INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team IPSO

Invariant Preserving Solvers

Rennes

THEME NUM

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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 [46], [37], [36] 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

Keywords: *Hamiltonian system*, *Lie-group system*, *invariant*, *numerical integrator*, *ordinary differential equation*, *reversible system*.

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

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

For a given y_0, the solution $y(t)$ at time t is denoted $\phi_t(y_0)$. For fixed t, ϕ_t becomes a function of y_0 called the *flow* of (1). From this point of view, a numerical scheme with step size h for solving (1) may be regarded as an approximation Φ_h of ϕ_h. One of the main questions of *geometric integration* is whether *intrinsic* properties of ϕ_t may be passed on to Φ_h.

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

3.1.1. Reversible ODEs

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

$$\rho \circ \phi_t = \phi_t^{-1} \circ \rho = \phi_{-t} \circ \rho. \tag{2}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

3.1.2. ODEs with an invariant manifold

The system (1) is said to have an invariant manifold g whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{3}$$

is kept *globally* invariant by ϕ_t. In terms of derivatives and for sufficiently differentiable functions f and g, this means that

$$\forall\, y \in \mathcal{M},\ g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [35] 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 ω, i.e. if

$$\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

3.1.4. Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository section, it is enough to present the so-called index-2 systems

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

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

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

and of the so-called hidden manifold

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

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

Keywords: *oscillatory solutions*, *second-order ODEs*, *step size restrictions*.

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

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

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

$$h\omega < C,$$

where C is a constant depending on the numerical method and where ω is the highest frequency of the problem, i.e. in this situation the square root of the largest eigenvalue of $\nabla^2 W$. In applications to molecular dynamics for instance, *fast* forces deriving from W (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another prominent example of highly-oscillatory systems is encountered in quantum dynamics where the Schrödinger equation is the model to be used. Assuming that the Laplacian has been discretized in space, one indeed gets the *time*-dependent Schrödinger equation:

$$i\dot{\psi}(t) = \tfrac{1}{\varepsilon} H(t)\psi(t), \tag{7}$$

where $H(t)$ is finite-dimensional matrix and where ε typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are confronted once again to two different time-scales, 1 and ε. In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

3.3. Geometric schemes for the Schrödinger equation

Keywords: *Schrödinger equation*, *energy conservation*, *variational splitting*.

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, ε is a (small) positive number representing the scaled Planck constant and i is the complex imaginary unit. The Hamiltonian operator H is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N} \frac{\varepsilon^2}{2m_k} \Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and Δ_{x_k} the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential V acts as a multiplication operator on ψ.

The multiplication by i in (8) plays the role of the multiplication by J in classical mechanics, and the energy $\langle \psi | H | \psi \rangle$ is conserved along the solution of (8), using the physicists' notations $\langle u|A|u\rangle = \langle u, Au\rangle$ where $\langle\ ,\ \rangle$ denotes the Hermitian L^2-product over the phase space. In quantum mechanics, the number N of particles is very large making the direct approximation of (8) very difficult.

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [42], [43] for reviews, and [34] for the case of Gaussian wave packets dynamics detailed in Section 5.1. 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:

$$\psi_1 = \exp(-i(\delta t)V/2)\exp(i(\delta t)\Delta)\exp(-i(\delta t)V/2)\psi_0 \tag{9}$$

where δt is the time increment (we have set all the parameters to 1 in the equation). As the Laplace operator is unbounded, we cannot apply the standard methods used in ODEs to derive long-time properties of these schemes. However, its projection onto finite dimensional submanifolds (such as Gaussian wave packets space or FEM finite dimensional space of functions in x) may exhibit Hamiltonian or Poisson structure, whose long-time properties turn out to be more tractable.

3.4. High-frequency limit of the Helmholtz equation

Keywords: *Helmholtz equation*, *high oscillations*, *waves*.

Participant: François Castella.

The Helmholtz equation modelizes 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

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x) u_\varepsilon = f_\varepsilon(x).$$

Here, ε is the small adimensional parameter that measures the typical wavelength of the signal, $n(x)$ is the space-dependent refraction index, and $f_\varepsilon(x)$ is a given (possibly dependent on ε) source term. The unknown is $u_\varepsilon(x)$. One may think of an antenna emitting waves in the whole space (this is the $f_\varepsilon(x)$), thus creating at any point x the signal $u_\varepsilon(x)$ along the propagation. The small $\alpha_\varepsilon > 0$ term takes into account damping of the waves as they propagate.

One important scientific objective typically is to describe the high-frequency regime in terms of *rays* propagating in the medium, that are possibly refracted at interfaces, or bounce on boundaries, etc. Ultimately, one would like to replace the true numerical resolution of the Helmholtz equation by that of a simpler, asymptotic model, formulated in terms of rays.

In some sense, and in comparison with, say, the wave equation, the specificity of the Helmholtz equation is the following. While the wave equation typically describes the evolution of waves between some initial time and some given observation time, the Helmholtz equation takes into account at once the propagation of waves over *infinitely long* time intervals. Qualitatively, in order to have a good understanding of the signal observed in some bounded region of space, one readily needs to be able to describe the propagative phenomena in the whole space, up to infinity. In other words, the “rays” we refer to above need to be understood from the initial time up to infinity. This is a central difficulty in the analysis of the high-frequency behaviour of the Helmholtz equation.

3.5. From the Schrödinger equation to Boltzmann-like equations

Keywords: *Boltzmann equation*, *Schrödinger equation*, *asymptotic model*.

Participant: François Castella.

The Schrödinger equation is the appropriate 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,

$$i\partial_t\psi(t,x) = -\tfrac{1}{2}\Delta_x\psi + V(x)\psi,$$

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 :

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v')\,[f(t,x,v') - f(t,x,v)]dv'.$$

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

Keywords: *manifold*, *spatial approximation*, *triangulation*.

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:

$$\begin{array}{rcl} \tilde{y}'(t) & = & \tilde{f}(\tilde{y}(t)), \\ \tilde{y}(0) & = & \tilde{y}_0, \end{array} \tag{10}$$

on an invariant manifold $\tilde{\mathcal{M}} = \{y \in \mathbb{R}^n; \tilde{g}(y) = 0\}$, where $\tilde{f}$ and $\tilde{g}$ 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 $\tilde{\mathcal{M}}$ for which an atlas consisting of *easily computable* charts exists. If this is the case, one can reformulate the vector field $\tilde{f}$ on each domain of the atlas in an *easy* way. The main obstacle of *parametrization* methods [45] or of *Lie-methods* [39] is then overcome.

The numerical solution obtained is this way obviously does not lie on the exact manifold: it lives on the approximate manifold $\tilde{\mathcal{M}}$. Nevertheless, it never drifts off the exact manifold considerably, if $\mathcal{M}$ and $\tilde{\mathcal{M}}$ 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 $\tilde{\mathcal{M}}$ 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 $\tilde{f}$ given $\tilde{g}$. By admissible, we mean tangent to the manifold $\tilde{\mathcal{M}}$, i.e. such that

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

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

$$\tilde{f}(y) = (I - P(y))f(y), \tag{11}$$

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

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's 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. Gaussian wave packets

Participant: Erwan Faou.

The work described in this section has been conducted in collaboration with Chr. Lubich, from the University of Tübingen (Germany).
Gaussian wavepacket dynamics is widely used in quantum molecular dynamics, see for instance [38], [33]. In this case, an approximation to the wave function $\psi(x,t)$ solution of (8) is sought for in the form

$$u(x,t) = e^{i\varphi(t)/\varepsilon} \prod_{k=1}^{N} \phi_k(x_k,t) \tag{12}$$

with

$$\phi_k(x_k,t) = \exp\left(\frac{i}{\varepsilon}\left(a_k(t)\,|x_k - q_k(t)|^2 + p_k(t)\cdot(x_k - q_k(t)) + c_k(t)\right)\right), \tag{13}$$

where $|\cdot|$ and $\cdot$ denote the Euclidean norm and inner product on $\mathbb{R}^d$, respectively. The parameters $q_k \in \mathbb{R}^d$ and $p_k \in \mathbb{R}^d$ represent the position and momentum average, respectively: $q_k = \langle\, u \,|\, x_k \,|\, u \,\rangle$ and $p_k = \langle\, u \,|\, -i\varepsilon\nabla_{x_k} \,|\, u \,\rangle$. Further, $a_k = \alpha_k + i\beta_k$ (with $\beta_k > 0$) is a complex width parameter, $c_k = \gamma_k + i\delta_k$ is a complex phase parameter, and φ is a real phase. (Only the sum of the phases $\varphi + \sum_k c_k$ is determined uniquely. The partition of the phases is made by convenience so that each ϕ_k is of unit norm.)

The Dirac-Frenkel-McLachlan variational principle yields equations of motion for these parameters. It turns out that this system of ordinary differential equations has a Poisson structure inherited from the Hamiltonian structure of the Schrödinger equation, and that to the semi classical limit $\varepsilon \to 0$, these equations tend to the finite dimensional Hamiltonian system $\dot{q}_k = p_k/m_k$, $\dot{p}_k = -\nabla_{q_k} V(q)$.

In [34], C. Lubich and E. Faou show that the projection of the splitting scheme (9) onto the sub-manifold made of Gaussian wave packets yields a numerical scheme that is a Poisson integrator, which can be computed explicitly. Using backward error analysis, this shows in particular the preservation of energy for exponentially long time. If the potential has a rotational symmetry so that the angular momentum is conserved in the full quantum dynamics, then the numerical integrator also preserves the angular momentum.

In the classical limit $\varepsilon \to 0$, the position and momentum approximations q_k^n, p_k^n converge to the position and momentum approximations obtained by applying the Störmer-Verlet method to the classical limit system $\dot{q}_k = p_k/m_k$, $\dot{p}_k = -\nabla_{q_k} V(q)$.

5.2. From the Bloch model to the rate equations

Participant: François Castella.

In references [28] and [29], we have studied the reaction of an atomic system under an applied laser field. The original equation is the aforementioned Bloch model, a Schrödinger like equation, and the laser field then takes the form of a highly oscillatory forcing term in the equation. Here, the dominant phenomenon lies in the resonant interaction between the oscillatory modes of the field and the natural oscillatory modes (= energy levels) of the atom itself.

Following the physical literature, we prove in this paper that this coupling is asymptotically described by a so-called rate equation, i.e. a linear Boltzmann equation. It describes the transitions of the electronic cloud between the atom's energy levels, as they are induced by the laser's forcing. The main difficulty in this analysis lies in the averaging out of high-oscillations, together with the sorting out of the "resonances" in the model.

This work has recently been extended in the following directions:

- First [10] in a joint work with T. Goudon (Lille) and P. Degond (Toulouse), the classical counterpart of the above question is analysed, i.e. the authors start from a classical, Vlasov-like, equation, and perform the natural averaging procedure.
- In [19], we also extend the analysis performed in [10] to force fields that are not necessarily periodi nor quasi-periodic in time. This requires new tools from homogenization theory.
- In [18], we also review the various models in laser-matter interaction, both at the quantum and at the classical level.
- Ina joint work [20] with Eric Dumas (Grenoble), the physically realistic situation of a true laser (described by a complete Maxwell system), interacting with an atom (described by the Bloch equations) is analysed. Again, resonances play a key role in the asymptotics, and the authors eventually prove that the fully coupled laser+atom system is well described by a Boltzmann equation (for the atom), which takes into account transition phenomena between energy levels, coupled with a Schroedinger equation (for the laser), which takes into account propagation in the forward direction and dispersion in the transverse plane.

5.3. From the Schrödinger to the Boltzmann equation

Participant: François Castella.

In references [27], we study the behavior of a system made up of a large number N of electrons. These electrons are all coupled through a given potential. This is a simplified version of a gas of electrons as it may be encountered in true semi-conductor devices. Following the physically relevant orders of magnitude, we study this system over large time intervals, and when the coupling is weak. It is well known in the semi-conductor-physics literature that such a situation is well described, asymptotically, by a nonlinear Boltzmann equation.

In Ref. [27], we give a partial result that indeed establishes the convergence of the original Schrödinger equation toward the nonlinear Boltzmann equation. In Ref. [9], we study the case when the fermionic behaviour of the electrons is taken into account, i.e. when the Pauli exclusion principle is used. We compute the associated corrective terms in the limiting Boltzmann equation. In [17], we give a complete convergence result for particles with no statistics: we prove the natural series expansion expressing the state of the system at time t indeed converges *term-by-term* towards the natural solution to the Boltzmann equation.

5.4. High frequency limit of the Helmholtz equation

Participant: François Castella.

In Ref. [30], we study the so-called radiation condition at infinity in the high-frequency Helmholtz equation. This leads us to a very precise analysis of the geometric features of wave propagation in a medium with variable refraction index. In some sense, we prove that, if the refraction index is such that the rays are not captured in bounded regions of space, then the Sommerfeld radiation condition at infinity is a reasonable boundary condition along the high-frequency process. This criterion is shown to be "optimal" in that rays captured in bounded regions do provide anomalous propagative phenomena that rule out the Sommerfeld radiation condition. We use here a wave packets approach, in a similar spirit as in [34]. This result is somewhat extended in a new text with T. Jecko [11], where we prove a new and optimal bound in the context of Helholtz-like equations.

5.5. An algebraic approach to invariant preserving integrators

Participants: Philippe Chartier, Erwan Faou.

Given a system of differential equations (1), a B-series $B(\alpha)$ is a formal expression of the form

$$B(a) \quad = \quad id_{\mathbb{R}^n} + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)}\, a(t)\, F(t) \tag{14}$$

where the index set $\mathcal{T}$ is the set of rooted trees , $|\cdot|$, σ and F are real functions defined on $\mathcal{T}$, and where a is a function defined on $\mathcal{T}$ as well which characterizes the B-series itself. In this work, conducted in collaboration with A. Murua from the University of Basque Country, we provide algebraic conditions for the preservation of general invariants (quadratic, polynomial or Hamiltonian) by numerical methods which can be written as B-series. The existence of a modified invariant is also investigated and turns out to be equivalent, up to a conjugation, to the preservation of the exact invariant. A striking corollary is that a *symplectic* method is formally conjugate to a method that preserves the Hamitonian exactly. Another surprising consequence is that the underlying one-step method of a symmetric multistep scheme is formally conjugate to a canonical B-series when applied to Newton's equations of motion.

To be more specific, we prove in Ref. [12] the following results:

1. a B-series integrator possesses a modified invariant for all problems with an invariant if and only if it is conjugate to the exact flow;
2. a B-series integrator possesses a modified invariant for all problems with a *quadratic* invariant if and only if it is conjugate to a *symplectic* method;
3. a B-series integrator possesses a modified Hamiltonian for all *Hamiltonian* problems if and only if it is conjugate to a method that preserves the Hamiltonian exactly;
4. a symplectic B-series is formally conjugate to a B-series that preserves the Hamiltonian exactly.

5.6. An algebraic counterpart of modified equations

Participants: Philippe Chartier, Gilles Vilmart.

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

In [32], we derive a new composition law obtained by substituting a B-series into the vector field appearing in another B-series. We derive explicit formulas for the computation of this law and study its algebraic properties. We then focus on the specific case of Hamiltonian vector fields. It is shown that this new law allows a convenient derivation of the modified equation occurring in backward error analysis or in numerical methods based on generating functions.

The above idea has been taken up in [13]. In a more general context (no restriction to B-series) the following problem is considered: for a given one-step method (typically very simple and of low order), find a differential equation written as a formal series in powers of the step size h, such that the numerical solution of the method applied to this modified differential equation yields the exact solution in the sense of formal power series. Truncating the series gives raise to new integrators of arbitrarily high order. The article [14], written in honour of Michel Crouzeix, summarizes the main results of [13] and shows possible applications of the new integrators. The implicit midpoint rule is used as an illustrating example.

In [13], modified differential equations are introduced for pairs of integration methods: Consider a system of differential equations

$$\dot{y} = f(y), \qquad y(0) = y_0, \tag{15}$$

and two numerical integrators $y_{n+1} = \Phi_{f,h}(y_n)$ and $y_{n+1} = \Psi_{f,h}(y_n)$. The problem that we address in this article is the study of a modified differential equation, written as a formal series in powers of the step size h,

$$\dot{y} = \tilde{f}(y) = f(y) + hf_2(y) + h^2 f_3(y) + \dots, \qquad y(0) = y_0, \tag{16}$$

such that the numerical solution of the method Ψ applied to (15) is (formally) equal to the numerical solution of the method Φ applied to the modified differential equation (16), i.e.,

$$\Phi_{\tilde{f},h}(y) = \Psi_{f,h}(y). \tag{17}$$

This permits us to present a unified theory and extensions of topics like:

- *backward error analysis,* which is obtained by letting $\Phi_{\tilde{f},h}(y)$ be the exact flow of the differential equation (16). Consequently, the numerical solution of $\Psi_{f,h}(y)$ becomes the exact flow of (16). This theory is fundamental for the analysis of geometric integrators and it is treated in much detail in the monographs of Sanz-Serna & Calvo [46], Hairer, Lubich & Wanner [36], and Leimkuhler & Reich [40].
- *exact integration methods,* which are obtained by letting $\Psi_{f,h}(y)$ be the exact flow of (15) and by taking for $\Phi_{f,h}(y)$ a simple numerical integrator. Truncating the modified equation, high order numerical integrators are constructed in this way. This approach is popular for Hamiltonian systems through the work of Feng Kang. It also permits the construction of symplectic elementary differential Runge–Kutta methods as first considered by Murua.

This paper also explains the connection with some exact integration methods – generating function methods for Hamiltonian systems, and a recent modification by McLachlan & Zanna of the discrete Moser–Veselov algorithm for the free rigid body.

5.7. Accurate rigid body integrators

Participants: Philippe Chartier, Gilles Vilmart.

The Discrete Moser–Veselov algorithm is an integrable discretization of the equations of motion for the free rigid body. It is symplectic and time-reversible, and it conserves all first integrals of the system. The only drawback is its low order. In the publication [16] the ideas of [13] are employed to derive a modification of this algorithm to arbitrarily high order which has negligible overhead but considerably improves the accuracy. For step sizes that are not excessively large, this algorithm gives the exact solution (up to round-off) much faster than using Jacobi elliptic functions for the exact solution of the free rigid body.

5.8. Symplectic integrators in sub-Riemannian geometry: the Martinet case

Participant: Gilles Vilmart.

By the Pontryagin maximum principle, the solution of an optimal control problem is related to the solution of a Hamiltonian system with a very special structure. We are interested to connect the knowledge in geometric numerical integration with that in the numerical treatment of control problems. In the report [24] we compare the performances of symplectic and non-symplectic integrators for the computation of normal geodesics and conjugate points in a sub-Riemannian example. We study the Martinet case, first with the flat metric and then with a one parameter perturbation leading to non integrable geodesics. From our computations we deduce that near the abnormal directions a symplectic method is much more efficient for this optimal control problem. The explanation relies on the theory of backward error analysis in geometric numerical integration.

5.9. Preserving first integrals and volume forms of additively split systems

Participant: Philippe Chartier.

This a joint work with Ander Murua, from the University of San Sebastian.

Preserving volume forms is a necessary requirement in several well-identified applications, such as molecular dynamics or meteorology, while preserving first integrals is vastly recognized as fundamental in a very large number of physical situations. Although the requirements appear somehow disconnected, they lead to algebraic conditions which have strong similarities and this is the very reason why we address these questions together.
In Ref. [23], we show in particular that a method that preserves the volume must also preserve all first integrals and as a consequence, that no volume-preserving B-series method exists apart from the composition of exact flows. This result generalizes to split vector fields a known result of Feng Kang and Shang Zai-jui.

It is however interesting to consider specific classes of problems, for which volume-preserving integrators can be constructed. For instance, it is clear that symplectic methods are volume-preserving for Hamiltonian systems: we show that symplectic conditions are in general necessary for a method to be volume-preserving and indeed sufficient for the special class of Hamiltonian problems. In a similar spirit, we derive simplified conditions for partitioned systems with two functions and three functions. The results obtained for two functions corroborate already known ones and results for more than three functions (and their straightforward generalization to more functions) appear to be completely new.

5.10. Splitting methods for the linear Schrödinger equation

Participants: Erwan Faou, Guillaume Dujardin.

In Ref. [25], we consider the linear Schrödinger equation on a one dimensional torus and its time-discretization by splitting methods. Assuming a non-resonance condition on the stepsize and a small size of the potential, we show that the numerical dynamics can be reduced over exponentially long time to a collection of two dimensional symplectic systems for asymptotically large modes. For the numerical solution, this implies the long time conservation of the energies associated with the double eigenvalues of the free Schrödinger operator. The method is close to standard techniques used in finite dimensional perturbation theory, but extended here to infinite dimensional operators. Some results in this direction are already published in [26].

5.11. Molecular dynamics in a shaker

Participant: Erwan Faou.

In molecular dynamics, we study the statistical properties of classical dynamical systems preserving a given measure and an energy depending on the situation: while Hamiltonian systems preserve the standard Liouville measure on energy surfaces, Nosé-Hoover systems preserve a Boltzmann-like measure describing the dynamics at constant temperature. A standard problem is that if these systems preserve the correct measure, they are in general not ergodic, and exhibit usually hidden invariants making the simulations irrelevant.

Here, we introduce extensions of these systems by simply adding time-dependent terms in the symplectic structure itself. By doing so, we *shake* the system without changing the measure and energy conservation properties. These *shakers* seem to increase considerably the ergodic properties of the system. They can depend on time in a deterministic way (typically, depend on a collection of harmonic oscillator) or be stochastic processes. In ref. [15] we apply this idea to the case of Nosé-Hoover systems.

5.12. Spatial approximation for solving ODEs

Participants: Philippe Chartier, Erwan Faou.

Consider a Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H(q,p), \\ \dot{p} & = & -\nabla_q H(q,p), \end{array} \right. \tag{18}$$

where $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$, and with a separable Hamiltonian H of the form

$$H(q,p) = \tfrac{1}{2} p^T p + V(q),$$

where $V(q)$ is the potential function. In many applications, such as for instance molecular dynamics, it is of importance that the numerical flow used to compute the solution of 18 preserves the volume form and the Hamiltonian. However, it is generally admitted that no standard method can satisfy both requirements, apart from exceptional situations such as for instance a quadratic Hamiltonian. A possible approach could be to solve in sequence the d Hamiltonian systems with Hamiltonians

$$\begin{array}{rcl} H^{[i]}(q_i,p_i) & = & \frac{1}{2} p_i^2 + V^{[i]}(q_i) + \frac{1}{2} \sum_{j \neq i} \overline{p}_j^T \overline{p}_j, \\ V^{[i]}(q_i) & = & V\left(\overline{q}_1, ..., \overline{q}_{i-1}, q_i, \overline{q}_{i+1}, ..., \overline{q}_d\right), \end{array}$$

obtained by freezing all components (denoted with a bar) except the two conjugate coordinates q_i and p_i. If each subsystem can be solved exactly and the same step-size is used for all, the resulting "numerical" method preserves the desired quantities, since each sub-step is symplectic and preserves $H^{[i]}$ (and thus H). Considering that each subsystem is of dimension 2 and thus integrable, it can be hoped that an exact solution is indeed obtainable in some specific situations. Nevertheless, such situations are rather non-generic, though it is important to mention at this stage the special case of *multi-quadratic* potentials, i.e. potentials such that for all $i = 1, ..., d$ and all $q \in \mathbb{R}^d$, $V^{[i]}$ is *quadratic* in q_i. In this context, the method described above has been introduced in by R. Quispel and R.I. McLachlan in [44].

In order to retain the possibility of solving exactly each sub-system and at the same time to cover more general problems, we give up the requirement of exact Hamiltonian preservation and we consider a multi-quadratic piecewise approximation of H. If instead of 18 we now solve

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H^\tau(q,p), \\ \dot{p} & = & -\nabla_q H^\tau(q,p), \end{array} \right. \tag{19}$$

where $H^\tau(q,p) = \frac{1}{2} p^T p + V^\tau(q)$ is a $C^{1,1}$ multi-quadratic approximation of H, the aforementioned procedure applied with exact solution of the sub-systems gives a first-order method which preserves H^τ exactly as well as the volume form. If $\sup_K |H - H^\tau| \leq C_K \, \tau^2$ for a compact subset K of $\mathbb{R}^d \times \mathbb{R}^d$ containing the numerical solution, then H is conserved up to an error of size $\mathcal{O}(\tau^2)$ over arbitrarily long intervals of integration (including infinite ones).

Note that this approach remains valid for more general Hamiltonians (non-separable for instance), provided an exact solution can be computed, so that all theoretical results concerning the conservation of energy and volume will be stated for general Hamiltonians. In contrast, we will describe the implementation of the method with quadratic B-splines only for the case of separable Hamiltonians.

In Ref. [21], [22]We prove the main properties of the flow of Hamiltonian systems with globally Lipschiz derivative: in particular, we show that the exact flow remains symplectic, volume preserving and Hamiltonian preserving, though in a weaker sense. We also prove the existence of a Taylor expansion in the sense of distribution and establish the order of a general composition of flows for split systems. We next consider the B-splines approximation of separable Hamiltonians in the one-dimensional case ($(q, p) \in \mathbb{R}^2$): an explicit expression of the exact solution is given that serves as a basis for higher dimensions and the numerical scheme used here is shown to be of order 1. Numerical results for three different test problems show that the usual behaviour of geometric integrators is retained.

6. Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

Participants: Francois Castella, Philippe Chartier, Erwan Faou.

Alcatel contract.
partners : INRIA, Alcatel CIT
time : from December 2003 until December 2005.

The results presented in this section have been obtained jointly with the engineers from the laboratory of optronics from Alcatel Marcoussis. This project with Alcatel is devoted to the mathematical and numerical aspects of a model for a n^{th} order cascaded Raman device. In their discretized version, the equations involve waves traveling backward and forward in the cavity, and interacting together via the Raman gain. In its most general form, a n-th order cascaded Raman fiber laser is described by a set of partial differential equations. However, it has become common, based on the experience that only a few frequencies contribute significantly to the phenomenon, to discretize the full spectrum and to simulate the resulting system of ordinary differential equations. Using a change of variable, the questions of existence and uniqueness of a solution have been solved and a more efficient and more stable algorithm has been proposed and implemented [31], [41]. However, this initial work has emphasized some limitations, and it now appears necessary to consider a more elaborated model, including the whole spectrum of frequencies: while the previous model describes in a reasonable way the so-called Self-Phase-Modulation (SPM), and the Cross-Phase-Modulation (XPM) effects, it does not take into account the so-called Four-Wave-Mixing (FWM). Is it possible to modify the model in order to encode FWM ?

Let us be more precise. The above model is a high-frequency model that is asymptotic to the Maxwell system. Here, the nonlinear terms stem from cubic nonlinearities at the Maxwell level, that encode the reaction of the fiber to the applied laser field. In that picture, FWM terms correspond to nonlinear terms that have been neglected in the asymptotic process leading from Maxwell's equations to the above Lotka-Volterra like model. The question is thus to recover those neglected terms upon making a refined asymptotic analysis that takes into account the true physical orders of magnitude of the various phenomena.

This model is currently under development and should certainly require a different numerical technique. The end of the contract has consequently been postponed to 2005.

7. Other Grants and Activities

7.1. National Grants

Participants: François Castella, Philippe Chartier, Erwan Faou.

7.1.1. ACI Molecular Simulation 2004-2006

The ARC Prestissimo will now be continued through the newly funded ACI (Action Concertée incitative) 2004-2006 entitled “Simulation Moléculaire” and taking place within the program “Nouvelles Interfaces des Mathématiques”. This action associates 20 researchers and 8 teams :

- E. Cancès (MICMAC-CERMICS),
- Y. Achdou (Laboratoire J.L. Lions, Université Paris VI) ,
- O. Atabek (Laboratoire Photo-physique Moléculaire, Université Paris Sud Orsay),
- P. Rouchon (Centre Automatique et Systèmes, Ecole des Mines de Paris),
- G. Zerah (Service Physique de la Matière Condensée, CEA-DAM, Ile-de-France),
- A. Savin (Laboratoire de Chimie Théorique, Université Paris VI),
- M. Shoenauer (Projet TAO, INRIA),
- P. Chartier (Equipe IPSO, INRIA).

The main objective of this action is to propose new numerical schemes for the simulation of molecules, both at the atomistic scale (this was the focus of PRESTISSIMO) and at the quantum scale. The main objective of this ACI is to improve the numerical methods in many aspects of molecular simulation and at different scales : quantum, atomistic, and higher... The idea is to bring together mathematicians with various skills (PDEs/ODE, control, optimization...) and chemists and physicists in order to have the largest possible impact on applications. The kick-off meeting took place at CERMICS in october under the leadership of Claude Le Bris.

7.1.2. ACI High-frequency methods for ordinary and partial differential equations 2003-2006

The team is involved in a recently accepted ACI named “High-frequency methods for ordinary and partial differential equations”, François Castella being in charge of the project. The other partners of the action are listed below:

- Laboratoire de Modélisation et de Calcul - IMAG - CNRS UMR 5523 B.P. 53 - 38041 Grenoble Cedex 9
- Département de Mathématiques - Université des Sciences et Technologies de Lille

The main objective of this ACI is to settle a work-group dedicated to the study of high frequency methods for ordinary differential and partial differential equations. The methods we have in mind include homogeneization for PDEs, averaging for ODEs, kinetic methods and geometric optics. The idea is to share some of the techniques used in the PDE and ODE communities with possible applications to Hamiltonian systems, molecular and population dynamics, semi-conductors and laser-matter interactions.

7.1.3. ANR Grant INGEMOL 2005-2008

The INGEMOL project is concerned with the numerical simulation of differential equations by so-called geometric methods, i.e. methods preserving some of the qualitative features of the exact solution. Conserving the energy or the symmetry is often physically relevant and of paramount importance in some applications such as molecular simulation or propagation of laser waves in fibers (these are the main applications considered within the project, though several others are possible: robotics, celestial mechanics). Though a lot has been achieved by numerical analysts in the domain of numerical integration during the last two decades, with most significantly the introduction of symplectic schemes and their analysis through backward error techniques, a lot remains to be done in situations where the existing theory fails to give a useful answer; the goal of the INGEMOL project is to help solving these difficulties in some well-identified cases : 1. whenever symmetric multi-step methods are used for Hamiltonian systems, 2. whenever splitting methods are used for the Schrödinger equation, 3. whenever the system under consideration has highly-oscillating solutions.

Taking into account in the theory the unboundedness of the operators or the high oscillations of the solutions allows for the construction, in a second step, of more appropriate numerical schemes with fewer or none of the present restrictions.

Eventually, it is planned to implement the new schemes with in view their application to the simulation of laser waves and to molecular simulation.

P. Chartier is coordinator of the project. INGEMOL associates the following persons and teams:

- F. Castella, P. Chartier, M. Crouzeix, G. Dujardin, E. Faou, G. Vilmart: IPSO
- Ch. Chipot: Structure et réactivité des systèmes moléculaire complexes, CNRS, Nancy.
- S. Descombes: ENS LYON.
- E. Cancès, C. Le Bris, F. Legoll, T. Lelièvre, G. Stoltz: CERMICS, ENPC, Marne-la-Vallée.

7.1.4. PAI Procope "Intégration géométrique et applications à la dynamique moléculaire quantique et classique"

This is an exchange program between the ipso team and the numerical analysis group in Tübingen, headed by C. Lubich. E. Faou is the coordinator of the french part of this project. In 2006, this program financed the following one-week visits:

- D. Cohen, V. Gradinaru and M. Loy from Tübingen
- E. Faou (2 times), G. Dujardin and G. Vilmart from IPSO.

This program is valid for two years (2006 and 2007).

8. Dissemination

8.1. Program committees, editorial Boards and organization of conferences

- P. Chartier is chair of the scientific committee of the international conference SciCADE'07.
- P. Chartier is member of the scientific committee of the "Journées en l'honneur de Michel Crouzeix" of CANUM'06.
- P. Chartier has organized a mini-symposium at CANUM'06.
- P. Chartier is member of the editorial board of M2AN.
- E. Faou is chair of the organization committee of the international conference SciCADE'07.
- F. Castella is a member of the organizing commitee of the GdR "GRIP" (Systèmes de Particules - leader : Th. Goudon).
- F. Castella has organized the summer school of the GDR "EAPQ" (Amplitude equations, leader : E. Lombardi).
- F. Castella has organized with F. Golse (ENS Paris) the conference "Systèmes à grand nombre de particules: approches déterministes et stochastiques" in Rennes. The proceedings of this conference will be published in "Communications in Mathematical Sciences".
- F. Castella has organized the summer school of the GDR "CHANT".
- F. Castella has organized, jointly with S. Descombes (ENS Lyon), a workshop on 'Structure preserving schemes for evolution equations', at E.N.S. Lyon.
- F. Castella has organized, jointly with M. Gutnic, S. Salmon, E. Sonnendrücker, a workshop on 'Numerical methods for kinetic and hyperbolic equations', at University of Strasbourg.

- F. Castella is the director of the GdR CNRS 'CHANT' ('equations Cinetiques et Hyperboliques : Aspects Numeriques, Theoriques, et de modelisation'). [budget=15000 Euros per year, approximately 300 persons, and about 4 events organized per year].

8.2. INRIA and University committees

- P. Chartier is member of the COST (Advisory Committee for Scientific and Technological Orientations) at INRIA.
- P. Chartier is member of the Comité des Projets at INRIA-Rennes.
- E. Faou is member of the Commission Personnel at INRIA-Rennes (until october 2006).
- E. Faou is member of the Commission d'Evaluation at INRIA.
- E. Faou is member of commission de spécialistes, section 26, of the Ecole Normale Supérieure de Cachan.
- F. Castella is the leader of an "Action Concertée Incitative" "Jeunes chercheuses et jeunes chercheur" on *High-frequency methods for ordinary and partial differential equations*.
- F. Castella is member of the evaluation committee of the Austrian Graduate Program "Differential Equations Models in Science and Engineering" (leader : C. Schmeiser, Vienna).
- F. Castella is member of commission de spécialistes, section 26, of INSA, University of Rennes I.
- F. Castella is member of commission de spécialistes, section 26, of the Ecole Normale Supérieure de Cachan.

8.3. Teaching

- E. Faou is oral examiner at ENS Cachan Bruz ("agrégation").

8.4. Participation in conferences

- P. Chartier was invited to give a talk at the Workshop on Geometric Numerical Integration, in Oberwolfach, March 2006.
- P. Chartier was invited to give a talk at the Castellon Conference on Geometric Integration, September 2006.
- P. Chartier was invited to give a talk at the GDR Chant "Structure preserving schemes for evolution equations", ENS-Lyon, November 2006.
- E. Faou was invited to give a talk in the Workshop on Geometric Numerical Integration, in Oberwolfach, March 2006.
- E. Faou was invited to give a talk to the "Journées techniques asymptotiques", ENSTA, june 2006.
- E. Faou was invited to give a talk in the Castellon Conference on Geometric Integration, September 2006.
- F. Castella gave seminars at the Ecole Polytechnique.
- F. Castella was invited to give a talk at the conference "Classical and Quantum Mechanical Models of Many-Particle Systems" - Oberwolfach.
- F. Castella was invited to give a talk at the conference "Mathematical and Numerical Aspects of Quantum Chemistry Problems" - Oberwolfach.
- G. Dujardin was invited to give a talk at the Congrès National d'Analyse Numérique, Lorient, June 2006.
- G. Vilmart was invited to give a talk at the Workshop "Mathematical methods for molecular simulation", CIRM, Lumigny, January 2006.

- G. Vilmart was invited to give a talk at the Castellon Conference on Geometric Integration, September 2006.
- G. Vilmart was invited to give a talk at the GDR Chant "Structure preserving schemes for evolution equations", ENS-Lyon, November 2006.

8.5. International exchanges

8.5.1. Visits

- P. Chartier visited the University of San Sabastian for one week, at the invitation of A. Murua.
- E. Faou visited the University of Tübingen in april and in december 2006 using the PAI exchange program between the numerical analysis group in Tübingen and the team IPSO.
- G. Dujardin visited the University of Tübingen in october 2006 using the PAI exchange program between the numerical analysis group in Tübingen and the team IPSO.
- G. Vilmart visited the University of Tübingen in october 2006 using the PAI exchange program between the numerical analysis group in Tübingen and the team IPSO.

8.5.2. Visitors

The team has invited the following persons :

- D. Cohen on a one-week visit.
- V. Gradinaru on a one-week visit.
- M. Loy on a one-week visit.

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