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Activity Report 2015

Project-Team IPSO

Invariant Preserving SOlvers

IN COLLABORATION WITH: Institut de recherche mathématique de Rennes (IRMAR)

RESEARCH CENTER
Rennes - Bretagne-Atlantique

THEME
Numerical schemes and simulations

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Project-Team IPSO

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6.1.2. - Stochastic Modeling (SPDE, SDE)
6.1.4. - Multiscale modeling
6.1.5. - Multiphysics modeling
6.2. - Scientific Computing, Numerical Analysis & Optimization
6.2.1. - Numerical analysis of PDE and ODE
6.2.2. - Numerical probability
6.2.3. - Probabilistic methods

Other Research Topics and Application Domains:

1. - Life sciences
1.1. - Biology
1.1.10. - Mathematical biology
4. - Energy
4.1. - Fossile energy production
4.1.3. - Fusion
5. - Industry of the future
5.3. - Nanotechnology and Biotechnology

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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 [61], [58], [57] 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. Research Program

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

Participants: François Castella, Philippe Chartier, Erwan Faou.

ordinary differential equation, numerical integrator, invariant, Hamiltonian system, reversible system, Lie-group system

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 [56] 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:

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

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

Participants: François Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Méhats, Mohammed Lemou.

second-order ODEs, oscillatory solutions, Schrödinger and wave equations, step size restrictions.

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 faced once again with two different time-scales, 1 and ε. In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

3.3. Geometric schemes for the Schrödinger equation

Participants: François Castella, Philippe Chartier, Erwan Faou, Florian Méhats.

Schrödinger equation, variational splitting, energy conservation.

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 [60], [59] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

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

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

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

3.4. High-frequency limit of the Helmholtz equation

Participant: François Castella.

waves, Helmholtz equation, high oscillations.

The Helmholtz equation models the propagation of waves in a medium with variable refraction index. It is a simplified version of the Maxwell system for electro-magnetic waves.

The high-frequency regime is characterized by the fact that the typical wavelength of the signals under consideration is much smaller than the typical distance of observation of those signals. Hence, in the high-frequency regime, the Helmholtz equation at once involves highly oscillatory phenomena that are to be described in some asymptotic way. Quantitatively, the Helmholtz equation reads

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

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

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

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

3.5. From the Schrödinger equation to Boltzmann-like equations

Participant: François Castella.

Schrödinger equation, asymptotic model, Boltzmann equation.

The Schrödinger equation is the appropriate way to describe transport phenomena at the scale of electrons. However, for real devices, it is important to derive models valid at a larger scale.

In semi-conductors, the Schrödinger equation is the ultimate model that allows to obtain quantitative information about electronic transport in crystals. It reads, in convenient adimensional units,

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

where $V(x)$ is the potential and $\psi(t,x)$ is the time- and space-dependent wave function. However, the size of real devices makes it important to derive simplified models that are valid at a larger scale. Typically, one wishes to have kinetic transport equations. As is well-known, this requirement needs one to be able to describe "collisions" between electrons in these devices, a concept that makes sense at the macroscopic level, while it does not at the microscopic (electronic) level. Quantitatively, the question is the following: can one obtain the Boltzmann equation (an equation that describes collisional phenomena) as an asymptotic model for the Schrödinger equation, along the physically relevant micro-macro asymptotics? From the point of view of modelling, one wishes here to understand what are the "good objects", or, in more technical words, what are the relevant "cross-sections", that describe the elementary collisional phenomena. Quantitatively, the Boltzmann equation reads, in a simplified, linearized, form :

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v')\,[f(t,x,v') - f(t,x,v)]dv'. \tag{12}$$

Here, the unknown is $f(x,v,t)$, the probability that a particle sits at position x, with a velocity v, at time t. Also, $\sigma(v,v')$ is called the cross-section, and it describes the probability that a particle "jumps" from velocity v to velocity v' (or the converse) after a collision process.

4. Highlights of the Year

4.1. Highlights of the Year

4.1.1. Awards

E. Faou received the SIAM Germund Dahlquist prize in september 2015.

5. New Results

5.1. Uniformly accurate numerical schemes for highly-oscillatory Klein-Gordon and nonlinear Schrödinger equation

The work [20] is devoted to the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called "Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. The method is based on two main ingredients. First, we embed our problem in a suitable "two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

5.2. Higher-order averaging, formal series and numerical integration III: error bounds

In earlier works, it has been shown how formal series like those used nowadays to investigate the properties of numerical integrators may be used to construct high- order averaged systems or formal first integrals of Hamiltonian problems. With the new approach the averaged system (or the formal first integral) may be written down immediately in terms of (i) suitable basis functions and (ii) scalar coefficients that are computed via simple recursions. In [21], we show how the coefficients/basis functions approach may be used advantageously to derive exponentially small error bounds for averaged systems and approximate first integrals.

5.3. Stroboscopic averaging for the nonlinear Schrödinger equation

In [18], we are concerned with an averaging procedure, -namely Stroboscopic averaging-, for highly-oscillatory evolution equations posed in a (possibly infinite dimensional) Banach space, typically partial differential equations (PDEs) in a high-frequency regime where only one frequency is present. We construct a high-order averaged system whose solution remains exponentially close to the exact one over long time intervals, possesses the same geometric properties (structure, invariants,...) as compared to the original system, and is non-oscillatory. We then apply our results to the nonlinear Schrdinger equation on the d-dimensional torus T^d, or in R^d with a harmonic oscillator, for which we obtain a hierarchy of Hamiltonian averaged models. Our results are illustrated numerically on several examples borrowed from the recent literature.

5.4. Uniformly accurate time-splitting schemes for NLS in the semiclassical limit

In [42], we construct new numerical methods for the nonlinear Schrödinger equation in the semiclassical limit. We introduce time-splitting schemes for a phase-amplitude reformulation of the equation where the dimensionless Planck constant is not a singular parameter anymore. Our methods have an accuracy which is spectral in space, of second or fourth-order in time, and independent of the Planck constant before the formation of caustics. The scheme of second-order preserves exactly the L^2 norm of the solution, as the flow of the nonlinear Schrödinger equation does. In passing, we introduce a new time-splitting method for the eikonal equation, whose precision is spectral in space and of second or fourth-order in time.

5.5. Gyroaverage operator for a polar mesh

In [33], we are concerned with numerical approximation of the gyroaverage operators arising in plasma physics to take into account the effects of the finite Larmor radius corrections. This work extended a previous approach to polar geometries. A direct method is proposed in the space configuration which consists in integrating on the gyrocircles using interpolation operator (Hermite or cubic splines). Numerical comparisons with a standard method based on a Padé approximation are performed: (i) with analytical solutions, (ii) considering the 4D drift-kinetic model with one Larmor radius and (iii) on the classical linear DIII-D benchmark case. In particular, we show that in the context of a drift-kinetic simulation, the proposed method has similar computational cost as the standard method and its precision is independent of the radius.

5.6. Asymptotic Preserving scheme for a kinetic model describing incompressible fluids

The kinetic theory of fluid turbulence modeling developed by Degond and Lemou "Turbulence models for incompressible fluids derived from kinetic theory" (J. Math. Fluid Mech. 2002) is considered for further study, analysis and simulation. Starting with the Boltzmann like equation representation for turbulence modeling, a relaxation type collision term is introduced for isotropic turbulence. In order to describe some important turbulence phenomenology, the relaxation time incorporates a dependency on the turbulent microscopic energy and this makes difficult the construction of efficient numerical methods. To investigate this problem, we focus

here on a multi-dimensional prototype model and first propose an appropriate change of frame that makes the numerical study simpler. Then, a numerical strategy to tackle the stiff relaxation source term is introduced in the spirit of Asymptotic Preserving Schemes. Numerical tests are performed in a one-dimensional framework on the basis of the developed strategy to confirm its efficiency.

5.7. Numerical schemes for kinetic equations in the diffusion and anomalous diffusion limits. Part I: the case of heavy-tailed equilibrium

In [44], we propose some numerical schemes for linear kinetic equations in the diffusion and anomalous diffusion limit. When the equilibrium distribution function is a Maxwellian distribution, it is well known that for an appropriate time scale, the small mean free path limit gives rise to a diffusion type equation. However, when a heavy-tailed distribution is considered, another time scale is required and the small mean free path limit leads to a fractional anomalous diffusion equation. Our aim is to develop numerical schemes for the original kinetic model which works for the different regimes, without being restricted by stability conditions of standard explicit time integrators. First, we propose some numerical schemes for the diffusion asymptotics; then, their extension to the anomalous diffusion limit is studied. In this case, it is crucial to capture the effect of the large velocities of the heavy-tailed equilibrium, so that some important transformations of the schemes derived for the diffusion asymptotics are needed. As a result, we obtain numerical schemes which enjoy the Asymptotic Preserving property in the anomalous diffusion limit, that is: they do not suffer from the restriction on the time step and they degenerate towards the fractional diffusion limit when the mean free path goes to zero. We also numerically investigate the uniform accuracy and construct a class of numerical schemes satisfying this property. Finally, the efficiency of the different numerical schemes is shown through numerical experiments.

5.8. Comparison of numerical solvers for anisotropic diffusion equations arising in plasma physics

In [25], we are concentrated to the comparison of numerical schemes to approximate anisotropic diffusion problems arising in tokamak plasma physics. We focus on the spatial approximation by using finite volume method and on the time discretization. This latter point is delicate since the use of explicit integrators leads to a severe restriction on the time step. Then, implicit and semi-implicit schemes are coupled to finite volumes space discretization and are compared for some classical problems relevant for magnetically confined plasmas. It appears that the semi-implicit approaches (using ARK methods or directional splitting) turn out to be the most efficient on the numerical results, especially when nonlinear problems are studied on refined meshes, using high order methods in space.

5.9. Hamiltonian splitting for the Vlasov-Maxwell equations

In [23], a new splitting is proposed for solving the Vlasov-Maxwell system. This splitting is based on a decomposition of the Hamiltonian of the Vlasov–Maxwell system and allows for the construction of arbitrary high order methods by composition (independent of the specific deterministic method used for the discretization of the phase space). Moreover, we show that for a spectral method in space this scheme satisfies Poisson's equation without explicitly solving it. Finally, we present some examples in the context of the time evolution of an electromagnetic plasma instability which emphasizes the excellent behavior of the new splitting compared to methods from the literature.

5.10. Multiscale numerical schemes for kinetic equations in the anomalous diffusion limit

In [24], we construct numerical schemes to solve kinetic equations with anomalous diffusion scaling. When the equilibrium is heavy-tailed or when the collision frequency degenerates for small velocities, an appropriate scaling should be made and the limit model is the so-called anomalous or fractional diffusion model. Our first

scheme is based on a suitable micro-macro decomposition of the distribution function whereas our second scheme relies on a Duhamel formulation of the kinetic equation. Both are Asymptotic Preserving (AP): they are consistent with the kinetic equation for all fixed value of the scaling parameter $\varepsilon > 0$ and degenerate into a consistent scheme solving the asymptotic model when epsilon tends to 0. The second scheme enjoys the stronger property of being uniformly accurate (UA) with respect to epsilon. The usual AP schemes known for the classical diffusion limit cannot be directly applied to the context of anomalous diffusion scaling, since they are not able to capture the important effects of large and small velocities. We present numerical tests to highlight the efficiency of our schemes.

5.11. High-order Hamiltonian splitting for Vlasov-Poisson equations

In [40], we consider the Vlasov-Poisson equation in a Hamiltonian framework and derive new time splitting methods based on the decomposition of the Hamiltonian functional between the kinetic and electric energy. Assuming smoothness of the solutions, we study the order conditions of such methods. It appears that these conditions are of Runge-Kutta-Nyström type. In the one dimensional case, the order conditions can be further simplified, and efficient methods of order 6 with a reduced number of stages can be constructed. In the general case, high-order methods can also be constructed using explicit computations of commutators. Numerical results are performed and show the benefit of using high-order splitting schemes in that context. Complete and self-contained proofs of convergence results and rigorous error estimates are also given.

5.12. Asymptotic Preserving numerical schemes for multiscale parabolic problems

In [45], we consider a class of multiscale parabolic problems with diffusion coefficients oscillating in space at a possibly small scale ε. Numerical homogenization methods are popular for such problems, because they capture efficiently the asymptotic behaviour as $\varepsilon \to 0$, without using a dramatically fine spatial discretization at the scale of the fast oscillations. However, known such homogenization schemes are in general not accurate for both the highly oscillatory regime $\varepsilon \to 0$ and the non oscillatory regime $\varepsilon \to 1$. In this paper, we introduce an Asymptotic Preserving method based on an exact micro-macro decomposition of the solution which remains consistent for both regimes.

5.13. Parallelization of an advection-diffusion problem arising in edge plasma physics using hybrid MPI/OpenMP programming

In [35], we present a hybrid MPI/OpenMP parallelization strategy for an advection-diffusion problem, arising in a scientific application simulating tokamak's edge plasma physics. This problem is the hotspot of the system of equations numerically solved by the application. As this part of the code is memory-bandwidth limited, we show the benefit of a parallel approach that increases the aggregated memory bandwidth in using multiple computing nodes. In addition, we designed some algorithms to limit the additional cost, induced by the needed extra inter nodal communications. The proposed solution allows to achieve good scalings on several nodes and to observe 70% of relative efficiency on 512 cores. Also, the hybrid parallelization allows to consider larger domain sizes, unreachable on a single computing node.

5.14. Numerical schemes for kinetic equations in the anomalous diffusion limit. Part II: degenerate collision frequency

In [43], which is the continuation of [44], we propose numerical schemes for linear kinetic equation which are able to deal with the fractional diffusion limit. When the collision frequency degenerates for small velocities it is known that for an appropriate time scale, the small mean free path limit leads to an anomalous diffusion equation. From a numerical point of view, this degeneracy gives rise to an additional stiffness that must be treated in a suitable way to avoid a prohibitive computational cost. Our aim is therefore to construct a class of numerical schemes which are able to undertake these stiffness. This means that the numerical schemes are able to capture the effect of small velocities in the small mean free path limit with a fixed set of numerical parameters. Various numerical tests are performed to illustrate the efficiency of our methods in this context.

5.15. Analysis of the Monte-Carlo error in a hybrid semi-Lagrangian scheme

In [17] we consider Monte-Carlo discretizations of partial differential equations based on a combination of semi-lagrangian schemes and probabilistic representations of the solutions. The goal of this paper is twofold. First we give rigorous convergence estimates for our algorithm: In a simple setting, we show that under an anti-CFL condition on the time-step δt and on the mesh size δx and for a reasonably large number of independent realizations N, we control the Monte-Carlo error by a term of order $\mathcal{O}(\sqrt{\delta t/N})$. Then, we show various applications of the numerical method in very general situations (nonlinear, different boundary conditions, higher dimension) and numerical examples showing that the theoretical bound obtained in the simple case seems to persist in more complex situations.

5.16. Resonant time steps and instabilities in the numerical integration of Schrödinger equations

In [30], we consider the linear and non linear cubic Schrödinger equations with periodic boundary conditions, and their approximations by splitting methods. We prove that for a dense set of arbitrary small time steps, there exists numerical solutions leading to strong numerical instabilities preventing the energy conservation and regularity bounds obtained for the exact solution. We analyze rigorously these instabilities in the semi-discrete and fully discrete cases.

5.17. Collisions of almost parallel vortex filaments

In [38], we investigate the occurrence of collisions in the evolution of vortex filaments through a system introduced by Klein, Majda and Damodaran, and by Zakharov. We first establish rigorously the existence of a pair of almost parallel vortex filaments, with opposite circulation, colliding at some point in finite time. The collision mechanism is based on the one of the self-similar solutions of the model, described in our previous work. In the second part of this paper we extend this construction to the case of an arbitrary number of filaments, with polygonal symmetry, that are perturbations of a configuration of parallel vortex filaments forming a polygon, with or without its center, rotating with constant angular velocity.

5.18. On numerical Landau damping for splitting methods applied to the Vlasov-HMF model

In [49] we consider time discretizations of the Vlasov-HMF (Hamiltonian Mean-Field) equation based on splitting methods between the linear and non-linear parts. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that the numerical solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping. Moreover, we prove that the modified state is close to the continuous one and provide error estimates with respect to the time stepsize.

5.19. A kinetic model for the transport of electrons in a graphen layer

In [50], a kinetic model for the transport of electrons in graphene is derived with the tools of semiclassical analysis. The underlying quantum model is a massless Dirac equation, whose eigenvalues display a conical singularity responsible for non adiabatic transitions between the two modes. Our kinetic model takes the form of two Boltzmann equations coupled by a collision operator modeling these transitions. This collision term includes a Landau-Zener transfer term and a jump operator whose presence is essential in order to ensure a good energy conservation during the transitions. We propose an algorithmic realization of the semi-group solving the kinetic model, by a particle method. In the last section, a series of numerical experiments are given in order to study the influences of the various sources of errors between the quantum and the kinetic models.

5.20. Dimension reduction for dipolar Bose-Einstein condensates in the strong interaction regime

In [39], we study dimension reduction for the three-dimensional Gross-Pitaevskii equation with a long-range and anisotropic dipole-dipole interaction modeling dipolar Bose-Einstein condensation in a strong interaction regime. The cases of disk shaped condensates (confinement from dimension three to dimension two) and cigar shaped condensates (confinement to dimension one) are analyzed. In both cases, the analysis combines averaging tools and semiclassical techniques. Asymptotic models are derived, with rates of convergence in terms of two small dimensionless parameters characterizing the strength of the confinement and the strength of the interaction between atoms.

5.21. The Interaction Picture method for solving the generalized nonlinear Schrödinger equation in optics

The "interaction picture" (IP) method studied in [13] is a very promising alternative to Split-Step methods for solving certain type of partial differential equations such as the nonlinear Schrödinger equation used in the simulation of wave propagation in optical fibers. The method exhibits interesting convergence properties and is likely to provide more accurate numerical results than cost comparable Split-Step methods such as the Symmetric Split-Step method. In this work we investigate in detail the numerical properties of the IP method and carry out a precise comparison between the IP method and the Symmetric Split-Step method.

5.22. Nonlinear stability criteria for the HMF Model

In [52], we study the nonlinear stability of a large class of inhomogeneous steady state solutions to the Hamiltonian Mean Field (HMF) model. Under a simple criterion, we prove the nonlinear stability of steady states which are decreasing functions of the microscopic energy. To achieve this task, we extend to this context the strategy based on generalized rearrangement techniques which was developed recently for the gravitational Vlasov-Poisson equation. Explicit stability inequalities are established and our analysis is able to treat non compactly supported steady states to HMF, which are physically relevant in this context but induces additional difficulties, compared to the Vlasov-Poisson system.

5.23. Dimension reduction for rotating Bose-Einstein condensates with anisotropic confinement

In [54], we consider the three-dimensional time-dependent Gross-Pitaevskii equation arising in the description of rotating Bose-Einstein condensates and study the corresponding scaling limit of strongly anisotropic confinement potentials. The resulting effective equations in one or two spatial dimensions, respectively, are rigorously obtained as special cases of an averaged three dimensional limit model. In the particular case where the rotation axis is not parallel to the strongly confining direction the resulting limiting model(s) include a negative, and thus, purely repulsive quadratic potential, which is not present in the original equation and which can be seen as an effective centrifugal force counteracting the confinement.

5.24. Dimension reduction for anisotropic Bose-Einstein condensates in the strong interaction regime

In [14], we study the problem of dimension reduction for the three dimensional Gross-Pitaevskii equation (GPE) describing a Bose-Einstein condensate confined in a strongly anisotropic harmonic trap. Since the gas is assumed to be in a strong interaction regime, we have to analyze two combined singular limits: a semi-classical limit in the transport direction and the strong partial confinement limit in the transversal direction. We prove that both limits commute together and we provide convergence rates. The by-products of this work are approximated models in reduced dimension for the GPE, with a priori estimates of the approximation errors.

5.25. Models of dark matter halos based on statistical mechanics: I. The classical King model

In [22], we consider the possibility that dark matter halos are described by the Fermi-Dirac distribution at finite temperature. This is the case if dark matter is a self-gravitating quantum gas made of massive neutrinos at statistical equilibrium. This is also the case if dark matter can be treated as a self-gravitating collisionless gas experiencing Lynden-Bell's type of violent relaxation. In order to avoid the infinite mass problem and carry out a rigorous stability analysis, we consider the fermionic King model. In this paper, we study the non-degenerate limit leading to the classical King model. This model was initially introduced to describe globular clusters. We propose to apply it also to large dark matter halos where quantum effects are negligible. We determine the caloric curve and study the thermodynamical stability of the different configurations. Equilibrium states exist only above a critical energy E_c in the microcanonical ensemble and only above a critical temperature T_c in the canonical ensemble.

5.26. Numerical study of a quantum-diffusive spin model for two-dimensional electron gases

In [15], we investigate the time evolution of spin densities in a two-dimensional electron gas subjected to Rashba spin-orbit coupling on the basis of the quantum drift-diffusive model. This model assumes the electrons to be in a quantum equilibrium state in the form of a Maxwellian operator. The resulting quantum drift-diffusion equations for spin-up and spin-down densities are coupled in a non-local manner via two spin chemical potentials (Lagrange multipliers) and via off-diagonal elements of the equilibrium spin density and spin current matrices, respectively. We present two space-time discretizations of the model, one semi-implicit and one explicit, which comprise also the Poisson equation in order to account for electron-electron interactions. In a first step pure time discretization is applied in order to prove the well-posedness of the two schemes, both of which are based on a functional formalism to treat the non-local relations between spin densities. We then use the fully space-time discrete schemes to simulate the time evolution of a Rashba electron gas confined in a bounded domain and subjected to spin-dependent external potentials. Finite difference approximations are first order in time and second order in space. The discrete functionals introduced are minimized with the help of a conjugate gradient-based algorithm, where the Newton method is applied in order to find the respective line minima. The numerical convergence in the long-time limit of a Gaussian initial condition towards the solution of the corresponding stationary Schrödinger- Poisson problem is demonstrated for different values of the numerical parameters. Moreover, the performances of the semi-implicit and the explicit scheme are compared.

5.27. Numerical analysis of the nonlinear Schrödinger equation with white noise dispersion

In [16], we focus to the numerical study of a nonlinear Schrödinger equation in which the coefficient in front of the group velocity dispersion is multiplied by a real valued Gaussian white noise. We first perform the numerical analysis of a semi-discrete Crank-Nicolson scheme in the case when the continuous equation possesses a unique global solution. We prove that the strong order of convergence in probability is equal to one in this case. In a second step, we numerically investigate, in space dimension one, the behavior of the solutions of the equation for different power nonlinearities, corresponding to subcritical, critical or supercritical nonlinearities in the deterministic case. Numerical evidence of a change in the critical power due to the presence of the noise is pointed out.

5.28. A regularity result for quasilinear stochastic partial differential equations of parabolic type

In [27], we consider a quasilinear parabolic stochastic partial differential equation driven by a multiplicative noise and study regularity properties of its weak solution satisfying classical a priori estimates. In particular,

we determine conditions on coefficients and initial data under which the weak solution is Hölder continuous in time and possesses spatial regularity that is only limited by the regularity of the given data. Our proof is based on an efficient method of increasing regularity: the solution is rewritten as the sum of two processes, one solves a linear parabolic SPDE with the same noise term as the original model problem whereas the other solves a linear parabolic PDE with random coefficients. This way, the required regularity can be achieved by repeatedly making use of known techniques for stochastic convolutions and deterministic PDEs.

5.29. Diffusion limit for the radiative transfer equation perturbed by a Wiener process

The aim of [28] is the rigorous derivation of a stochastic non-linear diffusion equation from a radiative transfer equation perturbed with a random noise. The proof of the convergence relies on a formal Hilbert expansion and the estimation of the remainder. The Hilbert expansion has to be done up to order 3 to overcome some difficulties caused by the random noise.

5.30. Invariant measure of scalar first-order conservation laws with stochastic forcing

In [29], under an hypothesis of non-degeneracy of the flux, we study the long-time behaviour of periodic scalar first-order conservation laws with stochastic forcing in any space dimension. For sub-cubic fluxes, we show the existence of an invariant measure. Moreover for sub-quadratic fluxes we show uniqueness and ergodicity of the invariant measure. Also, since this invariant measure is supported by L^p for some p small, we are led to generalize to the stochastic case the theory of L^1 solutions developed by Chen and Perthame in 2003.

5.31. An integral inequality for the invariant measure of a stochastic reaction-diffusion equation

In [46], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove an integral inequality for the invariant measure ν of a stochastic reaction-diffusion equation. Then we discuss some consequences as an integration by parts formula which extends to ν a basic identity of the Malliavin Calculus. Finally, we prove the existence of a surface measure for a ball and a half-space of H.

5.32. Estimate for P_tD for the stochastic Burgers equation

In [47], we consider the Burgers equation on $H = L^2(0,1)$ perturbed by white noise and the corresponding transition semigroup P_t. We prove a new formula for P_tD_φ (where $\varphi : H \to \mathbb{R}$ is bounded and Borel) which depends on φ but not on its derivative. Then we deduce some new consequences for the invariant measure ν of P_t as its Fomin differentiability and an integration by parts formula which generalises the classical one for gaussian measures.

5.33. Existence of the Fomin derivative of the invariant measure of a stochastic reaction-diffusion equation

In [48], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove existence of the Fomin derivative of the corresponding transition semigroup P_t. The main tool is a new estimate for $P_tD\varphi$ in terms of $\|\varphi\|_{L^2(H,\nu)}$, where ν is the invariant measure of P_t.

5.34. Global behavior of N competing species with strong diffusion: diffusion leads to exclusion

In [19], we study the following problem. For a large class of models involving several species competing for a single resource in a *homogeneous* environment, it is known that the competitive exclusion principle holds: only one species survives eventually. Various works indicate though that coexistence of many species is possible when the competition occurs in a *heterogeneous* environment. We propose here a spatially heterogeneous system modeling several species competing for a single resource, and migrating in the spatial domain. For this model, it is known, at least in particular cases, that if migrations are *slow* enough, then coexistence occurs. In this paper we show at variance that if the spatial migrations are *fast* enough, then our system can be approximated by a spatially homogeneous system, called aggregated model, which can be explicitly computed, and we show that if the competitive exclusion principle holds for the aggregated model, then it holds as well for the original, spatially heterogeneous model. In other words, we show the persistence of the competitive exclusion principle in the spatially heterogeneous situation when migrations are fast. As a consequence, for fast migrations only one species may survive, namely the best competitor *in average*. We last study which is the best competitor *in average* on some examples, and draw some ecological consequences.

5.35. Randomized message-passing test-and-set

In [37] and [34], we present a solution to the well-known Test&Set operation in an asynchronous system prone to process crashes. Test&Set is a synchronization operation that, when invoked by a set of processes, returns yes to a unique process and returns no to all the others. Recently many advances in implementing Test&Set objects have been achieved, however all of them target the shared memory model. In this paper we propose an implementation of a Test&Set object in the message passing model. This implementation can be invoked by any number $p \leq n$ of processes where n is the total number of processes in the system. It has an expected individual step complexity in $O(\log p)$ against an oblivious adversary, and an expected individual message complexity in $O(n)$. The proposed Test&Set object is built atop a new basic building block, called selector, that allows to select a winning group among two groups of processes. We propose a message-passing implementation of the selector whose step complexity is constant. We are not aware of any other implementation of the Test&Set operation in the message passing model.

6. Partnerships and Cooperations

6.1. National Initiatives

6.1.1. ANR Programme blanc international (BLAN) LODIQUAS 2012-2015

Participants: Philippe Chartier, Florian Méhats, François Castella, Mohammed Lemou.

The project, entitled "LODIQUAS" (for: Low DImensional QUANtum Systems), received fundings for 4 postdocs (48 months) and one pre-doc (36 months). The whole project involves the following researchers : Norbert Mauser (Vienna), Erich Gornik (Vienna), Mechthild Thalhammer (Innsbruck), Christoph Naegerl (Innsbruck), Jörg Schmiedmayer (Vienna), Hans-Peter Stimming (Vienna),Francis Nier (Rennes), Raymond El Hajj (Rennes), Claudia Negulescu (Toulouse), Fanny Delebecque (Toulouse), Stéphane Descombes (Nice), Christophe Besse (Lille).
The expected scientific and technological progress brought by the present project are as follows.

Quantum technology as the application of quantum effects in macroscopic devices has an increasing importance, not only for far future goals like the quantum computer, but already now or in the near future. The present project is mainly concerned with the mathematical and numerical analysis of these objects, in conjunction with experimental physicists. On the side of fermions quantum electronic structures like resonant tunnelling diodes show well studied non classical effects like a negative differential resistance that are exploited for novel devices. On the side of bosons the creation and manipulation of Bose Einstein Condensates (the first creation of BECs by Ketterle et al merited a Nobel prize) has become a standard technique that allows to study fundamental quantum concepts like matter-wave duality with increasingly large objects and advanced quantum effects like decoherence, thermalization, quantum chaos. In state-of-the-art experiments e.g. with ultracold atoms in optical lattices the bosonic or fermionic nature of quantum objects can change and it makes a lot of sense to treat the models in parallel in the development of mathematical methods. The experimental progress in these fields is spectacular, but the mathematical modelling and analysis as well as the numerical simulation are lagging behind. Low dimensional models are mostly introduced in a heuristic way and there is also a need for systematic derivations and comparison with the 3-d models. To close the gap is a main goal of this project that aims to deliver reliable tools and programme packages for the numerical simulation of different classes of quantum systems modelled by partial differential equation of NLS type. Virtually all participants have a strong track record of international collaboration, they grew up with the concept of the European Research Area where science knows no boundaries and scientists used to work in different countries, as it was the case in a pronounced way in mathematics and in quantum physics in the thirties of the last century. The Pre- and Post-Docs to be funded by this project will be trained in this spirit of mobility between scientific fields and between places.
This project gave rise to the following scientific achievements
PhD students
Boris Pawilowski, has been hired as a PhD student, under the supervision of F. Nier and N. Mauser. His contract started october 2012, and the PhD thesis was defended on December 2015. His PhD subject is "Mean field limit for discrete models and nonlinear discrete Schrödinger equations".
Postdocs
Loïc Le Treust has been hired as a Postdoc, under the supervision of F. Méhats (main) and N. Mauser. His contract started October 2013, and it did last two years, in Rennes and Vienna.
Yong Zhang, under contract in Vienna, has been invited for several one month periods in Rennes. There are works in progress with F. Méhats and P. Chartier.
Kristelle Roidot, had a six months contract in Vienna, and this gave rise to works with N. Mauser, C. Klein, J.-C. Saut, S. Descombes.
Workshops
July 2012, kick-off meeting of the LODIQUAS project, WPI, Vienna (one week, approx. 40 people, amongst which most of the participants of the project).
February 2013, WPI, Vienna, with a similar organization as the kick-off meeting.
July 2013, WPI, Vienna. At the WPI for one week. "Quantized Vortices in Superfluidity and Superconductivity and Related Problems", organisers W. Bao, C. Bardos, Q. Du, N. Mauser.
September 2013, WPI Vienna, "Modified dispersion for dispersive equations and systems ", organisers R. Carles, Mauser, J.C. Saut.
September 2013, WPI Vienna, "Modified dispersion for dispersive equations and systems ", organisers R. Carles, Mauser, J.C. Saut.
October 2014, WPI Vienna, "Blow-up and Dispersion in nonlinear Schrödinger and Wave equations", organizers G. Lebeau, A. Jüngel, O. Ivanovici, J.-C. Saut, H.-P. Stimming.
December 2014, Saint-Malo, "Lodiquas Meeting", organisers F. Castella and P. Chartier.
December 2015, Dinard, "Joint Lodiquas and Ipso Meeting",

6.1.2. ANR MOONRISE: 2015-2019

Participants: Nicolas Crouseilles, Philippe Chartier, Florian Méhats, François Castella, Mohammed Lemou.

The project *Moonrise* submitted by F. Méhats has been funded by the ANR for 4 years, for the period 2015-2019. This project aims at exploring modeling, mathematical and numerical issues originating from the presence of high-oscillations in nonlinear PDEs from the physics of nanotechnologies (quantum transport) and from the physics of plasmas (magnetized transport in tokamaks). The partners of the project are the IRMAR (Rennes), the IMT (Toulouse) and the CEA Cadarache. In the IPSO team, F. Castella, P. Chartier, N. Crouseilles and M. Lemou are members of the project Moonrise.

6.1.3. IPL (FRATRES)

IPSO is associated to IPL FRATRES which started in june 2015. The aim of this project is to organize Inria teams activities which develop mathematical and numerical tools in magnetically confined nuclear fusion. The ambition is to prepare the next generation of numerical modeling methodologies able to use in an optimal way the processing capabilities of modern massively parallel architectures. This objective requires close collaboration between a) applied mathematicians and physicists that develop and study mathematical models of PDE; b) numerical analysts developing approximation schemes; c) specialists of algorithmics proposing solvers and libraries using the many levels of parallelism offered by the modern architecture and d) computer scientists. The project road map ambitions to contribute in close connection with National and European initiatives devoted to nuclear Fusion to the improvement and design of numerical simulation technologies applied to plasma physics and in particular to the ITER project for magnetic confinement fusion.

6.2. European Initiatives

6.2.1. FP7 & H2020 Projects

6.2.1.1. Geopardi

Title: Numerical integration of Geometric Partial Differential Equations

Programm: FP7

Duration: September 2011 - August 2016

Coordinator: E. Faou

Inria contact: E. Faou

'The goal of this project is to develop new numerical methods for the approximation of evolution equations possessing strong geometric properties such as Hamiltonian systems or stochastic differential equations. In such situations the exact solutions endow with many physical properties that are consequences of the geometric structure: Preservation of the total energy, momentum conservation or existence of ergodic invariant measures. However the preservation of such qualitative properties of the original system by numerical methods at a reasonable cost is not guaranteed at all, even for very precise (high order) methods. The principal aim of geometric numerical integration is the understanding and analysis of such problems: How (and to which extend) reproduce qualitative behavior of differential equations over long time? The extension of this theory to partial differential equations is a fundamental ongoing challenge, which require the invention of a new mathematical framework bridging the most recent techniques used in the theory of nonlinear PDEs and stochastic ordinary and partial differential equations. The development of new efficient numerical schemes for geometric PDEs has to go together with the most recent progress in analysis (stability phenomena, energy transfers, multiscale problems, etc..) The major challenges of the project are to derive new schemes by bridging the world of numerical simulation and the analysis community, and to consider deterministic and stochastic equations, with a general aim at deriving hybrid methods. We also aim to create a research platform devoted to extensive numerical simulations of difficult academic PDEs in order to highlight new nonlinear phenomena and test numerical methods.'

6.2.1.2. EUROfusion 2015-2017

N. Crouseilles and M. Lemou are members of the EUROFusion project entitled "Enabling research project for the implementation of the fusion roadmap". The leader is E. Sonnendrücker (IPP Garching, Germany).

6.3. International Initiatives

6.3.1. Inria International Partners

6.3.1.1. Informal International Partners

Several IPSO members have international collaborations

- L. Einkemmer, University of Innsbruck. Collaboration on numerical schemes for Vlasov-Maxwell equations with N. Crouseilles and E. Faou.
- M. Thalhammer, University of Innsbruck. Collaboration on multi-revolution methods for the Schrödinger equation and Dirac equation with F. Méhats and P. Chartier.
- S. Jin, University of Madison. Collaboration on numerical schemes for highly-oscillatory problems with N. Crouseilles and M. Lemou.
- G. Vilmart, University of Geneva. Collaboration on uniformly accurate methods for highly-oscillatory problems with F. Méhats and P. Chartier
- F. Casas, University Jaume. Collaboration on splitting methods for Vlasov equations with N. Crouseilles and E. Faou.

6.4. International Research Visitors

6.4.1. Visits of International Scientists

6.4.1.1. Internships

S. Jin (University of Madison) spent 2 months at IRMAR (University of Rennes) within the framework of the Labex H. Lebesgue semester "PDEs and long time behavior", to collaborate with N. Crouseilles and M. Lemou.

6.4.2. Visits to International Teams

6.4.2.1. Research stays abroad

- P. Chartier: invitation at the University of Geneva (Switzerland), by G. Vilmart (one month in July).
- F. Méhats: invitation at the University of Geneva (Switzerland), by G. Vilmart (one week).
- F. Méhats: invitation at the Beijing Computational Science Research Center (China), by W. Bao (10 days).
- M. Lemou: invitation at the University of Wisconsin-Madison (US), by S. Jin (two weeks, october 2015).
- M. Lemou: invitation at the University of Geneva (Switzerland), by G. Vilmart (two weeks, july 2015).
- A. Debussche participated to the semester "New challenges in PDE: Deterministic dynamics and randomness in high and infinite dimensional systems" at MSRI (Berckeley, US).

7. Dissemination

7.1. Promoting Scientific Activities

7.1.1. Scientific events organisation

7.1.1.1. Member of the organizing committees

- M. Lemou and F. Méhats organized the CHL (Labex) workshop *Mathematical problems and modelization in kinetic theory*, Rennes, May 26-29 2015.

- E. Faou organized with B. Grébert, E. Paturel and L. Thomann (Univ. Nantes) the CHL (Labex) Summer school *PDE and large time asymptotics*, Nantes, June 22 - July 3 2015.
- N. Crouseilles and P. Chartier organized the CHL (Labex) workshop *Multiscale numerical methods for differential equations*, Rennes, August 25-27, 2015.
- F. Castella and P. Chartier organized the IPSO-LODIQUAS workshop with the support of the ANR LODIQUAS and MOONRISE, Dinard, December 9-11 2015.
- M. Lemou organized a mini-symposium at the 9th International Conference on Computational Physics (ICCP9): *numerical methods for quantum and kinetic problems*, Singapore, Junary 7-11 2015.
- N. Crouseilles and M. Lemou organized a mini-symposium at the national Congrès SMAI 2015: *Numerical Approaches for Stiff PDEs*, Les Karellis, June 8-12, 2015.

7.1.2. Scientific events selection

7.1.2.1. Member of the conference program committees

- P. Chartier was member of the scientific committee of ENUMATH 2015, 14-18 september, Ankara, Turkey.

7.1.3. Journal

7.1.3.1. Member of the editorial boards

- P. Chartier is member of the editorial board of *Mathematical Modelling and Numerical Analysis*.
- A. Debussche is editor in chief of *Stochastic Partial Differential Equations: analysis and computations*.
- A. Debussche is member of the editorial board of *Potential Analysis*.
- A. Debussche is member of the editorial board of *Journal of Evolution Equations*.
- A. Debussche is member of the editorial board of *Differential and Integral Equations*.
- A. Debussche is member of the editorial board of *ESAIM: proceedings*.
- A. Debussche is member of the editorial board of the collection *Mathématiques et Applications*.

7.1.3.2. Reviewer - Reviewing activities

The members of the team reviewed numerous papers for numerous international journals (Comm. Math. Phys., SIAM journals, J. Comput. Phys., $\cdots$).

7.1.4. Invited talks

- P. Chartier gave a talk at *The 9th International Conference on Computational Physics*, Singapore, January 7-11, 2015.
- E. Faou gave a talk at the seminar of analysis, at the university of Toulouse, January, 2015.
- E. Faou gave a talk at the Seminar ANEDP, University of Lille 1, January, 2015.
- P. Chartier gave a seminar at the University of Geneva, March 10, 2015.
- E. Faou gave a talk at ENS Lyon in the physics department, May 2015.
- E. Faou gave a talk at the workshop *Mathematical Methods in Quantum Molecular Dynamics*, organized by G. Hagedorn, C. Lasser and C. Le Bris, Oberwolfach, Germany, June, 2015.
- N. Crouseilles gave a talk in the seminar of the analysis team at the University of Toulouse III, June, 2015.
- P. Chartier gave a talk at the workshop *Modelling and Numerics for Quantum Systems*, Toulouse, September 2-4, 2015.
- E. Faou gave the Dahlquist prize lecture at the *Scicade conference*, Potsdam, Germany, September, 2015.

- P. Chartier gave a colloquium at the '*School of Mathematics in Georgia Tech*, Atlanta, USA, October 29, 2015.
- E. Faou gave a talk in the seminar of the analysis team at the University of Bordeaux I, October, 2015.
- F. Méhats gave seminars in Geneva (Switzerland), Beijing (China), Reims and Lyon.
- M. Lemou gave a talk at the Ki-Net international conference: *Asymptotic Preserving and Multiscale Methods for Kinetic and Hyperbolic Problems*, Madison (USA), May 4-8, 2015.
- M. Lemou gave a talk at the *International Congress on Industrial and Applied Mathematics, ICIAM 2015. Mini-symposium "Analysis and algorithm for coupling of kinetic and fluid equations*, Beijing (China), August 10-14, 2015.
- M. Lemou gave a talk at the *International workshop on kinetic problems in the honor of W. Strauss, R. Glassey and J. Schaeffer: Recent progress in collisionless models*, Imperial College, London, September 7-11, 2015.
- M. Lemou gave two conferences at the university of Wisconsin-Madison during his visit, between october 3 and october 17, 2015.
- A. Debussche gave a talk at the workshop *New challenges in PDE: Deterministic dynamics and randomness in high and infinite dimensional systems*, MSRI, Berkeley (USA), October 19-30, 2015.

7.1.5. Research administration

- F. Méhats has been the head of the IRMAR (UMR CNRS 6625), since June 2015,
- P. Chartier is scientific vice-deputy of the Inria-Rennes center.
- P. Chartier is member of the "Commission d'évaluation" of Inria.
- N. Crouseilles is member of the scientific council of ENS Rennes.
- N. Crouseilles is partly in charge of the weekly numerical analysis seminar at ENS Rennes.
- A. Debussche leads the H. Lebesgue Center (Labex) with San Vu Ngoc (coordinator) and L. Guillopé.
- E. Faou is member of the scientific council of the Pôle universitaire Léonard de Vinci, since september 2015.
- E. Faou is member of the CNU 26, since december 2015.
- M. Lemou is member of the scientific council of ENS Rennes.
- M. Lemou is member of the scientific council of the H. Lebesgue Center (Labex).
- M. Lemou is head of the "numerical analysis IRMAR team".
- F. Castella is head of the european ANR project "Lodiquas", described above.
- F. Castella is member of the "Conseil d'UFR de Mathématiques".

7.2. Teaching - Supervision - Juries

7.2.1. Teaching

Licence : P. Chartier, "Ordinary differential equations", 36 ETDH, L3, ENS Rennes.

Master : P. Chartier, "Numerical geometric integration and averaging methods", 36ETDH, M2, University of Rennes I.

Master : N. Crouseilles, "Numerical methods for kinetic equations", 18ETDH, M2, University of Rennes I.

Licence : N. Crouseilles, "Numerical methods", 36 ETDH, L3, ENS Rennes.

Master : M. Lemou, "Introduction to PDEs: hyperbolic systems and conservation laws.", 36ETDH, M2, University of Rennes I.

Master : F. Castella, “Pseudo-differential calculus.", 24ETDH, M2, University of Rennes I.

Master : F. Castella, “Kinetic equations.", 60ETDH, M1, University of Rennes I.

7.2.2. Supervision

PhD G. Leboucher, "Stroboscopic averaging methods for highly-oscillatory partial differential equations", University of Rennes I, defended on December 8, 2015. Advisors: P. Chartier and F. Méhats.

PhD H. Hivert, started in september 2012. Advisors: N. Crouseilles and M. Lemou.

PhD R. Horsin, started in september 2013. Advisors: E. Faou and F. Rousset.

PhD M. Malo, started in september 2015. Advisors: M. Lemou and F. Méhats.

PhD J. Sauzeau, started in september 2012. Advisors: P. Chartier and F. Castella.

PhD M. Tusseau, started in september 2013. Advisors: A. Debussche and F. Méhats.

7.2.3. Juries

- F. Méhats was referee on the thesis of A. Trescases (ENS Cachan). Defended on September 11, 2015.
- M. Lemou was member of the thesis committee, Phd of Xavier Valentin at Ecole Centrale de Paris. Defended on december 16, 2015.
- M. Lemou was referee on the thesis of T. Leroy (Paris 6) that will be defended on Junary 5, 2016.

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

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[12] A. ABDULLE, G. VILMART, K. ZYGALAKIS. *Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics*, in "SIAM Journal on Numerical Analysis", 2015, vol. 53, n^{o} 1, pp. 1-16, to appear in SIAM J. Numer. Anal., 23 pages [*DOI :* 10.1137/140962644], https://hal.archives-ouvertes.fr/hal-00965354

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