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ACTIVITY REPORT

Project-Team

MINGUS

Multi-scale Numerical Geometric Schemes

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

DOMAIN

**Applied Mathematics, Computation and
Simulation**

THEME

Numerical schemes and simulations

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Project-Team MINGUS

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- B5.1.1. – Quantum systems
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1 Team members, visitors, external collaborators

Research Scientists

- Nicolas Crouseilles [Team leader, Inria, Senior Researcher, HDR]
- Philippe Chartier [Inria, Senior Researcher, HDR]
- Erwan Faou [Inria, Senior Researcher, HDR]
- Mohammed Lemou [CNRS, Senior Researcher, HDR]

Faculty Members

- François Castella [Univ de Rennes I, Professor, HDR]
- Arnaud Debussche [École normale supérieure de Rennes, Professor, HDR]
- Florian Méhats [Univ de Rennes I, Professor, HDR]

PhD Students

- Gregoire Barrue [École normale supérieure de Rennes]
- Quentin Chauleur [École normale supérieure de Rennes]
- Josselin Massot [Univ de Rennes I]
- Angelo Rosello [École normale supérieure de Rennes, until Aug 2020]
- Leopold Tremant [Inria]

Technical Staff

- Yves Mocquard [Inria, Engineer]

Administrative Assistants

- Marie-Noëlle Georgeault [Inria, until May 2020]
- Stephanie Gosselin Lemaile [Inria]

Visiting Scientist

- Yingzhe Li [Academy of Mathematics and Systems Science - Chine, until Feb 2020]

External Collaborator

- Pierre Navaro [CNRS]

2 Overall objectives

2.1 Presentation

In applications involving complex physics, such as plasmas and nanotechnologies, numerical simulations serve as a prediction tool supplementing real experiments and are largely endorsed by engineers or researchers. Their performances rely not only on computational power, but also on the efficiency of the underlying numerical method and the complexity of the underlying models. The contribution of applied mathematics is then required, on the one hand for a better understanding of qualitative properties and a better identification of the different regimes present in the model, and on the other hand, for a more sounded construction of new models based on asymptotic analysis. This mathematical analysis is expected to greatly impact the design of *multiscale* numerical schemes.

The proposed research group MINGUS will be dedicated to the mathematical and numerical analysis of (possibly stochastic) partial differential equations (PDEs), originating from plasma physics and nanotechnologies, with emphasis on *multiscale* phenomena either of **highly-oscillatory**, of **dissipative** or **stochastic** types. These equations can be also encountered in applications to rarefied gas dynamics, radiative transfer, population dynamics or laser propagation, for which the multiscale character is modelled by a scale physical parameter ε .

Producing accurate solutions of multiscale equations is extremely challenging owing to severe restrictions to the numerical methods imposed by fast (or stiff) dynamics. *Ad-hoc* numerical methods should aim at capturing the slow dynamics solely, instead of resolving finely the stiff dynamics at a formidable computational cost. At the other end of the spectrum, the separation of scales -as required for numerical efficiency- is envisaged in asymptotic techniques, whose purpose is to describe the model in the limit where the small parameter ε tends to zero. MINGUS aspires to accommodate sophisticated tools of mathematical analysis and heuristic numerical methods in order to produce simultaneously rich asymptotic models and efficient numerical methods.

To be more specific, MINGUS aims at finding, implementing and analysing new multiscale numerical schemes for the following physically relevant multiscale problems:

- **Highly-oscillatory Schrödinger equation for nanoscale physics:** In quantum mechanics, the Schrödinger equation describes how the quantum state of some physical system changes with time. Its mathematical and numerical study is of paramount importance to fundamental and applied physics in general. We wish to specifically contribute to the mathematical modeling and the numerical simulation of confined quantum mechanical systems (in one or more space dimensions) possibly involving stochastic terms. Such systems are involved in quantum semi-conductors or atom-chips, as well as in cold atom physics (Bose-Einstein condensates) or laser propagation in optical fibers.

The prototypical equation is written

$$i\varepsilon\partial_t\psi^\varepsilon = \frac{\varepsilon^2}{\beta}\Delta\psi^\varepsilon + |\psi^\varepsilon|^2\psi^\varepsilon + \psi^\varepsilon\xi \quad (1)$$

where the function $\psi^\varepsilon = \psi^\varepsilon(t, x) \in \mathbb{C}$ depends on time $t \geq 0$ and position $x \in \mathbb{R}^3$, $\xi = \xi(x, t)$ is a white noise and where the small parameter ε is the Planck's constant describing the microscopic/macroscopic ratio. The limit $\varepsilon \rightarrow 0$ is referred to as the semi-classical limit. The regime $\varepsilon = 1$ and $\beta \rightarrow 0$ (this can be for instance the relative length of the optical fiber) is highly-oscillatory. The noise ξ acts as a potential, it may represent several external perturbations. For instance temperature effects in Bose-Einstein condensation or amplification in optical fibers. The highly oscillatory regime combined with noise introduces new challenges in the design of efficient schemes.

- **Highly-oscillatory or highly-dissipative kinetic equations:** Plasma is sometimes considered as the fourth state of matter, obtained for example by bringing a gas to a very high temperature. A globally neutral gas of neutral and charged particles, called plasma, is then obtained and is described by a kinetic equation as soon as collective effects dominate as compared to binary collisions. A situation of major importance is magnetic fusion in which collisions are not predominant. In order to confine such a plasma in devices like tokamaks (ITER project) or stellarators, a large magnetic field is used to endow the charged particles with a cyclotronic motion around field lines. Note that kinetic models are also widely used for modeling plasmas in earth magnetosphere or in rarefied gas dynamics.

Denoting $f^\varepsilon = f^\varepsilon(t, x, v) \in \mathbb{R}^+$ the distribution function of charged particles at time $t \geq 0$, position $x \in \mathbb{R}^3$ and velocity $v \in \mathbb{R}^3$, a typical kinetic equation for f^ε reads

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + \left(E + \frac{1}{\varepsilon} (v \times B) \right) \cdot \nabla_v f^\varepsilon = \frac{1}{\beta} Q(f^\varepsilon) + f^\varepsilon m^\varepsilon \quad (2)$$

where (E, B) is the electro-magnetic field (which may itself depend on f through Maxwell's equations), m^ε is a random process (which may describe absorption or creation of particles) and Q is a collision operator. The dimensionless parameters ε, β are related to the cyclotronic frequency and the mean free path. Limits $\varepsilon \rightarrow 0$ and $\beta \rightarrow 0$ do not share the same character (the former is oscillatory and the latter is dissipative) and lead respectively to gyrokinetic and hydrodynamic models. The noise term m^ε is correlated in space and time. At the limit $\varepsilon \rightarrow 0$, it converges formally to a white noise and stochastic PDEs are obtained.

MINGUS project is the follow-up of IPSO, ending in december in 2017. IPSO original aim was to extend the analysis of geometric schemes from ODEs to PDEs. During the last evaluation period, IPSO also considered the numerical analysis of geometric schemes for (S)PDEs, possibly including multiscale phenomena. Breakthrough results [41, 43, 44, 47] have been recently obtained which deserve to be deepened and extended. It thus appears quite natural to build the MINGUS team upon these foundations.

The objective of MINGUS is twofold: the construction and the analysis of numerical schemes (such as "Uniformly Accurate numerical schemes", introduced by members of the IPSO project) for multiscale (S)PDEs originating from physics. In turn, this requires (i) a deep mathematical understanding of the (S)PDEs under consideration and (ii) a strong involvement into increasingly realistic problems, possibly resorting to parallel computing. For this aspect, we intend to benefit from the Inria Selalib software library which turns out to be the ideal complement of our activities.

3 Research program

The MINGUS project is devoted to the mathematical and numerical analysis of models arising in plasma physics and nanotechnology. The main goal is to construct and analyze numerical methods for the approximation of PDEs containing multiscale phenomena. Specific multiscale numerical schemes will be proposed and analyzed in different regimes (namely highly-oscillatory and dissipative). The ultimate goal is to dissociate the physical parameters (generically denoted by ε) from the numerical parameters (generically denoted by h) with a uniform accuracy. Such a task requires mathematical prerequisite of the PDEs.

Then, for a given stiff (highly-oscillatory or dissipative) PDE, the methodology of the MINGUS team will be the following

- Mathematical study of the asymptotic behavior of multiscale models.
This part involves averaging and asymptotic analysis theory to derive asymptotic models, but also long-time behavior of the considered models.

- Construction and analysis of multiscale numerical schemes.
This part is the core of the project and will be deeply inspired from the mathematical prerequisite. In particular, our ultimate goal is the design of *Uniformly Accurate* (UA) schemes, whose accuracy is independent from ε .
- Validation on physically relevant problems.
The last goal of the MINGUS project is to validate the new numerical methods, not only on toy problems, but also on realistic models arising in physics of plasmas and nanotechnologies. We will benefit from the Selalib software library which will help us to scale-up our new numerical methods to complex physics.

3.1 Dissipative problems

In the dissipative context, the asymptotic analysis is quite well understood in the deterministic case and multiscale numerical methods have been developed in the last decades. Indeed, the so-called Asymptotic-Preserving schemes has retained a lot of attention all over the world, in particular in the context of collisional kinetic equations. But, there is still a lot of work to do if one is interested in the derivation high order asymptotic models, which enable to capture the original solution for all time. Moreover, this analysis is still misunderstood when more complex systems are considered, involving non homogeneous relaxation rates or stochastic terms for instance. Following the methodology we aim at using, we first address the mathematical analysis before deriving multiscale efficient numerical methods.

A simple model of dissipative systems is governed by the following differential equations

$$\begin{cases} \frac{dx^\varepsilon(t)}{dt} = \mathcal{G}(x^\varepsilon(t), y^\varepsilon(t)), & x^\varepsilon(0) = x_0, \\ \frac{dy^\varepsilon(t)}{dt} = -\frac{y^\varepsilon(t)}{\varepsilon} + \mathcal{H}(x^\varepsilon(t), y^\varepsilon(t)), & y^\varepsilon(0) = y_0, \end{cases} \quad (3)$$

for given initial condition $(x_0, y_0) \in \mathbb{R}^2$ and given smooth functions \mathcal{G}, \mathcal{H} which possibly involve stochastic terms.

3.1.1 Asymptotic analysis of dissipative PDEs (*F. Castella, P. Chartier, A. Debussche, E. Faou, M. Lemou*)

Derivation of asymptotic problems

Our main goal is to analyze the asymptotic behavior of dissipative systems of the form ((3)) when ε goes to zero. The *center manifold theorem* [40] is of great interest but is largely unsatisfactory from the following points of view

- a constructive approach of h and x_0^ε is clearly important to identify the high-order asymptotic models: this would require expansions of the solution by means of B-series or word-series [42] allowing the derivation of error estimates between the original solution and the asymptotic one.
- a better approximation of the transient phase is strongly required to capture the solution for small time: extending the tools developed in averaging theory, the main goal is to construct a suitable change of variable which enables to approximate the original solution for all time.

Obviously, even at the ODE level, a deep mathematical analysis has to be performed to understand the asymptotic behavior of the solution of (3). But, the same questions arise at the PDE level. Indeed, one certainly expects that dissipative terms occurring in collisional kinetic equations (2) may be treated theoretically along this perspective. The key new point indeed is to see the center manifold theorem as a change of variable in the space on unknowns, while the standard point of view leads to considering the center manifold as an asymptotic object.

Stochastic PDEs

We aim at analyzing the asymptotic behavior of stochastic collisional kinetic problems, that is equation of the type (2). The noise can describe creation or absorption (as in (2)), but it may also be a forcing term or a random magnetic field. In the parabolic scaling, one expects to obtain parabolic SPDEs at the limit. More precisely, we want to understand the fluid limits of kinetic equations in the presence of noise. The

noise is smooth and non delta correlated. It contains also a small parameter and after rescaling converges formally to white noise. Thus, this adds another scale in the multiscale analysis. Following the pioneering work by Debussche and Vovelle, [43], some substantial progresses have been done in this topic.

More realistic problems may be addressed such as high field limit describing sprays, or even hydrodynamic limit. The full Boltzmann equation is a very long term project and we wish to address simpler problems such as convergences of BGK models to a stochastic Stokes equation.

The main difficulty is that when the noise acts as a forcing term, which is a physically relevant situation, the equilibria are affected by the noise and we face difficulties similar to that of high field limit problems. Also, a good theory of averaging lemma in the presence of noise is lacking. The methods we use are generalization of the perturbed test function method to the infinite dimensional setting. We work at the level of the generator of the infinite dimensional process and prove convergence in the sense of the martingale problems. A further step is to analyse the speed of convergence. This is a prerequisite if one wants to design efficient schemes. This requires more refined tools and a good understanding of the Kolmogorov equation.

3.1.2 Numerical schemes for dissipative problems (*All members*)

The design of numerical schemes able to reproduce the transition from the microscopic to macroscopic scales largely matured with the emergence of the Asymptotic Preserving schemes which have been developed initially for collisional kinetic equations (actually, for solving (2) when $\beta \rightarrow 0$). Several techniques have flourished in the last decades. As said before, AP schemes entail limitations which we aim at overcoming by deriving

- AP numerical schemes whose numerical cost diminishes as $\beta \rightarrow 0$,
- Uniformly accurate numerical schemes, whose accuracy is independent of β .

Time diminishing methods

The main goal consists in merging Monte-Carlo techniques [38] with AP methods for handling *automatically* multiscale phenomena. As a result, we expect that the cost of the so-obtained method decreases when the asymptotic regime is approached; indeed, in the collisional (i.e. dissipative) regime, the deviational part becomes negligible so that a very few number of particles will be generated to sample it. A work in this direction has been done by members of the team.

We propose to build up a method which permits to realize the transition from the microscopic to the macroscopic description without domain decomposition strategies which normally oblige to fix and tune an interface in the physical space and some threshold parameters. Since it will permit to go over domain decomposition and AP techniques, this approach is a very promising research direction in the numerical approximation of multiscale kinetic problems arising in physics and engineering.

Uniformly accurate methods

To overcome the accuracy reduction observed in AP schemes for intermediate regimes, we intend to construct and analyse multiscale numerical schemes for (3) whose error is uniform with respect to ε . The construction of such a scheme requires a deep mathematical analysis as described above. Ideally one would like to develop schemes that preserve the center manifold (without computing the latter!) as well as schemes that resolve numerically the stiffness induced by the fast convergence to equilibrium (the so-called transient phase). First, our goal is to extend the strategy inspired by the central manifold theorem in the ODE case to the PDE context, in particular for collisional kinetic equations (2) when $\beta \rightarrow 0$. The design of Uniformly Accurate numerical schemes in this context would require to generalize two-scale techniques introduced by members of the team in the framework of highly-oscillatory problems [41].

Multiscale numerical methods for stochastic PDEs

AP schemes have been developed recently for kinetic equations with noise in the context of Uncertainty Quantification UQ [46]. These two aspects (multiscale and UQ) are two domains which usually come within the competency of separate communities. UQ has drawn a lot of attention recently to control the propagation of data pollution; undoubtedly UQ has a lot of applications and one of our goals will be to study how sources of uncertainty are amplified or not by the multiscale character of the model. We also wish to go much further and developing AP schemes when the noise is also rescaled and the limit is a

white noise driven SPDE, as described in section (3.1.1). For simple nonlinear problem, this should not present much difficulties but new ideas will definitely be necessary for more complicated problems when noise deeply changes the asymptotic equation.

3.2 Highly-oscillatory problems

As a generic model for highly-oscillatory systems, we will consider the equation

$$\frac{du^\varepsilon(t)}{dt} = \mathcal{F}(t/\varepsilon, u^\varepsilon(t)), \quad u^\varepsilon(0) = u_0, \quad (4)$$

for a given u_0 and a given periodic function \mathcal{F} (of period P w.r.t. its first variable) which possibly involves stochastic terms. Solution u^ε exhibits high-oscillations in time superimposed to a slow dynamics. Asymptotic techniques -resorting in the present context to *averaging* theory [50]- allow to decompose

$$u^\varepsilon(t) = \Phi_{t/\varepsilon} \circ \Psi_t \circ \Phi_0^{-1}(u_0), \quad (5)$$

into a fast solution component, the εP -periodic change of variable $\Phi_{t/\varepsilon}$, and a slow component, the flow Ψ_t of a non-stiff *averaged* differential equation. Although equation (5) can be satisfied only up to a small remainder, various methods have been recently introduced in situations where (4) is posed in \mathbb{R}^n or for the Schrödinger equation (1).

In the asymptotic behavior $\varepsilon \rightarrow 0$, it can be advantageous to replace the original singularly perturbed model (for instance (1) or (2)) by an approximate model which does not contain stiffness any longer. Such reduced models can be derived using asymptotic analysis, namely averaging methods in the case of highly-oscillatory problems. In this project, we also plan to go beyond the mere derivation of limit models, by searching for better approximations of the original problem. This step is of mathematical interest *per se* but it also paves the way of the construction of multiscale numerical methods.

3.2.1 Asymptotic analysis of highly-oscillatory PDEs (*All members*)

Derivation of asymptotic problems

We intend to study the asymptotic behavior of highly-oscillatory evolution equations of the form (4) posed in an infinite dimensional Banach space.

Recently, the stroboscopic averaging has been extended to the PDE context, considering nonlinear Schrödinger equation (1) in the highly-oscillatory regime. A very exciting way would be to use this averaging strategy for highly-oscillatory kinetic problem (2) as those encountered in strongly magnetized plasmas. This turns out to be a very promising way to re-derive gyrokinetic models which are the basis of tokamak simulations in the physicists community. In contrast with models derived in the literature (see [39]) which only capture the average with respect to the oscillations, this strategy allows for the complete recovery of the exact solution from the asymptotic (non stiff) model. This can be done by solving companion transport equation that stems naturally from the decomposition (5).

Long-time behavior of Hamiltonian systems

The study of long-time behavior of nonlinear Hamiltonian systems have received a lot of interest during the last decades. It enables to put in light some characteristic phenomena in complex situations, which are beyond the reach of numerical simulations. This kind of analysis is of great interest since it can provide very precise properties of the solution. In particular, we will focus on the dynamics of nonlinear PDEs when the initial condition is close to a stationary solution. Then, the long-time behavior of the solution is studied through mainly three axis

- *linear stability*: considering the linearized PDE, do we have stability of a stationary solution ? Do we have linear Landau damping around stable non homogeneous stationary states?
- *nonlinear stability*: under a criteria, do we have stability of a stationary solution in energy norm like in [47], and does this stability persist under numerical discretization? For example one of our goals is to address the question of the existence and stability of discrete travelling wave in space and time.

- do we have existence of damped solutions for the full nonlinear problem ? Around homogeneous stationary states, solutions scatter towards a modified stationary state (see [48, 44]). The question of existence of Landau damping effects around non homogeneous states is still open and is one of our main goal in the next future.

Asymptotic behavior of stochastic PDEs

The study of SPDEs has known a growing interest recently, in particular with the fields medal of M. Hairer in 2014. In many applications such as radiative transfer, molecular dynamics or simulation of optical fibers, part of the physical interactions are naturally modeled by adding supplementary random terms (the noise) to the initial deterministic equations. From the mathematical point of view, such terms change drastically the behavior of the system.

- In the presence of noise, highly-oscillatory dispersive equations presents new problems. In particular, to study stochastic averaging of the solution, the analysis of the long time behavior of stochastic dispersive equations is required, which is known to be a difficult problem in the general case. In some cases (for instance highly-oscillatory Schrödinger equation (1) with a time white noise in the regime $\varepsilon \ll 1$), it is however possible to perform the analysis and to obtain averaged stochastic equations. We plan to go further by considering more difficult problems, such as the convergence of a stochastic Klein-Gordon-Zakharov system to as stochastic nonlinear Schrödinger equation.
- The long-time behavior of stochastic Schrödinger equations is of great interest to analyze mathematically the validity of the Zakharov theory for wave turbulence (see [49]). The problem of wave turbulence can be viewed either as a deterministic Hamiltonian PDE with random initial data or a randomly forced PDEs where the stochastic forcing is concentrated in some part of the spectrum (in this sense it is expected to be a hypoelliptic problem). One of our goals is to test the validity the Zakharov equation, or at least to make rigorous the spectrum distribution spreading observed in the numerical experiments.

3.2.2 Numerical schemes for highly-oscillatory problems (*All members*)

This section proposes to explore numerical issues raised by highly-oscillatory nonlinear PDEs for which (4) is a prototype. Simulating a highly-oscillatory phenomenon usually requires to adapt the numerical parameters in order to solve the period of size ε so as to accurately simulate the solution over each period, resulting in a unacceptable execution cost. Then, it is highly desirable to derive numerical schemes able to advance the solution by a time step independent of ε . To do so, our goal is to construct *Uniformly Accurate* (UA) numerical schemes, for which the numerical error can be estimated by Ch^p (h being any numerical parameters) with C independent of ε and p the order of the numerical scheme.

Recently, such numerical methods have been proposed by members of the team in the highly-oscillatory context. [41]. They are mainly based on a separation of the fast and slow variables, as suggested by the decomposition (5). An additional ingredient to prove the uniformly accuracy of the method for (4) relies on the search for an appropriate initial data which enables to make the problem smooth with respect to ε .

Such an approach is assuredly powerful since it provides a numerical method which enables to capture the high oscillations in time of the solution (and not only its average) even with a large time step. Moreover, in the asymptotic regime, the potential gain is of order $1/\varepsilon$ in comparison with standard methods, and finally averaged models are not able to capture the intermediate regime since they miss important information of the original problem. We are strongly convinced that this strategy should be further studied and extended to cope with some other problems. The ultimate goal being to construct a scheme for the original equation which degenerates automatically into a consistent approximation of the averaged model, without resolving it, the latter can be very difficult to solve.

- Space oscillations:
When rapidly oscillating coefficients in **space** (*i.e.* terms of the form $a(x, x/\varepsilon)$) occur in elliptic or parabolic equations, homogenization theory and numerical homogenization are usually employed to handle the stiffness. However, these strategies are in general not accurate for all $\varepsilon \in]0, 1]$. Then, the construction of numerical schemes which are able to handle both regimes in an uniform way is of great interest. Separating fast and slow *spatial* scales merits to be explored in this context.

The delicate issue is then to extend the choice suitable initial condition to an *appropriate choice of boundary conditions* of the augmented problem.

- **Space-time oscillations:**
For more complex problems however, the recent proposed approaches fail since the main oscillations cannot be identified explicitly. This is the case for instance when the magnetic field B depends on t or x in (2) but also for many other physical problems. We then have to deal with the delicate issue of space-time oscillations, which is known to be a very difficult problem from a mathematical and a numerical point of view. To take into account the space-time mixing, a periodic motion has to be detected together with a phase S which possibly depends on the time and space variables. These techniques originate from **geometric optics** which is a very popular technique to handle highly-frequency waves.
- **Geometrical properties:**
The questions related to the geometric aspects of multiscale numerical schemes are of crucial importance, in particular when long-time simulations are addressed (see [45]). Indeed, one of the main questions of geometric integration is whether intrinsic properties of the solution may be passed onto its numerical approximation. For instance, if the model under study is Hamiltonian, then the exact flow is symplectic, which motivates the design of symplectic numerical approximation. For practical simulations of Hamiltonian systems, symplectic methods are known to possess very nice properties (see [45]). It is important to combine multiscale techniques to geometric numerical integration. All the problems and equations we intend to deal with will be addressed with a view to preserve intrinsic geometric properties of the exact solutions and/or to approach the asymptotic limit of the system in presence of a small parameter. An example of a numerical method developed by members of the team is the multi-revolution method.
- **Quasi-periodic case:**
So far, numerical methods have been proposed for the periodic case with single frequency. However, the quasi-periodic case ¹ is still misunderstood although many complex problems involve multi-frequencies. Even if the quasi-periodic averaging is doable from a theoretical point of view in the ODE case, (see [50]), it is unclear how it can be extended to PDEs. One of the main obstacle being the requirement, usual for ODEs like (4), for \mathcal{F} to be analytic in the periodic variables, an assumption which is clearly impossible to meet in the PDE setting. An even more challenging problem is then the design of numerical methods for this problem.
- **extension to stochastic PDEs:**
All these questions will be revisited within the stochastic context. The mathematical study opens the way to the derivation of efficient multiscale numerical schemes for this kind of problems. We believe that the theory is now sufficiently well understood to address the derivation and numerical analysis of multiscale numerical schemes. Multi-revolution composition methods have been recently extended to highly-oscillatory stochastic differential equations. The generalization of such multiscale numerical methods to SPDEs is of great interest. The analysis and simulation of numerical schemes for highly-oscillatory nonlinear stochastic Schrödinger equation under diffusion-approximation for instance will be one important objective for us. Finally, an important aspect concerns the quantification of uncertainties in highly-oscillatory kinetic or quantum models (due to an incomplete knowledge of coefficients or imprecise measurement of datas). The construction of efficient multiscale numerical methods which can handle multiple scales as well as random inputs have important engineering applications.

4 Application domains

4.1 Application domains

The MINGUS project aims at applying the new numerical methods on realistic problems arising for instance in physics of nanotechnology and physics of plasmas. Therefore, in addition to efforts devoted

¹replacing t/ε by $t\omega/\varepsilon$ in (4), with $\omega \in \mathbb{R}^d$ a vector of non-resonant frequencies

to the design and the analysis of numerical methods, the inherent large size of the problems at hand requires advanced mathematical and computational methods which are hard to implement. Another application is concerned with population dynamics for which the main goal is to understand how the spatial propagation phenomena affect the demography of a population (plankton, parasite fungi, ...). Our activity is mostly at an early stage in the process of transfer to industry. However, all the models we use are physically relevant and all have applications in many areas (ITER, Bose-Einstein condensate, wave turbulence, optical tomography, transport phenomena, population dynamics, ...). As a consequence, our research aims at reaching theoretical physicists or computational scientists in various fields who have strong links with industrial applications. In order to tackle as realistic physical problems as possible, a fundamental aspect will consist in working on the realization of numerical methods and algorithms which are able to make an efficient use of a large number of processors. Then, it is essential for the numerical methods developed in the MINGuS project to be thought through this prism. We will benefit from the strong expertise of P. Navaro in scientific computing and more precisely on the Selalib software library (see description below). Below, we detail our main applications: first, the modeling and numerical approximation of magnetized plasmas is our major application and will require important efforts in terms of software developments to scale-up our multiscale methods; second, the transport of charged particles in nanostructures has very interesting applications (like graphene material), for which our contributions will mainly focus on dedicated problems; lastly, applications on population dynamics will be dedicated to mathematical modeling and some numerical validations.

4.2 Plasmas problems

The Selalib (SEmi-LAgrangian LIBrary) software library² is a modular library for kinetic and gyrokinetic simulations of plasmas in fusion energy devices. Selalib is a collection of fortran modules aimed at facilitating the development of kinetic simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities and modules to help parallelization (both MPI and OpenMP), as well as pre-packaged simulations. Its main objective is to develop a documented library implementing several numerical methods for the numerical approximation of kinetic models. Another objective of the library is to provide physicists with easy-to-use gyrokinetic solvers. It has been originally developed by E. Sonnendrücker and his collaborators in the past CALVI Inria project, and has played an important role in the activities of the IPL FRATRES. P. Navaro is one of the main software engineer of this library and as such he played an important daily role in its development and its portability on supercomputers. Though Selalib has reached a certain maturity some additional works are needed to make available by the community. There are currently discussions for a possible evolution of Selalib, namely the writing of a new release which will be available for free download. Obviously, the team will be involved in this process. At the scientific level, Selalib is of great interest for us since it provides a powerful tool with which we can test, validate and compare our new methods and algorithms (users level). Besides numerical algorithms the library provides low-level utilities, input-output modules as well as parallelization strategies dedicated to kinetic problems. Moreover, a collection of simulations for typical test cases (of increasing difficulties) with various discretization schemes supplements the library. This library turns out to be the ideal complement of our activities and it will help us to scale-up our numerical methods to high-dimensional kinetic problems. During the last years, several experiments have been successfully performed in this direction (especially with PhD students) and it is important for us that this approach remains throughout. Then, we intend to integrate several of the numerical methods developed by the team within the Selalib library, with the strong help of P. Navaro (contributors level). This work has important advantages: (i) it will improve our research codes (in terms of efficiency but also of software maintenance point of view); (ii) it will help us to promote our research by making our methods available to the research community.

4.3 Quantum problems

Nowadays, a great challenge consists in the downscaling at the nanometer scale of electronic components in order to improve speed and efficiency of semiconductor materials. In this task, modeling and numerical simulations play an important role in the determination of the limit size of the nanotransistors. At the

²SELALIB, <http://selalib.gforge.inria.fr>

nanoscale, quantum effects have to be considered and the Schrödinger equation is prominent equation in this context. In the so-called semiclassical regime or when the transport is strongly confined, the solution endows space-time highly oscillations which are very difficult to capture numerically. An important application is the modeling of charged particles transport in graphene. Graphene is a sheet of carbone made of a single layer of molecule, organized in a bidimensional honeycomb crystal. The transport of charged particles in this structure is usually performed by Dirac equation (which is the relativistic counterpart of the Schrödinger equation). Due to the unusual properties of graphene -at room temperature, electrons moving in graphene behave as massless relativistic particles- physicists and compagnies are nowadays actively studying this material. Here, predicting how the material properties are affected by the uncertainties in the hexagonal lattice structure or in external potentials, is a major issue.

4.4 Population dynamics

The main goal is to characterize how spatial propagation phenomena (diffusion, transport, advection, ...) affect the time evolution of the demography of a population. In collaboration with Y. Lagadeuc (ECOBIO, Rennes), this question has been studied for plankton. In this context, mathematical models have been proposed and it has been shown that the spatial dynamic (in this context, due to the marine current) which is fast compared to demographic scales, can strongly modify the demographic evolution of the plankton. In collaboration with Ecole d'Agronomie de Rennes, a mathematical study on the demography of a parasite fungi of plants has been performed. In this context, the demography is specific: the fungi can proliferate through sexual reproduction or through parthenogenesis. This two ways of reproduction give rise mathematically to quadratic and linear growth rates with respect to the population variable. The demography is then coupled with transport (transport of fungi spore by wind). Here, the goal is to characterize the propagation of the fungi population by finding travelling waves solutions which are well adapted to describe the evolution of invasive fronts. Moreover, this approach enables to recover with a good agreement realistic examples (infection of ash or banana tree) for which experimental data are available. In these contexts, mathematical models are a powerful tool for biologists since measurements are very complicated to obtain and laboratory experiments hardly reproduce reality. The models derived are multiscale due to the nature of the underlying phenomena and the next step is to provide efficient numerical schemes.

5 New software and platforms

5.1 New software

5.1.1 Selalib

Name: SEMi-LAgrangian LIBrary

Keywords: Plasma physics, Semilagrangian method, Parallel computing, Plasma turbulence

Scientific Description: The objective of the Selalib project (SEMi-LAgrangian LIBrary) is to develop a well-designed, organized and documented library implementing several numerical methods for kinetic models of plasma physics. Its ultimate goal is to produce gyrokinetic simulations.

Another objective of the library is to provide to physicists easy-to-use gyrokinetic solvers, based on the semi-lagrangian techniques developed by Eric Sonnendrücker and his collaborators in the past CALVI project. The new models and schemes from TONUS are also intended to be incorporated into Selalib.

Functional Description: Selalib is a collection of modules conceived to aid in the development of plasma physics simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities from general and mathematical utilities and modules to aid in parallelization, up to pre-packaged simulations.

URL: <http://selalib.gforge.inria.fr/>

Contact: Philippe Helluy

Participants: Edwin Chacon Golcher, Pierre Navaro, Sever Hirstoaga, Eric Sonnendrücker, Michel Mehrenberger

Partners: Max Planck Insitute - Garching, Université de Strasbourg, CNRS, Université de Rennes 1

5.1.2 HOODESolver.jl

Name: Julia package for solving numerically highly-oscillatory ODE problems

Keywords: Ordinary differential equations, Numerical solver

Functional Description: Julia is a programming language for scientists with a syntax and functionality similar to MATLAB, R and Python. HOODESolver.jl is a julia package allowing to solve ordinary differential equations with sophisticated numerical techniques resulting from research within the MINGUS project team. To use it, just install Julia on your workstation.

Release Contributions: This is the first version of the package. It will evolve further because we want to have a better integration with the Julia organization on differential equations. This one already includes a lot of methods to numerically solve differential equations. This integration will allow us to have a larger audience and thus more feedback and possibly external collaborations.

Contact: Nicolas Crouseilles

Participants: Yves Mocquard, Pierre Navaro, Nicolas Crouseilles

Partners: Université de Rennes 1, CNRS

6 New results

In [17], we prove the nonlinear instability of inhomogeneous steady states solutions to the Hamiltonian Mean Field (HMF) model. We first study the linear instability of this model under a simple criterion by adapting the techniques developed by the authors recently. In a second part, we extend to the inhomogeneous case some techniques developed by the authors recently and prove a nonlinear instability result under the same criterion.

In [5], we consider the non linear wave equation (NLW) on the d -dimensional torus with a smooth nonlinearity of order at least two at the origin. We prove that, for almost any mass, small and smooth solutions of high Sobolev indices are stable up to arbitrary long times with respect to the size of the initial data. To prove this result we use a normal form transformation decomposing the dynamics into low and high frequencies with weak interactions. While the low part of the dynamics can be put under classical Birkhoff normal form, the high modes evolve according to a time dependent linear Hamiltonian system. We then control the global dynamics by using polynomial growth estimates for high modes and the preservation of Sobolev norms for the low modes. Our general strategy applies to any semi-linear Hamiltonian PDEs whose linear frequencies satisfy a very general non resonance condition. The (NLW) equation on a torus is a good example since the standard Birkhoff normal form applies only when $d = 1$ while our strategy applies in any dimension.

In [19], we study semigroups generated by accretive non-selfadjoint quadratic differential operators. We give a description of the polar decomposition of the associated evolution operators as products of a selfadjoint operator and a unitary operator. The selfadjoint parts turn out to be also evolution operators generated by time-dependent real-valued quadratic forms that are studied in details. As a byproduct of this decomposition, we give a geometric description of the regularizing properties of semigroups generated by accretive non-selfadjoint quadratic operators. Finally, by using the interpolation theory, we take advantage of this smoothing effect to establish subelliptic estimates enjoyed by quadratic operators.

In [22], we study the Boltzmann equation with external forces, not necessarily deriving from a potential, in the incompressible Navier-Stokes perturbative regime. On the torus, we establish local-in-time, for any time, Cauchy theories that are independent of the Knudsen number in Sobolev spaces.

The existence is proved around a time-dependent Maxwellian that behaves like the global equilibrium both as time grows and as the Knudsen number decreases. We combine hypocoercive properties of linearized Boltzmann operators with linearization around a time-dependent Maxwellian that catches the fluctuations of the characteristics trajectories due to the presence of the force. This uniform theory is sufficiently robust to derive the incompressible Navier-Stokes-Fourier system with an external force from the Boltzmann equation. Neither smallness, nor time-decaying assumption is required for the external force, nor a gradient form, and we deal with general hard potential and cutoff Boltzmann kernels. As a by-product the latest general theories for unit Knudsen number when the force is sufficiently small and decays in time are recovered.

In [37], we consider a particle system with a mean-field-type interaction perturbed by some common and individual noises. When the interacting kernels are sublinear and only locally Lipschitz-continuous, relying on arguments regarding the tightness of random measures in Wasserstein spaces, we are able to construct a weak solution of the corresponding limiting SPDE. In a setup where the diffusion coefficient on the environmental noise is bounded, this weak convergence can be turned into a strong $L^p(\Omega)$ convergence and the propagation of chaos for the particle system can be established. The systems considered include perturbations of the Cucker-Smale model for collective motion.

In [15], we derive the hydrodynamic limit of a kinetic equation where the interactions in velocity are modeled by a linear operator (Fokker-Planck or linear Boltzmann) and the force in the Vlasov term is a stochastic process with high amplitude and short-range correlation. In the scales and the regime we consider, the hydrodynamic equation is a scalar second-order stochastic partial differential equation. Compared to the deterministic case, we also observe a phenomenon of enhanced diffusion.

In [30], we consider multiscale stochastic spatial gene networks involving chemical reactions and diffusions. The model is Markovian and the transitions are driven by Poisson random clocks. We consider a case where there are two different spatial scales: a microscopic one with fast dynamic and a macroscopic one with slow dynamic. At the microscopic level, the species are abundant and for the large population limit a partial differential equation (PDE) is obtained. On the contrary at the macroscopic level, the species are not abundant and their dynamic remains governed by jump processes. It results that the PDE governing the fast dynamic contains coefficients which randomly change. The global weak limit is an infinite dimensional continuous piecewise deterministic Markov process (PDMP). Also, we prove convergence in the supremum norm.

In [20], we consider the gravitational N-body problem and introduces time-reparametrization functions that allow to define globally solutions of the N-body equations. First, a lower bound of the radius of convergence of the solution to the original equations is derived, which suggests an appropriate time-reparametrization. In the new fictitious time τ , it is then proved that any solution exists for all $t \in \mathbb{R}$, and that it is uniquely extended as a holomorphic function to a strip of fixed width. As a by-product, a global power series representation of the solutions of the N-body problem is obtained. Noteworthy, our global time-regularization remain valid in the limit when one of the masses vanishes. Finally, numerical experiments show the efficiency of the new time-regularization functions for some N-problems with close encounters.

In [32], we study a kinetic toy model for a spray of particles immersed in an ambient fluid, subject to some additional random forcing given by a mixing, space-dependent Markov process. Using the perturbed test function method, we derive the hydrodynamic limit of the kinetic system. The law of the limiting density satisfies a stochastic conservation equation in Stratonovich form, whose drift and diffusion coefficients are completely determined by the law of the stationary process associated with the Markovian perturbation.

In [31], we establish the existence of martingale solutions to a class of stochastic conservation equations. The underlying models correspond to random perturbations of kinetic models for collective motion such as the Cucker-Smale and Motsch-Tadmor models. By regularizing the coefficients, we first construct approximate solutions obtained as the mean-field limit of the corresponding particle systems. We then establish the compactness in law of this family of solutions by relying on a stochastic averaging lemma. This extends the results obtained by Karper, Mellet and Trivisa (SIAM, 2013) in the deterministic case.

In [34], we introduce specific solutions to the linear harmonic oscillator, named bubbles. They form resonant families of invariant tori of the linear dynamics, with arbitrarily large Sobolev norms. We use these modulated bubbles of energy to construct a class of potentials which are real, smooth, time dependent and uniformly decaying to zero with respect to time, such that the corresponding perturbed

quantum harmonic oscillator admits solutions which exhibit a logarithmic growth of Sobolev norms. The resonance mechanism is explicit in space variables and produces highly oscillatory solutions. We then give several recipes to construct similar examples using more specific tools based on the continuous resonant (CR) equation in dimension two.

In [14], we consider the transition semigroup P_t of the Φ_2^4 stochastic quantisation on the torus \mathbb{T}^2 and prove the following new estimate (Theorem 3.9)

$$|DP_t \varphi(x) \cdot h| \leq c t^{-\beta} |h|_{C^{-s}} \|\varphi\|_0 (1 + |x|_{C^{-\alpha}})^\gamma,$$

for some α, β, γ, s positive. Thanks to this estimate, we show that cylindrical functions are a core for the corresponding Kolmogorov equation. Some consequences of this fact are discussed in a final remark.

In [3], we study fractional hypoelliptic Ornstein-Uhlenbeck operators acting on $L^2(\mathbb{R}^n)$ satisfying the Kalman rank condition. We prove that the semigroups generated by these operators enjoy Gevrey regularizing effects. Two byproducts are derived from this smoothing property. On the one hand, we prove the null-controllability in any positive time from thick control subsets of the associated parabolic equations posed on the whole space. On the other hand, by using interpolation theory, we get global L^2 subelliptic estimates for these operators.

In [7], we develop a new strategy aimed at obtaining high-order asymptotic models for transport equations with highly-oscillatory solutions. The technique relies upon recent developments in averaging theory for ordinary differential equations, in particular normal form expansions in the vanishing parameter. Noteworthy, the result we state here also allows for the complete recovery of the exact solution from the asymptotic model. This is done by solving a companion transport equation that stems naturally from the change of variables underlying high-order averaging. Eventually, we apply our technique to the Vlasov equation with external electric and magnetic fields. Both constant and non-constant magnetic fields are envisaged, and asymptotic models already documented in the literature and re-derived using our methodology. In addition, it is shown how to obtain new high-order asymptotic models.

In [16], we consider stochastic and deterministic three-wave semi-linear systems with bounded and almost continuous set of frequencies. Such systems can be obtained by considering nonlinear lattice dynamics or truncated partial differential equations on large periodic domains. We assume that the nonlinearity is small and that the noise is small or void and acting only in the angles of the Fourier modes (random phase forcing). We consider random initial data and assume that these systems possess natural invariant distributions corresponding to some Rayleigh-Jeans stationary solutions of the wave kinetic equation appearing in wave turbulence theory. We consider random initial modes drawn with probability laws that are perturbations of these invariant distributions. In the stochastic case, we prove that in the asymptotic limit (small nonlinearity, continuous set of frequency and small noise), the renormalized fluctuations of the amplitudes of the Fourier modes converge in a weak sense towards the solution of the linearized wave kinetic equation around these Rayleigh-Jeans spectra. Moreover, we show that in absence of noise, the deterministic equation with the same random initial condition satisfies a generic Birkhoff reduction in a probabilistic sense, without kinetic description at least in some regime of parameters.

In [33], we consider the Nonlinear Schrödinger (NLS) equation and prove that the Gaussian measure with covariance $(1 - \partial_x^2)^{-\alpha}$ on $L^2(\mathbb{T})$ is quasi-invariant for the associated flow for $\alpha > 1/2$. This is sharp and improves a previous result obtained in the literature where the values $\alpha > 3/4$ were obtained. Also, our method is completely different and simpler, it is based on an explicit formula for the Radon-Nikodym derivative. We obtain an explicit formula for this latter in the same spirit as Cruzeiro. The arguments are general and can be used to other Hamiltonian equations.

In [27], we consider the nonlinear Schrödinger-Langevin equation for both signs of the logarithmic nonlinearity. We explicitly compute the dynamics of Gaussian solutions for large times, which is obtained through the study of a particular nonlinear differential equation of order 2. We then give the asymptotic behavior of general energy weak solutions under some regularity assumptions. Some numerical simulations are performed in order to corroborate the theoretical results.

In [28], we construct global dissipative solutions on the torus of dimension at most three of the defocusing isothermal Euler-Langevin-Korteweg system, which corresponds to the Euler-Korteweg system of compressible quantum fluids with an isothermal pressure law and a linear drag term with respect to the velocity. In particular, the isothermal feature prevents the energy and the BD-entropy (BD stands for Bresch-Desjardins) from being positive. Adapting standard approximation arguments we

first show the existence of global weak solutions to the defocusing isothermal Navier-Stokes-Langevin-Korteweg system. Introducing a relative entropy function satisfying a Gronwall-type inequality we then perform the inviscid limit to obtain the existence of dissipative solutions of the Euler-Langevin-Korteweg system.

In [36], we propose and analyze a new asynchronous rumor spreading protocol to deliver a rumor to all the nodes of a large-scale distributed network. This spreading protocol relies on what we call a k -pull operation, with $k \geq 2$. Specifically a k -pull operation consists, for an uninformed node s , in contacting $k - 1$ other nodes at random in the network, and if at least one of them knows the rumor, then node s learns it. We perform a thorough study of the total number $T_{k,n}$ together with their limiting values when n tends to infinity. We also analyze the limiting distribution of $(T_{k,n} - E(T_{k,n}))/n$ and prove that it has a double exponential distribution when n tends to infinity. Finally, we show that when $k > 2$, our new protocol requires less operations than the traditional 2-push-pull and 2-push protocols by using stochastic dominance arguments. All these results generalize the standard case $k = 2$.

In [6], the asymptotic behavior of the solutions of the second order linearized Vlasov-Poisson system around homogeneous equilibria is derived. It provides a fine description of some nonlinear and multidimensional phenomena such as the existence of Best frequencies. Numerical results for the $1D \times 1D$ and $2D \times 2D$ Vlasov-Poisson system illustrate the effectiveness of this approach.

The efficient numerical solution of many kinetic models in plasma physics is impeded by the stiffness of these systems. Exponential integrators are attractive in this context as they remove the CFL condition induced by the linear part of the system, which in practice is often the most stringent stability constraint. In the literature, these schemes have been found to perform well, e.g., for drift-kinetic problems. Despite their overall efficiency and their many favorable properties, most of the commonly used exponential integrators behave rather erratically in terms of the allowed time step size in some situations. This severely limits their utility and robustness. Our goal in [11] is to explain the observed behavior and suggest exponential methods that do not suffer from the stated deficiencies. To accomplish this we study the stability of exponential integrators for a linearized problem. This analysis shows that classic exponential integrators exhibit severe deficiencies in that regard. Based on the analysis conducted we propose to use Lawson methods, which can be shown not to suffer from the same stability issues. We confirm these results and demonstrate the efficiency of Lawson methods by performing numerical simulations for both the Vlasov-Poisson system and a drift-kinetic model of a ion temperature gradient instability.

In [18], a bracket structure is proposed for the laser-plasma interaction model introduced in the physical literature, and it is proved by direct calculations that the bracket is Poisson which satisfies the Jacobi identity. Then splitting methods in time are proposed based on the Poisson structure. For the quasi-relativistic case, the Hamiltonian splitting leads to three subsystems which can be solved exactly. The conservative splitting is proposed for the fully relativistic case, and three one-dimensional conservative subsystems are obtained. Combined with the splittings in time, in phase space discretization we use the Fourier spectral and finite volume methods. It is proved that the discrete charge and discrete Poisson equation are conserved by our numerical schemes. Numerically, some numerical experiments are conducted to verify good conservations for the charge, energy and Poisson equation.

In [23], the recent advances about the construction of a Trefftz Discontinuous Galerkin (TDG) method to a class of Friedrichs systems coming from linear transport with relaxation are presented in a comprehensive setting. Application to the $2D P_N$ model are discussed, together with the derivation of new high order convergence estimates and new numerical results for the P_1 and P_3 models. More numerical results in dimension 2 illustrate the theoretical properties.

In [9], we introduce a new methodology to design uniformly accurate methods for oscillatory evolution equations. The targeted models are envisaged in a wide spectrum of regimes, from non-stiff to highly-oscillatory. Thanks to an averaging transformation, the stiffness of the problem is softened, allowing for standard schemes to retain their usual orders of convergence. Overall, high-order numerical approximations are obtained with errors and at a cost independent of the regime.

In [4], a splitting strategy is introduced to approximate two-dimensional rotation motions. Unlike standard approaches based on directional splitting which usually lead to a wrong angular velocity and then to large error, the splitting studied here turns out to be exact in time. Combined with spectral methods, the so-obtained numerical method is able to capture the solution to the associated partial differential equation with a very high accuracy. A complete numerical analysis of this method is given in

this work. Then, the method is used to design highly accurate time integrators for Vlasov type equations: the Vlasov-Maxwell system and the Vlasov-HMF model. Finally, several numerical illustrations and comparisons with methods from the literature are discussed.

In [10], we introduce a new Monte Carlo method for solving the Boltzmann model of rarefied gas dynamics. The method works by reformulating the original problem through a micro-macro decomposition and successively in solving a suitable equation for the perturbation from the local thermodynamic equilibrium. This equation is then discretized by using unconditionally stable exponential schemes in time which project the solution over the corresponding equilibrium state when the time step is sent to infinity. The Monte Carlo method is designed on this time integration method and it only describes the perturbation from the final state. In this way, the number of samples diminishes during the time evolution of the solution and when the final equilibrium state is reached, the number of statistical samples becomes automatically zero. The resulting method is computationally less expensive as the solution approaches the equilibrium state as opposite to standard methods for kinetic equations which computational cost increases with the number of interactions. At the same time, the statistical error decreases as the system approaches the equilibrium state. In a last part, we show the behaviors of this new approach in comparison with standard Monte Carlo techniques and in comparison with spectral methods on different prototype problems.

In [8], we consider the three dimensional Vlasov equation with an inhomogeneous, varying direction, strong magnetic field. Whenever the magnetic field has constant intensity, the oscillations generated by the stiff term are periodic. The homogenized model is then derived and several state-of-the-art multiscale methods, in combination with the Particle-In-Cell discretisation, are proposed for solving the Vlasov-Poisson equation. Their accuracy as much as their computational cost remain essentially independent of the strength of the magnetic field. The proposed schemes thus allow large computational steps, while the full gyro-motion can be restored by a linear interpolation in time. In the linear case, extensions are introduced for general magnetic field (varying intensity and direction). Eventually, numerical experiments are exposed to illustrate the efficiency of the methods and some long-term simulations are presented.

In [13], for the one space dimensional semiclassical kinetic graphene model introduced in the literature, we propose a micro-macro decomposition based numerical approach, which reduces the computational dimension of the nonlinear geometric optics method based numerical method for highly oscillatory transport equation introduced recently. The method solves the highly oscillatory model in the original coordinate, yet can capture numerically the oscillatory space-time quantum solution pointwisely even without numerically resolving the frequency. We prove that the underlying micro-macro equations have smooth (up to certain order of derivatives) solutions with respect to the frequency, and then prove the uniform accuracy of the numerical discretization for a scalar model equation exhibiting the same oscillatory behavior. Numerical experiments verify the theory.

In [12], we develop generalized polynomial chaos (gPC) based stochastic Galerkin (SG) methods for a class of highly oscillatory transport equations that arise in semiclassical modeling of non-adiabatic quantum dynamics. These models contain uncertainties, particularly in coefficients that correspond to the potentials of the molecular system. We first focus on a highly oscillatory scalar model with random uncertainty. Our method is built upon the nonlinear geometrical optics (NGO) based method, developed recently for numerical approximations of deterministic equations, which can obtain accurate pointwise solution even without numerically resolving spatially and temporally the oscillations. With the random uncertainty, we show that such a method has oscillatory higher order derivatives in the random space, thus requires a frequency dependent discretization in the random space. We modify this method by introducing a new time variable based on the phase, which is shown to be non-oscillatory in the random space, based on which we develop a gPC-SG method that can capture oscillations with the frequency-independent time step, mesh size as well as the degree of polynomial chaos. A similar approach is then extended to a semiclassical surface hopping model system with a similar numerical conclusion. Various numerical examples attest that these methods indeed capture accurately the solution statistics pointwisely even though none of the numerical parameters resolve the high frequencies of the solution.

In [21], we used some classical microlocal estimates to prove the convergence of our splitting methods introduced in [4] (for example page A671). In this note, through Corollary 2 and Remark 1, we provide a detailed proof of these estimates. All the proofs rely on results presented in the book by Nicola and Rodino (Global pseudo-differential calculus on Euclidean spaces).

In [26], we consider a class of relaxation problems mixing slow and fast variations which can describe

population dynamics models or hyperbolic systems, with varying stiffness (from non-stiff to strongly dissipative), and develop a multi-scale method by decomposing this problem into a micro-macro system where the original stiffness is broken. We show that this new problem can therefore be simulated with a uniform order of accuracy using standard explicit numerical schemes. In other words, it is possible to solve the micro-macro problem with a cost independent of the stiffness (a.k.a. uniform cost), such that the error is also uniform. This method is successfully applied to two hyperbolic systems with and without non-linearities, and is shown to circumvent the phenomenon of order reduction.

In [25], we address the computational aspects of uniformly accurate numerical methods for solving highly-oscillatory evolution equations. In particular, we introduce an approximation strategy that allows for the construction of arbitrary high-order methods using solely the right-hand side of the differential equation. No derivative of the vector field is required, while uniform accuracy is retained. The strategy is then applied to two different formulations of the problem, namely the two-scale and the micro-macro formulations. Numerical experiments on the Hénon-Heiles system, as well as on the Klein-Gordon equation and a Vlasov type problem all confirm the validity of the new strategy.

In [24], we are concerned with the construction and analysis of a new class of methods obtained as double jump compositions with complex coefficients and projection on the real axis. It is shown in particular that the new integrators are symmetric and symplectic up to high orders if one uses a symmetric and symplectic basic method. In terms of efficiency, the aforementioned technique requires fewer stages than standard compositions of the same orders and is thus expected to lead to faster methods.

Highly oscillatory ordinary differential equations (ODEs) has a long history since they are ubiquitous to describe dynamical multi-scale physical phenomena in physics or chemistry. They can be obtained by appropriate spatial discretization of a partial differential equations or can directly describe the behavior of dynamical quantities. In addition to the standard difficulties coming their numerical resolution, highly oscillatory ODEs involve a stiffness (characterized by a parameter $\varepsilon \in]0, 1[$) creating high oscillations in the solution. Hence, to capture these small scales (or high oscillations), conventional methods have to consider a time step smaller than ε leading to unacceptable computational cost. In [35], we present HOODESolver.jl, a general-purpose library written in Julia dedicated to the efficient resolution of highly oscillatory ODEs. Details are given to explain how to simulate highly oscillatory ODEs using a Uniformly Accurate (UA) method ie the method able to capture the solution while keeping the time step (and then the computational cost) independent of the degree of stiffness ε .

In [29], we propose a numerical scheme to solve the semiclassical Vlasov-Maxwell equations for electrons with spin. The electron gas is described by a distribution function $f(t, \mathbf{x}, \mathbf{p}, \mathbf{s})$ that evolves in an extended 9-dimensional phase space $(\mathbf{x}, \mathbf{p}, \mathbf{s})$, where \mathbf{s} represents the spin vector. Using suitable approximations and symmetries, the extended phase space can be reduced to 5D: (x, p_x, \mathbf{s}) . It can be shown that the spin Vlasov-Maxwell equations enjoy a Hamiltonian structure that motivates the use of the recently developed geometric particle-in-cell (PIC) methods. Here, the geometric PIC approach is generalized to the case of electrons with spin. As a relevant example, we study the stimulated Raman scattering of an electromagnetic wave interacting with an underdense plasma, where the electrons are partially or fully spin polarized. It is shown that the Raman instability is very effective in destroying the electron polarization.

7 Bilateral contracts and grants with industry

7.1 Bilateral contracts with industry

- Contrat with RAVEL (one year, budget 15000 euros): this is a collaboration with the startup RAVEL on a one-year basis (with possible renewal at the end of the year). The objective is to study the mathematical foundations of artificial intelligence and in particular machine learning algorithms for data anonymized through homomorphic encryption.
Participants: P. Chartier, M. Lemou and F. Méhats.
- Contract with Cailabs. *Optical neural networks* (6 months, budget 3000 euros): This collaboration aims at exploring the possibility of deriving new fiber optics devices based on neural networks architecture.
Participants: P. Chartier, E. Faou, M. Lemou and F. Méhats.

- Master 2 seminar of Yoann Le Hénaff with Cailabs. Co-advised by E. Faou and members of Cailabs. Yoann is now doing a Master 2 internship with Cailabs with a co-funding PEPS AMIES.

8 Partnerships and cooperations

8.1 International initiatives

8.1.1 Inria associate team not involved in an ILL

ANTIODE

Title: *ANTIODE*

Duration: 2018 - 2020

Coordinator: Philippe Chartier

Partners:

- *mathematical department*, University of Wisconsin-Madison, USA (United States)

Inria contact: Philippe Chartier

Summary: The proposed associate team assembles the INRIA team MINGuS and the research group led by Prof. Shi Jin from the Department of Mathematics at the University of Wisconsin, Madison. The main scientific objective of ANTIODE consists in marrying uniformly accurate and uncertainty quantification techniques for multi-scale PDEs with uncertain data. Multi-scale models, as those originating e.g. from the simulation of plasma fusion or from quantum models, indeed often come with uncertainties. The main scope of this proposal is thus (i) the development of uniformly accurate schemes for PDEs where space and time high oscillations co-exist and (ii) their extension to models with uncertainties. Applications to plasmas (Vlasov equations) and graphene (quantum models) are of paramount importance to the project.

8.1.2 Participation in other international programs

SIMONS project: Wave turbulence Erwan Faou is one of the Principal investigators of the Simons Collaboration program *Wave Turbulence*. Head: Jalal Shatah (NYU). <https://cims.nyu.edu/wave-turbulence/>

Informal International Partners

- F. Casas (University of Jaume, Spain)
- L. Einkemmer (University of Innsbruck, Austria)
- P. Raphael (university of Cambridge, UK)
- E. Sonnendrucker (Max Planck, Germany)
- Y. Tsutsumi (University of Kyoto, Japan)
- G. Vilmart (University of Geneva, Switzerland)
- ...

8.2 International research visitors

8.2.1 Visits of international scientists

- Clarissa Astuto (PhD student, university of Catane, Italy) spent two months to work with M. Lemou (february and september 2020).

8.2.2 Visits to international teams

Research stays abroad

- P. Chartier, M. Lemou and F. Mehats visited G. Vilmart (University of Geneva, January 2020).

8.3 European initiatives

8.3.1 FP7 & H2020 Projects

- Participation to Eurofusion project headed by E. Sonnendrucker (Garching, Germany). ENR project MAGYK 2019-2021 on Mathematics and Algorithms for gyrokinetic and kinetic models. Participants: P. Chartier, N. Crouseilles, M. Lemou and F. Mehats.

8.3.2 ANR

MFG: 2016-2020 Mean Field Games (MFG) theory is a new and challenging mathematical topic which analyzes the dynamics of a very large number of interacting rational agents. Introduced ten years ago, the MFG models have been used in many areas such as, e.g., economics (heterogeneous agent models, growth modeling,...), finance (formation of volatility, models of bank runs,...), social sciences (crowd models, models of segregation) and engineering (data networks, energy systems...). Their importance comes from the fact that they are the simplest (stochastic control-type) models taking into account interactions between rational agents (thus getting beyond optimization), yet without entering into the issues of strategic interactions. MFG theory lies at the intersection of mean field theories (it studies systems with a very large number of agents), game theory, optimal control and stochastic analysis (the agents optimize a payoff in a possibly noisy setting), calculus of variations (MFG equilibria may arise as minima of suitable functionals) and partial differential equations (PDE): In the simplest cases, the value of each agent is found by solving a backward Hamilton-Jacobi equation whereas the distribution of the agents' states evolves according to a forward Fokker-Planck equation. The Master equation (stated in the space of probability measures) subsumes the individual and collective behaviors. Finally, modeling, numerical analysis and scientific computing are crucial for the applications. French mathematicians play a world-leading role in the research on MFG: The terminology itself comes from a series of pioneering works by J.-M. Lasry and P.-L. Lions who introduced most of the key ideas for the mathematical analysis of MFG; the last conference on MFG was held last June in Paris and organized by Y. Achdou, P. Cardaliaguet and J.-M. Lasry. As testified by the proposal, the number of researchers working on MFG in France (and also abroad) is extremely fast-growing, not only because the theoretical aspects are exciting and challenging, but also because MFG models find more and more applications. The aim of the project is to better coordinate the French mathematical research on MFG and to achieve significant progress in the theory and its applications.

The partners of the project are the CEREMADE laboratory (Paris Dauphine), the IRMAR laboratory (Rennes I), the university of Nice and of Tours.

ADA: 2019-2023 The aim of this project is to treat multiscale models which are both infinite-dimensional and stochastic with a theoretic and computational approach. Multiscale analysis and multiscale numerical approximation for infinite-dimensional problems (partial differential equations) is an extensive part of contemporary mathematics, with such wide topics as hydrodynamic limits, homogenization, design of asymptotic-preserving scheme. Multiscale models in a random or stochastic context have been analysed and computed essentially in finite dimension (ordinary/stochastic differential equations), or in very specific areas, mainly the propagation of waves, of partial differential equations. The technical difficulties of our project are due to the stochastic aspect of the problems (this brings singular terms in the equations, which are difficult to understand with a pure PDE's analysis approach) and to their infinite-dimensional character, which typically raises compactness and computational issues. Our main fields of investigation are: stochastic hydrodynamic limit (for example for fluids), diffusion-approximation for dispersive equations, numerical approximation of stochastic multiscale equations in infinite dimension. Our aim is to create the new tools - analytical, probabilistic and numerical - which are required to understand a large class of stochastic multiscale partial differential equations. Various modelling issues require this

indeed, and are pointing at a new class of mathematical problems that we wish to solve. We also intend to promote the kind of problems we are interested in, particularly among young researchers, but also to recognized experts, via schools, conference, and books. The partners are ENS Lyon (coordinator J. Vovelle) and ENS Rennes (coordinator A. Debussche).

8.3.3 Fédération de Recherche : Fusion par Confinement Magnétique

We are involved in the national research multidisciplinary group around magnetic fusion activities. As such, we answer to annual calls.

8.3.4 IPL SURF

A. Debussche and E. Faou are members of the IPL (Inria Project Lab) SURF: Sea Uncertainty Representation and Forecast. Head: Patrick Vidard.

8.3.5 AdT J-Plaff

This AdT started in october 2019 and will be finished in september 2021. An engineer has been hired (Y. Mocquard) to develop several packages in the Julia langage. The J-Plaff is shared with the Fluminance team.

8.3.6 GdR TRAG

The goal of the TRAG GDR is to gather french mathematicians who work on the rough path theory. <http://gdr-trag.math.cnrs.fr>

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

- Q. Chauleur and J. Massot co-organize the PhD students seminar Landau at IRMAR laboratory.
- N. Crouseilles co-organize the seminar « mathematics and application », ENS Rennes.
- E. Faou organizes the semester "Hamiltonian Methods in Dispersive and Wave Evolution Equations", ICERM, Brown University, USA in fall 2021.

9.1.2 Scientific events: selection

Reviewer

- A. Debussche was reviewer for ERC.
- M. Lemou was reviewer for the austrian call FWF, university of Graz.

9.1.3 Journal

Member of the editorial boards

- P. Chartier is a member of the editorial board of the journal Mathematical Modelling and Numerical Analysis (2007-).
- A. Debussche is a Editor in chief of the journal "Stochastics and Partial Differential Equations: Analysis and Computations" (2013-).
- A. Debussche is a member of the editorial board of the following journals:
 - ESAIM: PROCS (2012-),

- Journal of Evolution equation (2014-),
- Annales Henri Lebesgue (2018-),
- Annales de l’IHP Probabilités et Statistiques (2020-).
- A. Debussche is a member of the editorial board Mathematiques & Applications (SMAI).
- M. Lemou is a member of the editorial board of the journal Communications in Mathematical Science (CMS).

Reviewer - reviewing activities The members of the MINGUS team are reviewers of the journals in which they publish.

9.1.4 Invited talks

Obviously, many events during 2020 have been cancelled. Some of them have been put online. We specify the talks that have cancelled or organized online.

- F. Castella gave a lecture series (3h) at Ecole Agronomie de Rennes, January 2020.
- P. Chartier (workshop Multiscale Analysis and Methods for Dispersive PDEs and Fluid Equations, Singapore, February 2020). Cancelled.
- N. Crouseilles (workshop Oberwolfach, September 2020). Cancelled.
- N. Crouseilles (workshop Multiscale Analysis and Methods for Dispersive PDEs and Fluid Equations, Singapore, February 2020). Cancelled.
- N. Crouseilles (seminar Chinese Academy of Sciences, December 2020). Online.
- N. Crouseilles (seminar Structure preserving methods, University Wolfsburg, November 2020). Online.
- A. Debussche (STUOD workshop, september 21-24 2020). Online.
- A. Debussche (Analyse Appliquée et Modélisation, Monastir, Tunisia, October 15-18 2020). Cancelled.
- A. Debussche (plenary speaker, AIMS Conference, June 2020). Cancelled.
- E. Faou (conference Algorithms in Quantum Molecular Dynamics, CIRM, Luminy, Marseille, September 2020). Online.
- E. Faou (Seminar Enriques-Lebesgue, April 2020). Online.
- E. Faou gave a lecture series (8h) on wave turbulence in New-York University (January 2021). Online.
- M. Lemou (Nantes-Rennes analysis day, Rennes, January 2021).
- J. Massot (NumKin 2020, Garching, Germany, October 2020). Online. <https://www.ipp.mpg.de/numkin2020>
- J. Massot (CAN-J (Congrès d’Analyse Numérique pour les Jeunes), December 2020). Online. <https://indico.math.cnrs.fr/event/6098/overview>
- P. Navaro (introduction to the Julia langage, Inria Rennes, January 2020). <https://indico.math.cnrs.fr/event/6098/overview>
- L. Tremant (CAN-J (Congrès d’Analyse Numérique pour les Jeunes), December 2020). Online.

9.1.5 Scientific expertise

- N. Crouseilles is member of the Blaise Pascal prize committee (January 2020).
- N. Crouseilles is member of the Inria young researcher recruitment committee, Paris (July 2020).
- N. Crouseilles is member of the professor recruitment committee, ENS Rennes (May 2020).
- N. Crouseilles is member of the hiring committee for PhD recruitment for the university of Innsbruck within the European program (December 2020).
- N. Crouseilles is member of the scientific committee of the workshop Numerical Methods for Kinetic Equations 'NumKin21' <https://www.chairejeanmorlet.com/2356.html> council which is part of the semester 2021 "Kinetic theory : analysis, computation and applications", CIRM, Marseille.
- A. Debussche is member of the administrative Council of ENS Paris-Saclay.
- A. Debussche is a member of the External Advisory Board of the ERC synergie STUOD.
- A. Debussche is member of the professor recruitment committee, ENS Rennes (May 2020).
- A. Debussche is a member of the scientific council of the Federation Denis Poisson Orleans-Tours (2012-).
- E. Faou is member of the Scientific Council of the Pôle Universitaire Léonard de Vinci.
- M. Lemou is a member of the scientific council of ENS Rennes.
- M. Lemou is a member of the scientific council of the Labex center Henri Lebesgue.
- F. Méhats is scientific advisor for the start-up SpaceAble.
- F. Méhats is scientific advisor for the start-up Ravel.

9.1.6 Research administration

- N. Crouseilles is a member of the Inria evaluation committee (2018-).
- N. Crouseilles is a member of the IRMAR laboratory council (2016-).
- A. Debussche is the head of research at ENS Rennes.
- E. Faou is AMIES correspondent (Agency for Interaction in Mathematics with Business and Society) for Inria Rennes Bretagne atlantique and IRMAR laboratory.
- E. Faou is co-director of the Henri Lebesgue Center (Excellence laboratory of the program investissement avenir).
- M. Lemou is head of the analyse numerique team of IRMAR laboratory (2015-). 46 members.
- P. Navaro is a member of the bureau of the Groupe Calcul of CNRS.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

- Master :
 - E. Castella, Numerical methods for ODEs and PDEs, 60 hours, Master 1, University of Rennes 1.
 - N. Crouseilles, Numerical methods for PDEs, 24 hours, Master 1, ENS Rennes.
 - A. Debussche, Distribution and functional analysis, 30 hours, Master 1, ENS Rennes.

- E. Faou, Numerical transport, 24 hours, Master 2, University of Rennes 1.
- M. Lemou, Elliptic PDEs, 36 hours, Master 1, University of Rennes 1.
- P. Navaro (course Python-Fortran, Bordeaux). Cancelled. <https://pnavaro.github.io/python-fortran/>
- P. Navaro, Python courses, 20 hours, Master 2 Smart Data, ENSAI.
- P. Navaro, Scientific computing tools for big data, 20 hours, Master 2, University of Rennes.

9.2.2 Supervision

- PhD (ENS grant): G. Barrau , Approximation diffusion pour des  quations dispersives, University of Rennes I, started in september 2019, A. Debussche.
- PhD (ENS grant): Q. Chauleur, Equation de Vlasov singuli re et  quations reli es, University of Rennes I, started in september 2019, R. Carles (CNRS, Rennes) and E. Faou.
- PhD: Y. Li (Chinese Academy of Sciences), Structure preserving methods for Vlasov equations, march 2019-february 2020, Y. Sun (Chinese Academy of Sciences) and N. Crouseilles.
- PhD in progress (University of Rennes 1 grant): J. Massot, Exponential methods for hybrid kinetic models, started in october 2018, N. Crouseilles.
- PhD : A. Rosello (ENS grant), Approximation-diffusion pour des  quations cin tiques pour les mod les de type spray, ENS Rennes, defended in July 2020, A. Debussche and J. Vovelle (CNRS, Lyon).
- PhD in progress (Inria grant): L. Tr mant, Asymptotic analysis methods and numerical of dissipative multi-scale models: ODE with central manifold and kinetic models, started in october 2018, P. Chartier and M. Lemou.
- Postdoc: I. Almuslimani (Switzerland grant), Uniformly accurate methods for stochastic ODEs, started in December 2020, P. Chartier, M. Lemou and F. M hats.

9.2.3 Juries

The members of the MINGUS team were in the jury of the following PhD defenses.

- P. Chartier was in the jury defense of C. Offen (PhD thesis defended in June 2020, under the supervision of R. McLachlan, Massey-University, New-Zealand).
- P. Chartier was in the jury defense of I. Almuslimani (PhD thesis defended in november 2020, under the supervision of G. Vilmart, University of Geneva, Switzerland).
- N. Crouseilles was in the jury defense of Y. Li (PhD thesis defended in May 2020, under the supervision of Y. Sun, Chinese Academy of Science, China).
- A. Debussche was in the jury defense of A. Rosello (PhD thesis defended in July 2020, under the supervision of A. Debussche and J. Vovelle, ENS Rennes).
- M. Lemou was reviewer of the PhD thesis of C. Astuto (University of Catane).
- F. M hats was in the jury defense of T. Nguyen (PhD defended in October 2020, under the supervision of N. Seguin and B. Boutin, University Rennes 1).

The members of the team were in the jury of the following HDR defense.

- N. Crouseilles was in the jury defense of the habilitation of B. Decharme (defended in September 2020, M teo France, Toulouse).

9.3 Popularization

9.3.1 Interventions

- N. Crouseilles gave a conference for master students for University of Nantes and Ecole Centrale of Nantes to explain research opportunities at Inria (January 2021, online).
- N. Crouseilles participate to the program "introduction to research" by welcoming a first year student during one week. May 2020. Cancelled.

10 Scientific production

10.1 Major publications

- [1] J. Bernier, E. Faou and B. Grebert. 'Long time behavior of the solutions of NLW on the d-dimensional torus'. In: *Forum of Mathematics, Sigma* 8 (2020), E12. DOI: [10.1017/fms.2020.8](https://doi.org/10.1017/fms.2020.8). URL: <https://hal.archives-ouvertes.fr/hal-02151338>.
- [2] P. Chartier, N. Crouseilles, M. Lemou, F. Méhats and X. Zhao. 'Uniformly accurate methods for three dimensional Vlasov equations under strong magnetic field with varying direction'. In: *SIAM Journal on Scientific Computing* 42.2 (2020), B520–B547. DOI: [10.1137/19M127402X](https://doi.org/10.1137/19M127402X). URL: <https://hal.archives-ouvertes.fr/hal-02179534>.

10.2 Publications of the year

International journals

- [3] P. Alphonse and J. Bernier. 'Smoothing Properties of Fractional Ornstein-Uhlenbeck Semigroups and Null-Controllability'. In: *Bulletin des Sciences Mathématiques* 165 (Dec. 2020), article n° 102914. DOI: [10.1016/j.bulsci.2020.102914](https://doi.org/10.1016/j.bulsci.2020.102914). URL: <https://hal.archives-ouvertes.fr/hal-01888835>.
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- [8] P. Chartier, N. Crouseilles, M. Lemou, F. Méhats and X. Zhao. 'Uniformly accurate methods for three dimensional Vlasov equations under strong magnetic field with varying direction'. In: *SIAM Journal on Scientific Computing* 42.2 (2020), B520–B547. DOI: [10.1137/19M127402X](https://doi.org/10.1137/19M127402X). URL: <https://hal.archives-ouvertes.fr/hal-02179534>.
- [9] P. Chartier, M. Lemou, F. Méhats and G. Vilmart. 'A new class of uniformly accurate numerical schemes for highly oscillatory evolution equations'. In: *Foundations of Computational Mathematics* 20.1 (2020), pp. 1–33. DOI: [10.1007/s10208-019-09413-3](https://doi.org/10.1007/s10208-019-09413-3). URL: <https://hal.archives-ouvertes.fr/hal-01666472>.
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- [11] N. Crouseilles, L. Einkemmer and J. Massot. ‘Exponential methods for solving hyperbolic problems with application to kinetic equations’. In: *Journal of Computational Physics* 420 (Nov. 2020), p. 109688. DOI: [10.1016/j.jcp.2020.109688](https://doi.org/10.1016/j.jcp.2020.109688). URL: <https://hal.archives-ouvertes.fr/hal-02321916>.
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