.

## 5.12. Long-time behavior in scalar conservation laws

**Participant:** Arnaud Debussche.

In this joint work [22] with J. Vovelle (Université de Lyon 1), we consider the long-time behavior of the entropy solution of a first-order scalar conservation law on a Riemannian manifold. In the case of the torus, we show that, under a weak property of genuine non-linearity of the flux, the solution converges to its average value in $L^p$, $1 \leq p < +\infty$. We give a partial result in the general case.

## 5.13. Soliton dynamics for the Korteweg-de Vries equation with multiplicative homogeneous noise

**Participant:** Arnaud Debussche.

In this joint work [28] with A. de Bouard (CMAP, Polytechnique), we consider a randomly perturbed Korteweg-de Vries equation. The perturbation is a random potential depending both on space and time, with a white noise behavior in time, and a regular, but stationary behavior in space. We investigate the dynamics of the soliton of the KdV equation in the presence of this random perturbation, assuming that the amplitude of the perturbation is small. We estimate precisely the exit time of the perturbed solution from a neighborhood of the modulated soliton, and we obtain the modulation equations for the soliton parameters. We moreover prove a central limit theorem for the dispersive part of the solution, and investigate the asymptotic behavior in time of the limit process.

## 5.14. Weak order for the discretization of the stochastic heat equation

**Participant:** Arnaud Debussche.

In this joint work [21] with J. Printems (Université Paris XII), we study the approximation of the distribution of $X_t$ Hilbert–valued stochastic process solution of a linear parabolic stochastic partial differential equation written in an abstract form as

$$dX_t + AX_t\,dt = Q^{1/2}dW_t, \quad X_0 = x \in H, \quad t \in [0,T],$$

driven by a Gaussian space time noise whose covariance operator $Q$ is given. We assume that $A^{-\alpha}$ is a finite trace operator for some $\alpha > 0$ and that $Q$ is bounded from $H$ into $D(A^\beta)$ for some $\beta \geq 0$. It is not required to be nuclear or to commute with $A$.

The discretization is achieved thanks to finite element methods in space (parameter $h > 0$) and implicit Euler schemes in time (parameter $\Delta t = T/N$). We define a discrete solution $X_h^N$ and for suitable functions $\varphi$ defined on $H$, we show that

$$|E\,\varphi(X_h^N) - E\,\varphi(X_T)| = O(h^{2\gamma} + \Delta t^\gamma)$$

where $\gamma < 1 - \alpha + \beta$. Let us note that as in the finite dimensional case the rate of convergence is twice the one for pathwise approximations.

## 5.15. Hybrid stochastic simplifications for multiscale gene networks

**Participant:** Arnaud Debussche.

This joint work [18] with A. Crudu and O. Radulescu (Université Rennes 1) concerns stochastic simulation of gene networks by Markov processes. This has important applications in molecular biology. The complexity of exact simulation algorithms scales with the number of discrete jumps to be performed. Approximate schemes reduce the computational time by reducing the number of simulated discrete events. Also, answering important questions about the relation between network topology and intrinsic noise generation and propagation should be based on general mathematical results. These general results are difficult to obtain for exact models.

We propose a unified framework for hybrid simplifications of Markov models of multiscale stochastic gene networks dynamics. We discuss several possible hybrid simplifications, and provide algorithms to obtain them from pure jump processes. In hybrid simplifications, some components are discrete and evolve by jumps, while other components are continuous. Hybrid simplifications are obtained by partial Kramers-Moyal expansion which is equivalent to the application of the central limit theorem to a sub-model. By averaging and variable aggregation we drastically reduce simulation time and eliminate non-critical reactions. Hybrid and averaged simplifications can be used for more effective simulation algorithms and for obtaining general design principles relating noise to topology and time scales. The simplified models reproduce with good accuracy the stochastic properties of the gene networks, including waiting times in intermittence phenomena, fluctuation amplitudes and stationary distributions. The methods are illustrated on several gene network examples.

We conclude that hybrid simplifications can be used for onion-like (multi-layered) approaches to multi-scale biochemical systems, in which various descriptions are used at various scales. Sets of discrete and continuous variables are treated with different methods and are coupled together in a physically justified approach.

## 5.16. Moments analysis in Markov reward models.

**Participants:** François Castella, Guillaume Dujardin.

In this paper [13], we analyze the moments of the accumulated reward over the interval $(0, t)$ in a continuous-time Markov chain. We develop a numerical procedure to compute efficiently the normalized moments using the uniformization technique. Our algorithm involves auxiliary quantities whose convergence is analyzed, and for which we provide a probabilistic interpretation.

## 5.17. The strongly confined Schrödinger-Poisson system for the transport of electrons in a nanowire.

**Participant:** François Castella.

In [9], we study the limit of the three-dimensional Schrödinger-Poisson system with a singular perturbation, to model a quantum electron gas that is strongly confined near an axis. For well-prepared data, which are polarized on the ground space of the transversal Hamiltonian, the resulting model is the cubic defocusing nonlinear Schrödinger equation. Our main tool is a refined analysis of the Poisson kernel when acting on strongly confined densities. In that direction, an appropriate scaling of the initial data is required, to avoid divergent integrals when the gas concentrates on the axis.

## 5.18. An averaging technique for highly-oscillatory Hamiltonian problems.

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

In this work [11], we are concerned with the numerical solution of highly-oscillatory Hamiltonian systems with a stiff linear part. We construct an averaged system whose solution remains close to the exact one over bounded time intervals, possesses the same adiabatic and Hamiltonian invariants as the original system, and is non-stiff. We then investigate its numerical approximation through a method which combines a symplectic integration scheme and an acceleration technique for the evaluation of time-averages developped in an earlier work by the authors. Eventually, we demonstrate the efficiency of our approach on two test problems with one or several frequencies.

## 5.19. Propagation of Gevrey regularity over long times for the fully discrete Lie Trotter splitting scheme applied to the linear Schrödinger equation.

**Participants:** François Castella, Guillaume Dujardin.

In this work [12], we study the linear Schrödinger equation over the d-dimensional torus, with small values of the perturbing potential. We consider numerical approximations of the associated solutions obtained by a symplectic splitting method (to discretize the time variable) in combination with the Fast Fourier Transform algorithm (to discretize the space variable). In this fully discrete setting, we prove that the regularity of the initial datum is preserved over long times, i.e. times that are exponentially long with the time discretization parameter. We here refer to Gevrey regularity, and our estimates turn out to be uniform in the space discretization parameter. This paper extends the previous work by G. Dujardin and E. Faou, where a similar result has been obtained in the semi-discrete situation, i.e. when the mere time variable is discretized and space is kept a continuous variable.

## 5.20. Splitting methods with complex times for parabolic equations

**Participants:** François Castella, Philippe Chartier, Gilles Vilmart.

This is a joint work with S. Descombes, from the University of Nice.
Although the numerical simulation of the heat equation in several space dimension is now well understood, there remain a lot of challenges in the presence of an external source, *e.g.* for reaction-diffusion problems, or more generally for the complex Ginzburg-Landau equation. From a mathematical point of view, these belong to the class of semi-linear parabolic partial differential equations and can be represented in the general form

$$\frac{\partial u}{\partial t} = D\Delta u + F(u).$$

When one wishes to approximate the solution of the above parabolic non-linear problem, a method of choice is based on operator-splitting: the idea is to split the abstract evolution equation into two parts which can be solved explicitly or at least approximated efficiently.

For a positive step size $h$, the most simple numerical integrator is the Lie-Trotter splitting which is an approximation of order 1, while the symmetric version is referred to as the Strang splitting and is an approximation of order 2. For higher orders, one can consider general splitting methods of the form

$$e^{b_1 hV} e^{a_1 h\Delta} e^{b_2 hV} e^{a_2 h\Delta} \ldots e^{b_s hV} e^{a_s h\Delta}. \tag{17}$$

However, achieving higher order is not as straightforward as it looks. A disappointing result indeed shows that all splitting methods (or composition methods) with real coefficients must have negative coefficients $a_i$ and $b_i$ in order to achieve order 3 or more. The existence of at least one negative coefficient was shown in [55], [56], and the existence of a negative coefficient for both operators was proved in [42]. An elegant geometric proof can be found in [33]. As a consequence, such splitting methods *cannot* be used when one operator, like $\Delta$, is not time-reversible.

In order to circumvent this order-barrier, there are two possibilities. One can use a linear, convex (see [40], [41], [32] for methods of order 3 and 4) or non-convex (see [54], [39] where an extrapolation procedure is exploited), combinations of elementary splitting methods like (17). Another possibility is to consider splitting methods with *complex* coefficients $a_i$ and $b_i$ with positive real parts (see [37] in celestrial mechanics). In 1962/1963, Rosenbrock [52] considered complex coefficients in a similar context.

In [10], we consider splitting methods, and we derive new high-order methods using composition techniques originally developed for the geometric numerical integration of ordinary differential equations [44]. The main advantages of this approach are the following:

- the splitting method inherits the stability property of exponential operators;
- we can replace the costly exponentials of the operators by cheap low order approximations without altering the overall order of accuracy;
- using complex coefficients allows to reduce the number of compositions needed to achieve any given order;

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

**Participant:** Philippe Chartier.

In [17], 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.

## 5.22. An algebraic theory of order

**Participant:** Philippe Chartier.

This a joint work with Ander Murua, from the University of the Basque Country.

When one needs to compute the numerical solution of a differential equation of a specific type (ordinary, differential-algebraic, linear...) with a method of a given class of numerical schemes, a deciding criterion to pick up the right one is its order of convergence: the systematic determination of order conditions thus appears as a pivotal question in the numerical analysis of differential equations. Given a family of vector fields with some specific property (say for instance linear, additively split into a linear and a nonlinear part, scalar...) and a set of numerical schemes (rational approximations of the exponential, exponential integrators , Runge-Kutta methods...), a fairly general recipe consists in expanding into series both the exact solution of the problem and its numerical approximation: order conditions are then derived by comparing the two series term by term, once their independence has been established. Depending on the equation and on the numerical method, these series can be indexed by integers or trees, and can be expressed in terms of elementary differentials or commutators of Lie-operators. Despite the great variety of situations encountered in practice and of ad-hoc techniques, the problems raised are strikingly similar and can be described as follows:

(Q1) is it possible to construct a set of algebraically independent order conditions?

(Q2) what are the order conditions corresponding to a scheme obtained by composition of two given methods?

(Q3) are there numerical schemes within the class considered of arbitrarily high order for arbitrary vector field?

(Q4) are there numerical schemes within the set of methods considered that approximate modified fields?

The Butcher group [35] and its underlying Hopf algebra of rooted trees were originally formulated to address these questions for Runge-Kutta methods. In the past few years, these concepts turned out to have far-reaching applications in several areas of mathematics and physics: they were rediscovered in noncommutative geometry by Connes and Moscovici [38] and they describe the combinatorics of renormalization in quantum field theory as described by Kreimer [48]. In the present work, we show that the Hopf algebra of rooted trees associated to Butcher's group can be seen as a particular instance of a more general construction: given a group $G$ of integrations schemes (satisfying some natural assumptions), we exhibit a sub-algebra of the algebra of functions acting on $G$, which is graded, commutative and turns out to be a Hopf algebra. Within this algebraic framework, we then address the questions listed above and provide answers that are relevant to many practical situations.

The paper [16] introduces an algebraic concept, called *group of asbtract integration schemes*, composed of a group of integrators $G$, an algebra $H$ of functions on $G$ and a scaling map $\nu$ whose existence is essential to the subsequent results. We begin by proving that, under some reasonable assumptions of a purely algebraic nature, the algebra $H$ can be equipped with a co-product, an antipode and an embedded family of equivalence relations (called order), thus giving rise to a graded Hopf algebra structure. In particular, the co-product of $H$ is per se the key to the second question in our list. It furthermore endows the linear dual $H^*$ of $H$ with an algebra structure, where a new group $\mathbf{G}$ and a Lie-algebra $\mathbf{g}$ can be defined and related through the exponential and logarithm maps. These two structures are of prime interest, since $\mathbf{g}$ can be interpreted, in the more usual terminology of ODEs, as the set of "modified vector fields", while $\mathbf{G}$ can be intrepreted as the larger group of "integrators" containing $G$. We then prove that all elements of $\mathbf{G}$ can be "approximated" up to any order by elements of $G$. Although there seems to be no appropriate topology for $G$ and $\mathbf{G}$, we can interpret this result by saying that $G$ is dense in $\mathbf{G}$: this anwers the third and fourth questions in our list. Note that the proof of this result also provides a positive answer to the first question of our list.

Finally, we describe how our theory can be used to obtain order conditions for composition schemes.

# 6. Other Grants and Activities

## 6.1. National Grants

**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. In 2009, this program financed visits from P. Chartier, A. Murua and E. Faou, as well as participations to the Scicade 09 and Icnaam 09 conference to present the work of the associated team.

This program was valid for two years (2008 and 2009).

### *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 is 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 was guest editor-in-chief of a special issue of M2AN devoted to numerical methods for the integration of ODEs which appeared in July 2009.
- 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.

## 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").
- E. Faou was lecturer at the Ecole Normale Supérieure de Cachan Bretagne. Course: *Ordinary differential equations.*

## 7.4. Participation in conferences

- P. Chartier gave a seminar at CERMICS, November 12, 2009.
- P. Chartier gave a seminar at the University of Tuebingen, November 2, 2009.
- P. Chartier gave a talk at the Seventh International Conference of Numerical Analysis and Applied Mathematics (ICNAAM 2009), Crete, September 18-22, 2009 (Invited Plenary Speaker).
- P. Chartier participated to the Conference on Scientific Computing, Conference in honour of the 60th birthday of E. Hairer, Geneva, June 17-20, 2009 (Co-organiser of the mini-symposium "Algebraic tools in numerical analysis of ODEs").

- P. Chartier gave a talk at SciCADE09, Beijing, China, May 25-29, 2009 (Invited Speaker; co-organiser with H. Munthe-Kass of the mini-symposium “Butcher trees”; member of the scientific committee).
- P. Chartier gave a seminar at Jacques-Louis Lions Laboratory, Paris VI, April 10, 2009.
- P. Chartier gave a seminar at the University of Valladolid, March 25, 2009.
- E. Faou gave a mini-course in the Rencontres EDP/Probas, Institut Henri Poincaré, Paris, October 2009.
- E. Faou gave a talk in the ICNAAM 09 conference on the occasion of the 60th birthday of Ernst Hairer, September 2009.
- E. Faou gave a talk in the ICOSAHOM 09 conference, Trondheim (Norway), June 2009.
- E. Faou gave a talk in the SCICADE 09 conference in Beijing, China, May 2009.
- E. Faou gave a talk in the Seminar for Applied Mathematics, ETH Zuerich, April 2009.
- E. Faou gave a talk in the Numerical Analysis Seminar, University of Cambridge (UK), February 2009.
- F. Castella has been invited to the Workshop “Theory and Applications of Classical and Quantum Kinetic Theory”, Banff International Research Station, Canada, 2009.

## 7.5. International exchanges

### *7.5.1. Visits*

- P. Chartier visited the University of the Basque Country for two weeks.
- P. Chartier visited the University of Tuebingen for one week.
- E. Faou was invited in the Institute of Mathematics of the Academy of Mathematics and Systems Science (Chinese Academy of Sciences), Beijing, China, may 2009.
- E. Faou was invited in the university of Mexico (UNAM, Cuernavaca) in march 2009.

### *7.5.2. Visitors*

The team has invited the following persons :

- A. Murua for a one-week visit.

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# Year Publications

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