INRIA

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Project-Team IPSO

Invariant Preserving Solvers

Rennes - Bretagne-Atlantique

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 [65], [52], [50] 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

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

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

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

3.1.1. Reversible ODEs

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

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

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

3.1.2. ODEs with an invariant manifold

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

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

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

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

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [49] 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

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

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

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

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

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

$$h\omega < C,$$

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

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

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

where $H(t)$ is finite-dimensional matrix and where ε typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are 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 [57], [58] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

A particularly interesting case of study is given by symmetric splitting methods, such as the Strang splitting:

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

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

3.4. High-frequency limit of the Helmholtz equation

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

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2\Delta_x u_\varepsilon + n^2(x)u_\varepsilon = f_\varepsilon(x). \tag{10}$$

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

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

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

3.5. From the Schrödinger equation to Boltzmann-like equations

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,

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi + V(x)\psi, \tag{11}$$

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

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:

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

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 [63] or of *Lie-methods* [53] is then overcome.

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

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

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

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

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

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

4. Application Domains

4.1. Laser physics

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

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

Generally speaking, the demand in developing such models or schemes in the context of laser physics, or laser/matter interaction, is large. It involves both modeling and numerics (description of oscillations, structure preserving algorithms to capture the long-time behaviour, etc).

In a very similar spirit, but at a different level of modelling, one would like to understand the very coupling between a laser propagating in, say, a fiber, and the atoms that build up the fiber itself.

The standard, quantum, model in this direction is called the Bloch model: it is a Schrödinger like equation that describes the evolution of the atoms, when coupled to the laser field. Here the laser field induces a potential that acts directly on the atom, and the link bewteeen this potential and the laser itself is given by the so-called dipolar matrix, a matrix made up of physical coefficients that describe the polarization of the atom under the applied field.

The scientific objective here is twofold. First, one wishes to obtain tractable asymptotic models that average out the high oscillations of the atomic system and of the laser'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. 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 [15], 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 [39], [40] 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 [51] 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. 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 [18] 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 [41], 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. On the weak order of the Euler Schemes for stochastic Partial Differential Equations

Participant: Arnaud Debussche.

In this work [29], we give results on the order of convergence of the Euler scheme for a Stochastic Partial Differential Equation. The strong order of convergence has been studied by many authors. However, very few results are available for the weak order of convergence.

It is well known that the Euler scheme is of strong order $1/2$ and weak order 1 in the case of a stochastic differential equation. Two methods are available to prove this result. The first one uses the Kolmogorov equation associated to the stochastic equation and was first used by D. Talay. A second one has been recently discovered by A. Kohatsu-Higa and is based on Malliavin calculus.

In this article, we generalize such results to the infinite dimensional case. We show how to adapt Talay's method. The main difficulty is due to the presence of unbounded operators in the Kolmogorov equation. A tricky change of unknown allows to treat the case of a linear equation. It also works for an equation whose linear part defines a group, the nonlinear Schrödinger equation for instance. The case of a semilinear equations of parabolic type treated here is more difficult and we use Malliavin calculus, but not in the same way as in Kohatsu-Higa's method. We prove for instance that, in the case of a nonlinear heat equation in dimension one with a space time white noise, the Euler scheme has weak order $1/2$, it is well known that the strong order is $1/4$.

5.4. From the N-body Schrödinger equation to the quantum Boltzmann equation: a term-by-term convergence result in the weak-coupling regime

Participant: François Castella.

In this paper we analyze the asymptotic dynamics of a system of N quantum particles, in a weak coupling regime. Particles are assumed statistically independent at the initial time.

Our approach follows the strategy introduced by the authors in a previous work : we compute the time evolution of the Wigner transform of the one-particle reduced density matrix; it is represented by means of a perturbation series, whose expansion is obtained upon iterating the Duhamel formula; this approach allows us to follow the arguments developed by Lanford for classical interacting particles evolving in a low density regime.

We prove, under suitable assumptions on the interaction potential, that the complete perturbation series converges term-by-term, for all times, towards the solution of a Boltzmann equation.

The present paper completes the previous work: it is proved there that a subseries of the complete perturbation expansion converges uniformly, for short times, towards the solution to the nonlinear quantum Boltzmann equation. This previous result holds for (smooth) potentials having possibly non-zero mean value. The present text establishes that the terms neglected at once previously, on a purely heuristic basis, indeed go term-by-term to zero along the weak coupling limit, at least for potentials having zero mean.

Our analysis combines stationary phase arguments, with considerations on the nature of the various Feynman graphs entering the expansion.

5.5. Time averaging for the strongly confined nonlinear Schrödinger equation, using almost periodicity

Participant: François Castella.

We study the limiting behavior of a nonlinear Schrödinger equation describing a 3 dimensional gas that is strongly confined along the vertical, z direction. The confinement induces fast oscillations in time, that need to be averaged out. Since the Hamiltonian in the z direction is merely assumed confining, without any further specification, the associated spectrum is discrete but arbitrary, and the fast oscillations induced by the nonlinear equation entail countably many frequencies that are arbitrarily distributed. For that reason, averaging can not rely on small denominator estimates or like.

To overcome these difficulties, we prove that the fast oscillations are *almost periodic* in time, with values in a *Sobolev-like* space that we completely identify. We then exploit the existence of *long time averages* for almost periodic function to perform the necessary averaging procedure in our nonlinear problem.

5.6. Semiclassical resolvent estimates for Schrödinger operators with Coulomb singularities

Participant: François Castella.

Consider the Schrödinger operator with semiclassical parameter h, in the limit where h goes to zero. When the involved long-range potential is smooth, it is well known that the boundary values of the operator's resolvent at a positive energy λ are bounded by $O(h^{-1})$ if and only if the associated Hamilton flow is non-trapping at energy λ. In the present paper, we extend this result to the case where the potential may possess Coulomb singularities. Since the Hamilton flow then is not complete in general, our analysis requires the use of an appropriate regularization.

5.7. A reduced model for spatially structured predator-prey systems with fast spatial migrations and slow demographic evolutions

Participant: François Castella.

In [14], we consider a spatially structured predator-prey model where fast migrations occur inside a given spatial domain, while slow predator-prey interactions prescribe the demographic evolution. The unknowns of our model are the numbers of predators and prey at each time t and each site x of the domain. In the idealized limit where migrations are infinitely fast, we show one can approximate the global dynamics using the mere two unknowns corresponding to the total number of preys and predators, irrespective of their respective spatial repartition. Besides, the error term induced by this approximation can be made exponentially small with respect to the natural asymptotic parameter.

In doing so, we completely characterize how migrations do modify both the qualitative and quantitative properties of the global demography.

Our analysis relies on a convenient version of the central manifold theorem, in conjunction with a spectral gap estimate on the involved migration operator.

5.8. Methodology and Computing in Applied Probability

Participants: François Castella, Guillaume Dujardin.

In Ref. [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.

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

Participant: François Castella.

In [13], 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.

5.10. An averaging technique for highly-oscillatory Hamiltonian problems

Participants: François Castella, Philippe Chartier, Erwan Faou.

In the paper [12], 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 a previous paper. Eventually, we demonstrate the efficiency of our approach on two test problems with one or several frequencies.

5.11. 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

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

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 [68], [69], and the existence of a negative coefficient for both operators was proved in [48]. An elegant geometric proof can be found in [38]. As a consequence, such splitting methods *cannot* be used when one operator, like Δ, is not time-reversible.

In order to circumvent this order-barrier, there are two possibilities. One can use a linear, convex (see [46], [47], [36] for methods of order 3 and 4) or non-convex (see [66], [44] 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 [42] in celestrial mechanics). In 1962/1963, Rosenbrock [64] considered complex coefficients in a similar context.

In [11], 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 [50]. 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;

5.12. 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 aprooximations 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 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 [40] 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 [43] and they describe the combinatorics of renormalization in quantum field theory as described by Kreimer [55]. 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 [19] 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 ν 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 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.

5.13. Birkhoff normal form and splitting methods for semi linear Hamiltonian PDEs. Part I: Finite dimensional discretization

Participant: Erwan Faou.

In this work [31] we consider discretized Hamiltonian PDEs associated with a hamiltonian function that can be split into a linear unbounded operator and a regular non linear part. We consider splitting methods associated with this decomposition. In this first part, we consider the full discretization of this numerical method. Using a finite dimensional Birkhoff normal form result, we show the preservation of the actions of the numerical solution associated with the splitting method over arbitrary long time, provided the Sobolev norms of the initial data is small enough, and for asymptotically large level of space approximation. This result holds under generic non resonance conditions on the frequencies of the linear operator and on the step size. We apply this results to non linear Schrödinger equations as well as the non linear wave equation. Results concerning the case where there is no discretization in space (or equivalently for the abstract splitting methods) are given in a separate paper.

5.14. Birkhoff normal form and splitting methods for semi linear Hamiltonian PDEs. Part II: Abstract splitting

Participant: Erwan Faou.

This work [32] 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.

5.15. 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 [28],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 methods 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.

5.16. Computing semi-classical quantum dynamics with Hagedorn wavepackets

Participant: Erwan Faou.

In Ref. [33], 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 StörmerÐVerlet 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.

5.17. Conservative stochastic differential equations: Mathematical and numerical analysis

Participant: Erwan Faou.

In Ref. [24], 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.

5.18. Gauss-Hermite wavepacket dynamics: convergence of the spectral and pseudo-spectral approximation

Participant: Erwan Faou.

The time dependent linear Schrödinger equation for nuclei on the whole space is semi-discretised using Hermite and Gauss-Hermite basis functions. These are well suited on the one hand for the conservation properties of the numerical solution and, on the other hand, for their remarkable approximation properties. In Ref. [23], we investigate theoretically and numerically the convergence of the spectral and pseudospectral Gauss-Hermite semi-discretisation schemes.

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

Participant: Erwan Faou.

In Ref. [22], 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 ÒhybridÓ numerical schemes based on Monte Carlo approximations of the splitting method itself.

5.20. Exponential Runge-Kutta methods for the Schrödinger equation

Participant: Guillaume Dujardin.

In this work [30], we consider exponential Runge-Kutta methods of collocation type, and use them to solve linear and semi-linear Schrödinger Cauchy problems on the d-dimensional torus. The main results are that in both cases (linear and non-linear) and under suitable assumptions, an s-stage method is of order s. Sufficient conditions to achieve orders s + 1 and s + 2 are given. The effects of resonant time steps when solving linear problems on a finite time interval are explained and analyzed. This work is inspired by a recent work of M. Hochbruck and A. Ostermann, where exponential Runge-Kutta methods of collocation type are applied to parabolic Cauchy problems. The present results are compared with those obtained for parabolic problems, and numerical experiments are given to illustrate them.

5.21. 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

$$H(q,p) = \frac{1}{2} p^T p + V(q), \tag{19}$$

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

$$\begin{aligned} H^{[i]}(q_i,p_i) &= \frac{1}{2} p_i^2 + V^{[i]}(q_i) + \frac{1}{2} \sum_{j \neq i} \overline{p}_j^T \overline{p}_j, \\ V^{[i]}(q_i) &= V\left(\overline{q}_1, ..., \overline{q}_{i-1}, q_i, \overline{q}_{i+1}, ..., \overline{q}_d\right), \end{aligned} \tag{20}$$

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 [59].

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

$$\left\{ \begin{array}{rcl} \dot{q} &=& \nabla_p H^\tau(q,p), \\ \dot{p} &=& -\nabla_q H^\tau(q,p), \end{array} \right. \tag{21}$$

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. [17], 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.

5.22. A simple proof of the existence of adiabatic invariants for perturbed reversible problems

Participants: Philippe Chartier, Erwan Faou.

An adiabatic invariant is a property of a physical system which stays constant when changes are made slowly. In mechanics, an adiabatic change is a small perturbation of the Hamiltonian where the change of the energy is much slower than the orbital frequency (see for instance [35], [56]). The area enclosed by the different motions in phase space are then the adiabatic invariants. In the case of a perturbed Hamiltonian of the form

$$H(a,\theta) = H_0(a) + \epsilon H_1(a,\theta), \tag{22}$$

with $(a,\theta) \in \mathbb{R} \times [0,2\pi]^n$, the classical procedure for deriving the invariants of motion is to look for a change of variables, close to the identity, in powers of ϵ

$$\begin{aligned} I &= a + \epsilon J_1(a,\theta) + \epsilon^2 J_2(a,\theta) + ... \\ \varphi &= \theta + \epsilon K_1(a,\theta) + \epsilon^2 K_2(a,\theta) + ... \end{aligned} \tag{23}$$

in order to eliminate the angle variables of the Hamiltonian. This method, that goes back to Poincaré, was refined in the 20th century by Birkhoff [37], Kolmogorov/Arnold/Moser (KAM) [54], [34], Nekhoroshev [62], and forms now the classical perturbation theory.

Using this coordinate transform method, the classical conclusion is that the series, though divergent, are asymptotic in the sense that, for instance,

$$|I(t) - a(t) - \epsilon J_1(a(t),\theta(t)) - ... - \epsilon^{k-1} J_{k-1}(a(t),\theta(t))| \leq C\epsilon^k$$

for exponentially large time t. Hence, $I(t)$ is an adiabatic invariant for system (22), in the sense that its variation is small for a long time interval.

In the paper [16], we consider perturbed *reversible* systems for which the classical method can be applied (see for instance [61], [67], [50]). The systems we consider are of the following form:

$$\begin{aligned} \dot{a} &= \epsilon s(a,\theta) \in \mathbb{R}^m, \\ \dot{\theta} &= \omega + \epsilon\tau(a,\theta) \in [0,2\pi]^n, \end{aligned} \tag{24}$$

where ϵ is a small parameter, s is an odd function of θ and τ an even function of θ

$$\begin{aligned} s(a,-\theta) &= -s(a,\theta), \\ \tau(a,-\theta) &= \tau(a,\theta). \end{aligned} \tag{25}$$

For such systems, we propose an alternative construction of the invariants. It stems from the expansion of I itself and involves no change of variables in (a,θ): the procedure thus remains extremely basic. We assume here that ω is a constant vector, independent of a. This simplifies further some of the proofs while still covering most cases of interest[1]. We furthermore suppose that our model is nondegenerate, a not so serious limitation as most systems are nondegenerate (see [35]).

[1] The case of varying frequencies is more technically intricate and would require ultra-violet cut-off techniques. It is out of the scope of this paper.

Although the form of equations (25) seems very specific, a lot of systems in classical mechanics (reversible integrable ones to be precise) can be transformed into action-angle variables (see for instance Chapter XI in [50]). A prominent example of such a mechanical system is the Fermi-Pasta-Ulam model [45] which nicely illustrates the persistence of adiabatic quantities (in this model, an adiabatic invariant is built up from the oscillatory energies of the stiff springs).

Results derived in this paper apply to the Fermi-Pasta-Ulam equations as much as to many other systems in celestial mechnanics for instance. Moreover, they might be helpful to analyse geometric properties of numerical methods or to obtain stability results of a more theoretical nature such as those proved in [60] or [50] Chapter XI.

5.23. Rounding errors

Participant: Gilles Vilmart.

In several recent publications, numerical integrators based on Jacobi elliptic functions are proposed for solving the equations of motion of the rigid body. Although this approach yields theoretically the exact solution, a standard implementation shows an unexpected linear propagation of round-off errors. In Ref. [27], we explain how deterministic error contribution can be avoided, so that round-off behaves like a random walk. Key Words. rigid body integrator, Jacobi elliptic functions, probabilistic error propagation, long-time integration, compensated summation, quaternion, Discrete MoserÐVeselov algorithm.

5.24. The role of symplectic integrators in optimal control

Participant: Gilles Vilmart.

This is a joint work with M. Chyba and E. Hairer.
For general optimal control problems, PontryaginÕs maximum principle gives necessary optimality conditions which are in the form of a Hamiltonian differential equation. For its numerical integration, symplectic methods are a natural choice. The article [20] investigates to which extent the excellent performance of symplectic integrators for long-time integrations in astronomy and molecular dynamics carries over to problems in optimal control. Numerical experiments supported by a backward error analysis show that, for problems in low dimension close to a critical value of the Hamiltonian, symplectic integrators have a clear advantage. This is illustrated using the Martinet case in sub-Riemannian geometry. For problems like the orbital transfer of a spacecraft or the control of a submerged rigid body such an advantage cannot be observed. The Hamiltonian system is a boundary value problem and the time interval is in general not large enough so that symplectic integrators could benefit from their structure preservation of the flow. Key Words. symplectic integrator, backward error analysis, sub-Riemannian geometry, Martinet, abnormal geodesic, orbital transfer, submerged rigid body.

6. Other Grants and Activities

6.1. National Grants

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

6.1.1. 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, A. Debussche, 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.

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 2008, this program financed the following one-week visits:

- L. Gauckler from Tübingen
- E. Faou (1 time), G. Dujardin from IPSO.
- P. Chartier from IPSO.
- A. Murua from the Basque Country.

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

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 is guest editor-in-chief of a special issue of M2AN devoted to numerical methods for the integration of ODEs.
- E. Faou is the leader of the INRIA associated team MIMOL (2008–2010) grouping members of:
  - The IPSO team (INRIA Rennes, France, head: P. Chartier),
  - The numerical analysis group of the University of Tübingen, (Germany, head: C. Lubich),

  - The computer science department of the University of the Basque country, (Spain, San-Sebastian, head: A. Murua).

- F. Castella is **Co-organizer**, with R. Illner, of a session "Kinetic Methods in PDE's", in the framework of the second Canada-France mathematical congress, **Montreal**.
- F. Castella is **Co-organizer**, with D. Bresch, B. Desjardins and M. Peybernes, of the **summer school** of the GdR "CHANT", **Roscoff** (Finistère), 70 participants.
- F. Castella is the director of the GdR CNRS 'CHANT' (équations Cinétiques et Hyperboliques : Aspects Numériques, Théoriques, et de modélisation'). [budget=15000 Euros per year, approximately 300 persons, and about 4 events organized per year].
- 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 is oral examiner at ENS Cachan Bruz ("agrégation").
- E. Faou is lecturer at the Ecole Normale Supérieure de Cachan Bretagne. Course: *Ordinary differential equations.*

7.4. Participation in conferences

- P. Chartier gave a lecture at the Ecole CIMPA, Tlemcem, Algeria, May 2008.
- P. Chartier gave a talk at the conference "Splitting Methods in Time Integration" in Innsbruck, October 2008.
- P. Chartier gave a talk at the workshop "Numerical methods and Hopf algebras of trees" in Clermont-Ferrand, October 2008.
- P. Chartier was invited to give a talk at at Basel University, November 2008.
- P. Chartier was invited to give a talk at the University of Geneva, December 2008.
- P. Chartier was invited to give a talk at the University of Nice, December 2008.
- E. Faou was invited to give at the Canada-France congress in Montreal, June 2008. (Invitation to the mini-symposium: *Variational and Numerical Methods in Geometry, Physics and Chemistry*, organized by M.J. Esteban, L. Bronsard and E. Cancés).
- E. Faou attended the Workshop in Berder on Hamiltonian PDEs, organized by the university of Nantes.
- E. Faou gave a Seminar in the University of Pau (France), November 2008.
- E. Faou gave aSeminar in the Observatoire de Paris (Astronomy and dynamical systems team), October 2008.
- E. Faou gave a Seminar in the University of Lille (France), October 2008.
- E. Faou gave a Seminar in the University of Tübingen (Germany), June 2008.

- E. Faou gave a Seminar in the University of Mulhouse (France), March 2008.
- F. Castella gave a six hours lecture at *'Ecole de Physique des Houches'* on interacting particles systems, les Houches, France.
- F. Castella attented the Workshop "Mathematical Models for Transport in Macroscopic and Mesoscopic Systems", Berlin,Germany.
- A. Debussche gave a talk in the workshop Stochastic Partial Differential Equations and Applications - VIIIÓ, Levico Terme (Trento), 6-12 janvier2008
- A. Debussche gave a talk in the workshop Numerical Analysis of Stochastic PDEs 2008 (NASPDE08), ETH Zurich, 16-17 mai 2008 New Perspectives on Malliavin Calculus, CRM, Barcelona, 25 juin 2008
- A. Debussche gave a talk in the Journees MAS 2008, Rennes , 25-27 aout 2008.
- A. Debussche gave a talk in the workshop Stochastic Partial Differential Equations Computations & Applications, ICMS Edinburgh, 29 sept.-1er oct. 1008.
- G. Vilmart gave a talk at the workshop "Numerical methods and Hopf algebras of trees" in Clermont-Ferrand, October 2008.
- G. Vilmart gave a talk at the Fall Metting of the Swiss Mathematical Society, Berne (Switzerland) Oct. 2008
- G. Vilmart gave a talk at the Séminaire Mulhousien de mathématiques, Mulhouse (France), Oct. 2008
- G. Vilmart gave a talk at Fourth Graduate Colloquium, Swiss Doctoral Program in mathematics, Neuchâtel (Switzerland), Sep. 2008
- G. Vilmart attended the II International Summer School on Geometry, Mechanics, and Control, La Palma, Canary Islands (Spain), June 2008.
- G. Vilmart gave a talk at Colloque Numérique Suisse, Fribourg (Switzerland), Apr. 2008

7.5. International exchanges

7.5.1. Visits

- P. Chartier visited the University of the Basque Country for three weeks.
- E. Faou visited the University of Tübingen in june 2008 .

7.5.2. Visitors

The team has invited the following persons :

- L. Gauckler on a one-week visit.
- A. Murua on a a two-week visit.

8. Bibliography

Major publications by the team in recent years

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Year Publications

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[9] G. DUJARDIN. *Etudes de schémas de discrétisation en temps de l'équation de Schrödinger*, Thèse de Mathématiques, Ph. D. Thesis, Université de Rennes 1, 2008.

[10] G. VILMART. *Etude d'intégrateurs géométriques pour des équations différentielles*, Thèse de Mathématiques, Ph. D. Thesis, Université de Genève, 2008.

Articles in International Peer-Reviewed Journal

[11] F. CASTELLA, P. CHARTIER, S. DESCOMBES, G. VILMART. *Splitting methods with complex times for parabolic equations*, in "BIT Numer. Anal.", submitted, 2008.

[12] F. CASTELLA, P. CHARTIER, E. FAOU. *An averaging technique for highly-oscillatory Hamiltonian problems*, in "SIAM J. Numer. Anal.", to appear, 2008.

[13] F. CASTELLA, G. DUJARDIN, B. SERICOLA. *Moments analysis in Markov reward models.*, in "Methodology and Computing in Applied Probability", 2008.

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[16] P. CHARTIER, E. FAOU. *A simple proof of the existence of adiabatic invariants for perturbed reversible problems*, in "J. Phys. A: Math. Theor.", vol. 41, 2008.

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