## **RESEARCH CENTRE**

Inria Center at Rennes University

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Université Rennes 1, École normale supérieure de Rennes, CNRS

# 2022 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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## Keywords

#### Computer sciences and digital sciences

- A6.1.1. Continuous Modeling (PDE, ODE)
- A6.1.2. Stochastic Modeling
- A6.1.4. Multiscale modeling
- A6.2.1. Numerical analysis of PDE and ODE
- A6.2.7. High performance computing

## Other research topics and application domains

- B4.2.2. Fusion
- B5.11. Quantum systems
- B9.5.2. Mathematics

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## 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  $\varepsilon$ .

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  $\varepsilon$  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

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

where the function  $\psi^{\varepsilon} = \psi^{\varepsilon}(t, x) \in \mathbb{C}$  depends on time  $t \ge 0$  and position  $x \in \mathbb{R}^3$ ,  $\xi = \xi(x, t)$  is a white noise and where the small parameter  $\varepsilon$  is the Planck's constant describing the microscopic/macroscopic ratio. The limit  $\varepsilon \to 0$  is referred to as the semi-classical limit. The regime  $\varepsilon = 1$ and  $\beta \to 0$  (this can be for instance the relative length of the optical fiber) is highly-oscillatory. The noise  $\xi$  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  $t \ge 0$ , position  $x \in \mathbb{R}^3$  and velocity  $v \in \mathbb{R}^3$ , a typical kinetic equation for  $f^{\varepsilon}$  reads

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

where (E, B) is the electro-magnetic field (which may itself depend on f through Maxwell's equations),  $m^{\varepsilon}$  is a random process (which may describe absorption or creation of particles) and Q is a collision operator. The dimensionless parameters  $\varepsilon$ ,  $\beta$  are related to the cyclotronic frequency and the mean free path. Limits  $\varepsilon \to 0$  and  $\beta \to 0$  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  $m^{\varepsilon}$  is correlated in space and time. At the limit  $\varepsilon \to 0$ , 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 [38, 40, 41, 44] 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.

During the last period, some results have been obtained by the members of the team [1, 2, 3, 4, 5].

## **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  $\varepsilon$ ) 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

$$\begin{cases} \frac{dx^{\varepsilon}(t)}{dt} = \mathscr{G}(x^{\varepsilon}(t), y^{\varepsilon}(t)), & x^{\varepsilon}(0) = x_{0}, \\ \frac{dy^{\varepsilon}(t)}{dt} = -\frac{y^{\varepsilon}(t)}{\varepsilon} + \mathscr{H}(x^{\varepsilon}(t), y^{\varepsilon}(t)), & y^{\varepsilon}(0) = y_{0}, \end{cases}$$
(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, A. Debussche, E. Faou)

#### Derivation of asymptotic problems

Our main goal is to analyze the asymptotic behavior of dissipative systems of the form ((3)) when  $\varepsilon$  goes to zero. The *center manifold theorem* [37] is of great interest but is largely unsatisfactory from the following points of view

- a constructive approach of h and  $x_0^{\varepsilon}$  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 [39] 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 the rescaling, it converges formally to white noise. Thus, this adds another scale in the multiscale analysis. Following the pioneering work by Debussche and Vovelle, [40], 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 Asymptotic Preserving (ie AP) 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  $\beta$ .

Time diminishing methods

The main goal consists in merging Monte-Carlo techniques [35] 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 enables 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  $\varepsilon$ . 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 [38].

Multiscale numerical methods for stochastic PDEs

AP schemes have been developed recently for kinetic equations with noise in the context of Uncertainty Quantification UQ [43]. 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

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

for a given  $u_0$  and a given periodic function  $\mathscr{F}$  (of period *P* w.r.t. its first variable) which possibly involves stochastic terms. Solution  $u^{\varepsilon}$  exhibits high-oscillations in time superimposed to a slow dynamics. Asymptotic techniques -resorting in the present context to *averaging* theory [47]- allow to decompose

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

into a fast solution component, the  $\varepsilon P$ -periodic change of variable  $\Phi_{t/\varepsilon}$ , and a slow component, the flow  $\Psi_t$  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 [36]) 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 axes

- *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 [44], 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 [45, 41]). 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 present 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 a 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 [46]). 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  $\varepsilon$  so as to accurately simulate the solution over each period, resulting in an unacceptable execution cost. Then, it is highly desirable to derive numerical schemes able to advance the solution by a time step independent of  $\varepsilon$ . 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  $\varepsilon$  and p the order of the numerical scheme.

Recently, such numerical methods have been proposed by members of the team in the highlyoscillatory context. [38]. 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  $\varepsilon$ .

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 high-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 [42]). 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 [42]). 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 <sup>1</sup> 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 [47]), it is unclear how it can be extended to PDEs. One of the main obstacle being the requirement, usual for ODEs like (4), for  $\mathscr{F}$  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 data). 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 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 affects 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

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

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 library 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 thorough. 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 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 Social and environmental responsibility

#### 5.1 Footprint of research activities

A group called ECO-IRMAR has been created in the IRMAR laboratory to inform about the footprint of research activities at the level of the laboratory. The members of the team follow the advices proposed by this group.

## 6 Highlights of the year

The team hired Geoffrey Beck as a permanent Inria researcher.

## 7 New software and platforms

The MINGuS team maintains the three following softwares.

#### 7.1 New software

#### 7.1.1 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:** https://selalib.github.io

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

7.1.2 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

#### 7.1.3 PhaseLifting

Keyword: Python

**Functional Description:** Performs the phase bearing of a complex function defined on a grid, taking into account two criteria based on a non uniform weight map.

Author: Yoann Le Henaff

Contact: Erwan Faou

## 8 New results

Our results of the year are presented in the following three sections:

- multiscale numerical schemes (for dissipative or highly-oscillatory problems),
- · numerical schemes for Hamiltonian problems,
- analysis of PDEs and SPDEs.

#### 8.1 Multiscale numerical schemes

Participants: F. Castella, A. Crestetto, A. Debussche, N. Crouseilles, E. Faou, P. Navaro.

Multiscale (ie highly oscillatory or dissipative) ordinary differential equations (ODEs) have a long history since they are ubiquitous to describe dynamical multiscale physical phenomena in physics or chemistry. They can be obtained by appropriate spatial discretization of the partial differential equation or can directly describe the behavior of dynamical quantities. In addition to the standard difficulties coming from their numerical resolution, multiscale ODEs involve a stiffness (characterized by a parameter  $\varepsilon \in ]0, 1]$ ). creating strong gradients in the solution. Hence, to capture these small scales, conventional methods have to consider a time step smaller than  $\varepsilon$  leading to unacceptable computational cost. The team members proposed several strategies to overcome this stiffness.

In [6], we adapt the micro-macro methodology to stochastic differential equations for the purpose of numerically solving oscillatory evolution equations. The models we consider are addressed in a wide spectrum of regimes where oscillations may be slow or fast. We show that through an ad-hoc transformation (the micro-macro decomposition), it is possible to retain the usual orders of convergence of Euler-Maruyama method, that is to say, uniform weak order one and uniform strong order one half.

In [9], 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 [10], 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 [20], the design and analysis of high order accurate IMEX finite volume schemes for the compressible Euler-Poisson (EP) equations in the quasineutral limit is presented. As the quasineutral limit is singular for the governing equations, the time discretisation is tantamount to achieving an accurate numerical method. To this end, the EP system is viewed as a differential algebraic equation system (DAEs) via the method of lines. As a consequence of this vantage point, high order linearly semi-implicit (SI) time discretisation are realised by employing a novel combination of the direct approach used for implicit discretisation of DAEs and, two different classes of IMEX-RK schemes: the additive and the multiplicative. For both the time discretisation strategies, in order to account for rapid plasma oscillations in quasineutral regimes, the nonlinear Euler fluxes are split into two different combinations of stiff and non-stiff components. The high order scheme resulting from the additive approach is designated as a classical scheme while the one generated by the multiplicative approach possesses the asymptotic preserving (AP) property. Time discretisations for the classical and the AP schemes are performed by standard IMEX-RK and SI-IMEX-RK methods, respectively so that the stiff terms are treated implicitly and the non-stiff ones explicitly. In order to discretise in space a Rusanov-type central flux is used for the non-stiff part, and simple central differencing for the stiff part. AP property is also established for the space-time fully-discrete scheme obtained using the multiplicative approach. Results of numerical experiments are presented, which confirm that the high order schemes based on the SI-IMEX-RK time discretisation achieve uniform second order convergence with respect to the Debye length and are AP in the quasineutral limit.

In [29], we study the construction of multiscale numerical schemes efficient in the finite Larmor radius approximation of the collisional Vlasov equation. Following the paper of Bostan and Finot (2019), the

system involves two different regimes, a highly oscillatory and a dissipative regimes, whose asymptotic limits do not commute. In this work, we consider a Particle-In-Cell discretization of the collisional Vlasov system which enables to deal with the multiscale characteristics equations. Different multiscale time integrators are then constructed and analysed. We prove asymptotic properties of these schemes in the highly oscillatory regime and in the collisional regime. In particular, the asymptotic preserving property towards the modified equilibrium of the averaged collision operator is recovered. Numerical experiments are then shown to illustrate the properties of the numerical schemes.

#### 8.2 Numerical schemes for Hamiltonian PDEs

Participants: A. Crestetto, N. Crouseilles, E. Faou, P. Navaro.

The MINGuS team has a long history in the design and study of numerical schemes for Hamiltonian PDEs. The main examples are Schroedinger or Vlasov equations.

In [18], a novel second order family of explicit stabilized Runge-Kutta-Chebyshev methods for advection-diffusion-reaction equations is introduced. The new methods outperform existing schemes for relatively high Peclet number due to their favorable stability properties and explicitly available coefficients. The construction of the new schemes is based on stabilization using second kind Chebyshev polynomials first used in the construction of the stochastic integrator SK-ROCK. An adaptive algorithm to implement the new scheme is proposed. This algorithm is able to automatically select the suitable step size, number of stages, and damping parameter at each integration step. Numerical experiments that illustrate the efficiency of the new algorithm are presented.

In [30], we aim at constructing numerical schemes, that are as efficient as possible in terms of cost and conservation of invariants, for the Vlasov-Fokker-Planck system coupled with Poisson or Ampère equation. Splitting methods are used where the linear terms in space are treated by spectral or semi-Lagrangian methods and the nonlinear diffusion in velocity in the collision operator is treated using a stabilized Runge–Kutta–Chebyshev (RKC) integrator, a powerful alternative of implicit schemes. The new schemes are shown to exactly preserve mass and momentum. The conservation of total energy is obtained using a suitable approximation of the electric field. An *H*-theorem is proved in the semi-discrete case, while the entropy decay is illustrated numerically for the fully discretized problem. Numerical experiments that include investigation of Landau damping phenomenon and bump-on-tail instability are performed to illustrate the efficiency of the new schemes.

In [14], we focus on the numerical approximation of a hybrid fluid-kinetic plasma model for electrons, in which energetic electrons are described by a Vlasov kinetic model whereas a fluid model is used for the cold population of electrons. First, we study the validity of this hybrid modelling in a two dimensional context (one dimension in space and one dimension in velocity) against the full (stiff) Vlasov kinetic model and second, a four dimensional configuration is considered (one dimension in space and three dimensions in velocity). To do so, we consider two numerical Eulerian methods. The first one is based on the Hamiltonian structure of the hybrid system and the second approach, which is based on exponential integrators, enables to derive high order integrator and remove the CFL condition induced by the linear part. The efficiency of these methods, which are combined with an adaptive time stepping strategy, are discussed in the different configurations and in the linear and nonlinear regimes.

In [26], Lawson type numerical methods are studied to solve Vlasov type equations on a phase space grid. These time integrators are known to satisfy enhanced stability properties in this context since they do not suffer from the stability condition induced from the linear part. We introduce here a class of modified Lawson integrators in which the linear part is approximated in such a way that some geometric properties of the underlying model are preserved, which has important consequences for the analysis of the scheme. Several Vlasov-Maxwell examples are presented to illustrate the good behavior of the approach.

In [28], we consider a particular discretization of the harmonic oscillator which admits an orthogonal basis of eigenfunctions called Kravchuk functions possessing appealing properties from the numerical point of view. We analytically prove the almost second-order convergence of these discrete functions towards Hermite functions, uniformly for large numbers of modes. We then describe an efficient way to

simulate these eigenfunctions and the corresponding transformation. We finally show some numerical experiments corroborating our different results.

In [32], we propose an Eulerian-Lagrangian (EL) Runge-Kutta (RK) discontinuous Galerkin (DG) method for linear hyperbolic system. The method is designed based on the EL DG method for transport problems [J. Comput. Phy. 446: 110632, 2021], which tracks solution along approximations to characteristics in the DG framework, allowing extra large time stepping sizes with stability with respect to the classical RK DG method. Considering each characteristic family, a straightforward application of EL DG for hyperbolic system will be to transform to the characteristic variables, evolve them on associated characteristic related space-time regions, and transform them back to the original variables. However, the conservation could not be guaranteed in a general setting. In this paper, we formulate a conservative semi-discrete EL DG method by decomposing each variable into two parts, each of them associated with a different characteristic family. As a result, four different quantities are evolved in EL fashion and recombined to update the solution. The fully discrete scheme is formulated by using method-of-lines RK methods, with intermediate RK solutions updated on the background mesh. Numerical results for 1D and 2D wave equations are presented to demonstrate the performance of the proposed ELDG method. These include the high order spatial and temporal accuracy, stability with extra large time stepping size, and conservative property.

In [33], we study a grid-free particle method based on following the evolution of the characteristics of the Vlasov-Poisson system, and we show that it converges for smooth enough initial data. This method is built as a combination of well-studied building blocks-mainly time integration and integral quadratures-, hence allows to obtain arbitrarily high orders. By making use of the Non-Uniform Fast Fourier Transform (NUFFT), the overall computational complexity is  $\mathcal{O}(P + K^d \log K^d)$ , where *P* is the total number of particles and where we only keep the Fourier modes  $k \in \mathbb{Z}^d$  such that  $k_1^2 + \cdots + k_d^2 \leq K^2$ . Some numerical results are given for the Vlasov-Poisson system in the one-dimensional case.

In [21], a two-species Vlasov-Poisson model is described together with some numerical simulations, permitting to exhibit the formation of a plasma sheath. The numerical simulations are performed with two different methods: a first order classical finite difference (FD) scheme and a high order semi-Lagrangian (SL) scheme with Strang splitting; for the latter one, the implementation of (non-periodic) boundary conditions is discussed. The codes are first evaluated on a one-species case, where an analytical solution is known. For the two-species case, cross comparisons and the influence of the numerical parameters for the SL method are performed in order to have an idea of a reference numerical simulation.

In [22], we study, both theoretically and numerically, qualitative and quantitative properties of the solutions a Vlasov-Poisson system modeling the interaction between a plasma and a cylindrical Langmuir probe. In particular, we exhibit a class of radial solutions for which the electrostatic potential is increasing concave with a strong variation in the vicinity of the probe which scales as the inverse of the Debye length. These solutions are proven to exist provided the incoming distributions of particles from the plasma verify the so called generalized Bohm condition of plasma physics. Small perturbations of the radial semi-Maxwellian incoming distributions are then investigated numerically. We notably observe potential barriers that lead to the existence of unpopulated trapped orbits and to the presence of particles that by bypass the probe. Curves of the collected current versus its applied voltage are also presented.

Ultrafast laser pulses interacting with plasmas can give rise to a rich spectrum of physical phenomena, which have been extensively studied both theoretically and experimentally. Less work has been devoted to the study of polarized plasmas, where the electron spin may play an important role. In this short review [16], we illustrate the use of phase-space methods to model and simulate spin-polarized plasmas. This approach is based on the Wigner representation of quantum mechanics, and its classical counterpart, the Vlasov equation, which are generalized to include the spin degrees of freedom. Our approach is illustrated through the study of the stimulated Raman scattering of a circularly polarized electromagnetic wave interacting with a dense electron plasma.

In [31], we present a numerical method to solve the Vlasov-Maxwell equations for spin-1/2 particles, in a semiclassical approximation where the orbital motion is treated classically while the spin variable is fully quantum. Unlike the spinless case, the phase-space distribution function is a 2 × 2 matrix, which can also be represented, in the Pauli basis, as one scalar function  $f_0 \in \mathbb{R}$  and one three-component vector function  $\vec{f} \in \mathbb{R}^3$ . The relationship between this "vectorial" representation and the fully scalar representation on an extended phase space first proposed by Brodin et al. [Phys. Rev. Lett. 101, 245002 (2008)] is analyzed in detail. By means of suitable approximations and symmetries, the vectorial spin-Vlasov-Maxwell model

can be reduced to two-dimensions in the phase space, which is amenable to numerical solutions using a high-order grid-based Eulerian method. The vectorial model enjoys a Poisson structure that paves the way to accurate Hamiltonian split-time integrators. As an example, we study the stimulated Raman scattering of an electromagnetic wave interacting with an underdense plasma, and compare the results to those obtained earlier with the scalar spin-Vlasov-Maxwell model and a particle-in-cell code.

#### 8.3 Analysis of PDEs and SPDEs

Participants: G. Beck, F. Castella, A. Debussche, E. Faou.

In view of the construction of efficient multiscale numerical schemes, the study and analysis of PDEs or SPDEs is of great importance. Below is a list of some contributions of the team on this aspect.

In [7], we characterize geometrically the regularizing effects of the semigroups generated by accretive non-selfadjoint quadratic differential operators. As a byproduct, we establish the subelliptic estimates enjoyed by these operators, being expected to be optimal. These results prove conjectures by M. Hitrik, K. Pravda-Starov and J. Viola. The proof relies on a new representation of the polar decomposition of these semigroups. In particular, we identify the selfadjoint part as the evolution operator generated by the Weyl quantization of a time-dependent real-valued nonnegative quadratic form for which we prove a sharp anisotropic lower bound.

In [8], we consider the two-dimensional stochastic Gross-Pitaevskii equation, which is a model to describe Bose-Einstein condensation at positive temperature. The equation is a complex Ginzburg-Landau equation with a harmonic potential and an additive space-time white noise. We study the well-posedness of the model using an inhomogeneous Wick renormalization due to the potential, and prove the existence of an invariant measure and of stationary martingale solutions.

In [13], we consider the logarithmic Schroedinger equations with damping, also called Schroedinger-Langevin equation. On a periodic domain, this equation possesses plane wave solutions that are explicit. We prove that these solutions are asymptotically stable in Sobolev regularity. In the case without damping, we prove that for almost all value of the nonlinear parameter, these solutions are stable in high Sobolev regularity for arbitrary long times when the solution is close to a plane wave. We also show and discuss numerical experiments illustrating our results.

In [11], 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 Bresch-Desjardins-entropy 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 [12], we consider the isothermal Euler system with damping. We rigorously show the convergence of Barenblatt solutions towards a limit Gaussian profile in the isothermal limit  $\gamma \rightarrow 1$ , and we explicitly compute the propagation and the behavior of Gaussian initial data. We then show the weak  $L^1$ convergence of the density as well as the asymptotic behavior of its first and second moments.

In [15], 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 in the deterministic case.

In [34], we construct the infinitesimal generator of the Brox diffusion on a line with a periodic Brownian environment. This gives a new construction of the process and allows to solve the singular martingale problem. We prove that the associated semigroup is strong Feller with Gaussian lower and upper bounds. This also yields a construction of the Brox diffusion on a segment with periodic or Dirichlet boundary

conditions. In this bounded space, we prove that there exists a unique measure and the existence of a spectral gap giving exponential ergodicity of the diffusion.

In [27], we analyze a new asynchronous rumor spreading protocol to deliver a rumor to all the nodes of a large-scale distributed network. This protocol relies on successive pull operations involving *k* different nodes, with  $k \ge 2$ , and called *k*-pull operations. Specifically during a *k*-pull operation, an uninformed node a contacts k - 1 other nodes at random in the network, and if at least one of them knows the rumor, then node a learns it. We perform a detailed study in continuous-time of the total time  $\Theta$ , *k*, *n* needed for all the *n* nodes to learn the rumor. These results extend those obtained in a previous paper which dealt with the discrete-time case. We obtain the mean value, the variance and the distribution of  $\Theta$ , *k*, *n* together with their asymptotic behavior when the number of nodes *n* tends to infinity.

In [23], e consider the continuous Anderson operator  $H = \Delta + \xi$  on a two dimensional closed Riemannian manifold *S*. We provide a short self-contained functional analysis construction of the operator as an unbounded operator on  $L^2(S)$  and give almost sure spectral gap estimates under mild geometric assumptions on the Riemannian manifold. We prove a sharp Gaussian small time asymptotic for the heat kernel of *H* that leads amongst others to strong norm estimates for quasimodes. We introduce a new random field, called Anderson Gaussian free field, and prove that the law of its random partition function characterizes the law of the spectrum of *H*. We also give a simple and short construction of the polymer measure on path space and relate the Wick square of the Anderson Gaussian free field to the occupation measure of a Poisson process of loops of polymer paths. We further prove large deviation results for the polymer measure and its bridges.

Turbulent cascades characterize the transfer of energy injected by a random force at large scales towards the small scales. In hydrodynamic turbulence, when the Reynolds number is large, the velocity field of the fluid becomes irregular and the rate of energy dissipation remains bounded from below even if the fluid viscosity tends to zero. A mathematical description of the turbulent cascade is a very active research topic since the pioneering work of Kolmogorov in hydrodynamic turbulence and that of Zakharov in wave turbulence. In both cases, these turbulent cascade mechanisms imply power-law behaviors of several statistical quantities such as power spectral densities. For a long time, these cascades were believed to be associated with nonlinear interactions, but recent works have shown that they can also take place in a dynamics governed by a linear equation with a differential operator of degree 0. In this spirit, we construct a linear equation that mimics the phenomenology of energy cascades when the external force is a statistically homogeneous and stationary stochastic process. In the Fourier variable, this equation can be seen as a linear transport equation, which corresponds to an operator of degree 0 in physical space. Our results in [19] give a complete characterization of the solution: it is smooth at any finite time, and, up to smaller order corrections, it converges to a fractional Gaussian field at infinite time.

## 9 Bilateral contracts and grants with industry

Participants: E. Faou.

#### 9.1 Bilateral contracts with industry

· Contract with the Cailabs compagny.

A long standing collaboration has emerged between MINGuS and the company CAILABS whose main aim is the conception and construction of optical fibers. Most of the main objectives of this collaboration are strictly confidential. However they have strong common point with the scientific goals of the MINGuS project, for instance the development of efficient numerical methods for quantum simulation and many aspects of mathematical and physical analysis of quantum systems. The impact of this collaboration are very important both from the transfer of technology point of view and from the interaction with a very active startup providing very practical problems that are often very close to hot academic topics. We believe that this interaction will last long and continue to feed the scientific activity of the whole project with problem directly coming from the industrial and economical world.

- During his PhD thesis, Y. Le Hénaff will work during one month in Cailabs. Y. Le Hénaff already did his master thesis with Cailabs with a PEPS-AMIES contract in 2021.
- Agence Lebesgue.

Since 2019 E. Faou is head of the *Agence Lebesgue pour les mathématiques* whose role is precisely to increase the role of mathematics in the socio-economic world by facilitating contact between mathematicians and companies or institute working in distant sector of activity.

This is done by organizing events oriented to industrial companies and socio-economic partners (like the *Journée d'innovation mathématiques* which was organized this year or by organizing the *Semaine mathématiques et entreprises* (SEME) for student who work during one week on problems brought by some industrial companies (May 2022). These SEME are essentially funded by AMIES.

A last and important activity of the Agence Lebesgue is formation where mathematicians go to industries, companies of the private sector or other institutes to organize some crash course in some hot topics in mathematics, or on demand depending on the requirement of the partners. In particular, during the SEME, two PhD students of the team worked on a topic proposed by industrial partners which lead to the two following reports [24] and [25].

In this direction the Agence Lebesgue collaborated in 2020 with Stratinnov, a company of specialists in innovation, in order to increase the global impact of mathematics in the socio-economic local environment. This collaboration was very successful and is expected to continue with further development of a real *mathematical offer* in the perimeter of the Agence Lebesgue which covers mainly the Rennes and Nantes areas.

## 10 Partnerships and cooperations

#### **10.1** International initiatives

## 10.1.1 Inria associate team not involved in an IIL or an international program

#### Bubbles

Participants: Geoffrey Beck, Nicolas Crouseilles, Arnaud Debussche, Erwan Faou.

Title: Bubbles and modulations for solving Schroedinger equations

Duration: 2022 -> 2025

Coordinator: Pierre Raphaël (university of Cambridge), email: pr463@cam.ac.uk

#### Partners:

• university of Cambridge (Royaume-Uni)

Inria contact: Erwan Faou

**Summary:** The goal is to analyze the long time behavior of the Schroedinger equations, study weak turbulence phenomena to design new numerical integrators using modulations techniques.

Geo-CollVA

Participants: Nicolas Crouseilles, Arnaud Debussche, Erwan Faou, Pierre Navaro.

Title: Geometric numerical methods for collisional Vlasov equations

**Duration:** 2022 -> 2025

Coordinator: Yajuan Sun (Chinese Academy of Sciences), email: sunyj@lsec.cc.ac.cn

#### **Partners:**

• Chinese Academy of Sciences (Chine)

Inria contact: Nicolas Crouseilles

**Summary:** The main scientific objective of Geo-CollVa consists in investigating collision effects in numerical simulations of charged particles systems described by Hamiltonian PDEs. These PDEs involve a dissipative part and a Hamiltonian part, and the goal is to study these two parts in a unified numerical framework. The two main families of numerical methods (Lagrangian and Eulerian) will be studied.

#### ANTIPODE

Participants: Nicolas Crouseilles, Arnaud Debussche, Erwan Faou, Pierre Navaro.

Title: Asymptotic Numerical meThods for Oscillatory partial Differential Equations with uncertainties.

**Duration:** 2019 -> 2022

Coordinator: Shi Jin and Qin Li (university of Wisconsin-Madison), email: qinli@math.wisc.edu

**Partners:** 

• university of Wisconsin-Madison (USA)

Inria contact: Nicolas Crouseilles

**Summary:** The main scientific objective of ANTipODE consists in marrying uniformly accurate (UA) and uncertainty quantification (UQ) techniques for multi-scale PDEs with uncertain data, two domains which usually come within the competency of separate communities.

The ringing of an old alarm clock bell on an uneven table induces a fast swaying from one side to the other and a slow drift along the steepest slope. Though the clock's vibrations are not interesting per se (the drift is what matters), their computation is an absolute prerequisite to the overall motion, while the tiny step-size required for that renders the simulation prohibitively costly, or even impossible. Such discrepant scales are characteristic of multi-scale models, amongst which prominent examples originate from the simulation of fusion as envisaged in ITER or from quantum models. Besides, many real-life problems are also rife with sources of uncertainties which are amplified by oscillations.

#### **10.1.2** Participation in other International Programs

#### Simons collaboration on wave turbulence

Participants: Geoffrey Beck, Erwan Faou, Antoine Mouzard.

#### Wave turbulence

Partner Institution(s): New York University (USA), Princeton (USA), ENS Lyon (France).

#### 2020-2025

The goal of this project is to provide a first attempt for a systematic coordinated study of Wave Turbulence Theory in a large-scale project, bringing together state of the art skills in the areas of mathematics and physics, with theoretical, experimental, and numerical expertise.

#### 10.2 International research visitors

#### Other international visits to the team

- L. Einkemmer (university Innsbruck, Austria) visited the MINGuS team during one week (September 2022).
- P. Raphaël (university Cambridge, UK) visited the MINGuS team during one week (October 2022).
- M. Anandan (Indian Institute of Science, Bangalore, India) visited the MINGuS team during one month (June-July 2022).

#### 10.2.1 Visits to international teams

#### **Research stays abroad**

The members of the team visited some colleagues abroad or participated to the international event CEMRACS 2022 (CIRM Marseille, France).

- I. Almuslimani visited Prof. G. Vilmart during one week at Geneva university (December 2022).
- A. Crestetto spent 2 weeks at CIRM (Marseille, France) for a research project during the CEMRACS 2022.
- N. Crouseilles spent 2 weeks at CIRM (Marseille, France) for a research project during the CEMRACS 2022.
- E. Faou spent 2x1 month at the Newton institute for the semester Frontiers in numerical analysis of kinetic equations (Cambridge, April-May 2022, UK).
- X. Hong spent 4 weeks at CIRM (Marseille, France) for a research project during the CEMRACS 2022.
- X. Hong visited Prof. Q. Li during one week at UW-Madison (December 2022).
- X. Hong visited Prof. J. Qiu during one week at Delaware university (December 2022).
- Y. Le Hénaff spent 6 weeks at CIRM (Marseille, France) for a research project during the CEMRACS 2022.
- P. Navaro spent 6 weeks at CIRM (Marseille, France) during the CEMRACS 2022 to support several research projects in terms of performance computing and programming.
- D. Prel spent 6 weeks at CIRM (Marseille, France) for a research project during the CEMRACS 2022.

#### **10.3** National initiatives

• 2018-2023: participation IPL SURF headed by A. Vidard (Airsea team).

Participants: Arnaud Debussche, Erwan Faou.

This project aims at the modelling and simulation of coastal and littoral ocean circulation problems, including quantification. This project involves 7 Inria teams and Ifremer, BRGM and SHOM.

 2022: project funded by Fédération de Recherche Fusion par Confinement Magnétique, headed by N. Crouseilles. 5000 euros. Participants: Anais Crestetto, Nicolas Crouseilles, Erwan Faou, Pierre Navaro.

This project is focused on the design of numerical schemes for tokamak plasmas and involve 5 members (of the team but also colleagues from university of Nantes). This year, this budget enables to partly support the participation of 3 members to the CEMRACS 2022 (6 weeks at CIRM, Marseille France).

• 2019-2023: A. Debussche is the local coordinator of ANR project ADA, headed by J. Vovelle (ENS Lyon). 160000 euros

Participants: Arnaud Debussche.

This project focuses on multiscale models which are both infinite-dimensional and stochastic with a theoretic and computational approach. The project involved a group in Lyon and MINGuS members.

• 2019-2024 GdR TRAG on rough path theory.

Participants: Arnaud Debussche.

The goal of the TRAG GDR is to gather french mathematicians who work on the rough path theory. GDR TRAG.

• 2023-2027: E. Faou is the PI of the ANR project KEN (Kinetic, PDE and Numerics). The partners are R. Krikorian (Ecole Polytechnique) and B. Grébert (University Nantes). Budget total 391000 euros

Participants: Anais Crestetto, Nicolas Crouseilles, Erwan Faou.

The project involved a group in Nantes, Ecole Polytechnique and some MINGuS members.

• 2022: participation at the CEMRACS 2022 through several research groups. CEMRACS 2022

**Participants:** Anais Crestetto, Nicolas Crouseilles, Pierre Navaro.

#### 10.4 Regional initiatives

• 2021-2023: SPIN project, co-funded by the Brittany region council and the Labex Centre Henri Lebesgue), headed by N. Crouseilles. 90000 euros dedicated to 18 months of a postdoc contract for X. Hong. This project focuses on modelling and numerical schemes for spin plasmas in collaboration with physicists from university of Strasbourg.

Participants: Anais Crestetto, Nicolas Crouseilles, Erwan Faou, Pierre Navaro.

• 2022: N. Crouseilles obtained a "Défi" project from IRMAR to participate to the CEMRACS 2022.

Participants: Anais Crestetto, Nicolas Crouseilles, Pierre Navaro.

## 11 Dissemination

Participants: G. Beck, F. Castella, A. Crestetto, A. Debussche, N. Crouseilles, E. Faou, P. Navaro.

#### 11.1 Promoting scientific activities

#### 11.1.1 Scientific events: organisation

- A. Crestetto organized the conference of ANR MoHyCon (Pornichet, March 2022, France).
- A. Crestetto organized the Rennes-Nantes day (Nantes, April 2022, France).
- E. Faou organized the event SEME (semaine maths et entreprise) at university Rennes 1 (Rennes, May 2022, France).
- E. Faou organized the colloquium of the IRMAR laboratory.
- P. Navaro organized the "Journées Julia pour le calcul scientifique" (Paris, June 2022, France)

#### Member of the editorial boards

- A. Debussche: Editor in chief of "Stochastics and Partial Differential Equations: Analysis and Computations" (2013-)
- A. Debussche: Member of the editorial committee of ESAIM: PROCS (2012-).
- A. Debussche: Member of the editorial committee of Annales de l'IHP Probabiliteés et Statisques (2020-).
- A. Debussche: Member of the editorial committee of Journal of Evolution equation (2014-).
- A. Debussche: Member of the editorial committee of Annales Henri Lebesgue (2018-).
- A. Debussche: Member of the editorial committee of the collection de monographie : Mathématiques and Applications, sous l'égide de la SMAI.

**Reviewer - reviewing activities** Members of MINGuS reviewed papers from journals in which they usually publish their works.

#### 11.1.2 Invited talks

The MINGuS members gave the following invited talks (seminars, national or international events). Seminar

- I. Almuslimani gave a seminar at the university of Geneva (Geneva, December 2022, Switzerland).
- I. Almuslimani gave a seminar at the university of Compiègne (Compiègne, January 2023, France).
- A. Crestetto gave the seminar "Informatique scientifique et mathématiqus appliquées" organized by CEA-DAM Ile de France (March 2022, France).
- A. Crestetto gave an online seminar "Modeling, Computation, Nonlinearity, Randomness and Waves" organized by the university of Arizona (March 2022, France).

- N. Crouseilles gave an online seminar at the university of Wuhan (Wuhan, January 2022, China).
- E. Faou gave a seminar at the university of Rennes (Rennes, March 2022, France).
- E. Faou gave two seminars at the university of Paris 13 (Paris, March 2022, France).
- X. Hong gave a seminar at the university of Madison-Wisconsin (Madison, November 2022, USA).
- X. Hong gave a seminar at the university of Delaware (Delaware, November 2022, USA).
- X. Hong gave a seminar at the university of Rennes (Rennes, February 2022, France).
- X. Hong gave a seminar at the Michigan Technological university (Michigan, December 2021, USA).

#### National events

- I. Almuslimani gave a talk at the conference CANUM 2022 (Evian, June 2022, France).
- G. Beck gave a talk at the conference "Modélisation mathématique et simulation numérique pour le traitement d'image, l'énergie, le développement durable et la morphodynamique côtière" (Rouen, November 2022, France)
- A. Crestetto gave a talk at the conference CEA-SMAI-GAMNI (IHP Paris, January 2022, France).
- A. Crestetto gave a talk at the conference of PDE-GdR (Vannes, February 2022, France).
- N. Crouseilles gave a talk at the workshop ANR MoHyCon (Pornichet, March 2022).
- A. Debussche gave a talk at the conference EDP singulières et aléatoires at IECN (Nancy, December 2021, France).
- A. Mouzard gave a talk at the conference of GDR TRAG (Nanterre, June 2022, France).
- A. Mouzard gave a talk at the meeting ANR QuAMProcs (Bordeaux, October 2022, France).

#### International events

- I. Almuslimani gave a talk at the conference SciCADE 2022 (Reykjavik, July 2022, Island)
- G. Beck gave a talk at the workshop on Fluid Structure Interactions (Brussels, October 2022, Belgium).
- G. Beck gave a talk at the workshop Coastal flow models and boundary conditions (Toulouse, October 2022, France)
- G. Beck gave a talk at the annual meeting of the Simons Collaboration on Wave Turbulence (Lyon, December 2022, France).
- A. Crestetto gave a talk during the CEMRACS 2022 (Marseille, August 2022, France).
- A. Crestetto gave a talk at the conference Kinetic and hyperbolic equations: modeling, analysis and numerics (Toulouse, December 2022, France).
- N. Crouseilles gave an online talk during the conference "Modelling and Numerical Simulation of Non-Equilibrium Processes" organized by National university of Singapore (Singapore, February 2022).
- N. Crouseilles gave a talk during the Oberwolfach workshop (Oberwolfach, April 2022, Germany).
- N. Crouseilles gave a talk during the CEMRACS 2022 (Marseille, July 2022, France).
- N. Crouseilles gave an online talk during the 6th conference "Asia-Pacific Conference on Plasma Physics" (October 2022).

- N. Crouseilles gave a talk at the conference Kinetic and hyperbolic equations: modeling, analysis and numerics (Toulouse, December 2022, France).
- A. Debussche gave an online talk at the conference "Theory and Computational methods for SPDEs" (CMO and BIRS, September 2022, Mexico and Canada).
- A. Debussche gave a talk at the conference "Stochastic Transport in Upper Ocean Dynamics" at Imperial College (London, September 2022, UK).
- A. Debussche gave a talk at the conference on Stochastic Analysis and Stochastic Partial Differential Equations at CRM (Barcelona, June 2022, Spain).
- E. Faou gave a talk at the conference Dynamics of Hamiltonian PDEs (La Thuile, February 2022, Italy).
- E. Faou gave a talk at the conference ICMS Frontiers in The Interplay Between Probability and Kinetic Theory (Edinburgh, April 2022, UK).
- E. Faou gave a mini-course at the workshop "Formes normales et méthodes de splitting" (Pornichet, June 2022, France).
- A. Mouzard gave a talk at the annual meeting of the Simons Collaboration on Wave Turbulence (Lyon, December 2022, France).
- P. Navaro gave a talk at the NUMKIN-22 conference (Munich, November 2022, Germany).
- D. Prel gave a talk at the NUMKIN-22 conference (Munich, November 2022, Germany).

#### 11.1.3 Leadership within the scientific community

- N. Crouseilles is head of the MINGuS Inria team.
- A. Debussche is head of the team "Processus Stochastique" of IRMAR laboratory.
- E. Faou is head of the Labex Lebesgue.
- E. Faou is head of the Agence Lebesgue pour l'innovation en mathématiques.
- E. Faou participates to the AMIES network.

#### 11.1.4 Scientific expertise

- A. Crestetto is a member of the CNU 26.
- N. Crouseilles is a member of the Commission d'Evaluation Inria.
- N. Crouseilles was member of the hiring committee for the Inria young researcher position at Paris.
- N. Crouseilles was member of the hiring committee for the Inria senior researcher position.
- N. Crouseilles participates as a coordinator of the evaluation of some Inria teams.
- N. Crouseilles was member of the committee "moyens incitatifs Inria du centre de l'université de Rennes".
- A. Debussche was chair committee of the Junior Professor Inria position Modeliterre.
- E. Faou was member of the hiring committee of a professor position at university of Bordeaux 1.
- P. Navaro was member of the hiring committee CNRS "Ingénieur d'Etude" 106.
- P. Navaro participates to the "réseau Calcul" at MITI (Mission pour les Initiatives Transverses et Interdisciplinaires du CNRS).

#### 11.1.5 Research administration

- N. Crouseilles is member of the IRMAR council.
- N. Crouseilles: responsible for the university of Rennes 1 of the Fédération de recherche pour la fusion confinement magnétique.
- A. Debussche is member of the administration council of ENS Paris Saclay.
- A. Debussche is member of the research committee of university Rennes.
- E. Faou is member of the scientific committee of the Pôle Léonard de Vinci.

#### 11.2 Teaching - Supervision - Juries

#### 11.2.1 Teaching

Almost all the members of team teach. We list below the Master courses only.

- F. Castella, Numerical methods for ODEs and PDEs, 40 hours, Master 1, University of Rennes 1.
- F. Castella, Finite Elements, 36 hours, Master 2, University of Rennes 1.
- A. Crestetto is head of the Master MACS, Nantes university.
- N. Crouseilles, Numerical methods for PDEs, 24 hours, Master 1, ENS Rennes.
- N. Crouseilles, Numerical methods for kinetic equations, 36 hours, Master 2, University of Rennes 1.
- A. Debussche, Calcul stochastique, 36 hours, Master 2, University Rennes 1.
- P. Navaro (course "introduction to Julia langage, 2 hours, Inria Rennes).
- 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.

#### 11.2.2 Supervision

- I. Almuslimani (postdoc 2021-2023) advised by N. Crouseilles.
- G. Barrué (PhD ENS Rennes, 2019-2022) advised by A. Debussche. Defended July 2022, now postdoc at Orange, Cesson. Title: Approximation diffusion for dispersive equations.
- Q. Chauleur (PhD, Univ Rennes, 2019-2022) co-advised by R. Carles and E. Faou. Defended July 2022, now postdoc Inria Paradyse, Lille. Title: On the Schrödinger-Langevin equation and on the damped Euler system.
- F. Dufay (master 1 internship, 2022) co-advised by N. Crouseilles and P. Navaro.
- Y. Le Hénaff (PhD, Univ Rennes, 2021-2024) co-advised by N. Crouseilles and E. Faou. Title: High order modulated particle methods: theoretical and numerical studies.
- X. Hong (postdoc 2022-2023) advised by N. Crouseilles.
- T. Laborde (PhD, Naval Group, 2020-2023) co-advised by former members of the team. Due to the contract with Naval Group, his name still appears as a member of the team.
- A. Mouzard (postdoc 2021-2023) advised by E. Faou.
- R. Nader (postdoc 2023) advised by A. Debussche.
- D. Prel (PhD, Université Nantes, 2021-2024) co-advised by A. Crestetto and N. Crouseilles. Title: Multi-scale numerical methods for tokamak plasma simulations.

#### 11.2.3 Juries

- A. Crestetto participated to the PhD jury of M. Rigal (Sorbonne university, November 2022, France).
- A. Crestetto participated to the PhD jury of O. Michel (Paris Saclay university, November 2022, France).
- N. Crouseilles participated to the PhD jury of M. Tacu (Paris Saclay university, November 2022, France).

#### 11.3 Popularization

- A. Crestetto participated to the master class lectures "Sophie Kowalevski" to encourage women students to do mathematics (Angers, May 2022, France).
- A. Crestetto participated to the event "Fête de la Science" (Nantes, October 2022, France).
- N. Crouseilles participated to the livestorm organized by Inria Rennes. The goal was to gather experts to give some advises to PhD students for their applications (Rennes, October 2022, France).
- E. Faou organized the "Journée d'Innovation Mathématiques" (Rennes, May 2022, France).
- D. Prel participated to the event "Fête de la Science" (Nantes, October 2022, France).

#### 11.3.1 Internal or external Inria responsibilities

• N. Crouseilles is a member of the Commission d'Evaluation.

## 12 Scientific production

#### 12.1 Major publications

- F. Casas, N. Crouseilles, E. Faou and M. Mehrenberger. 'High-order Hamiltonian splitting for Vlasov-Poisson equations'. In: *Numerische Mathematik* 135.3 (2017), pp. 769–801. DOI: 10.1007/s00211-016-0816-z. URL: https://hal.inria.fr/hal-01206164.
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#### 12.2 Publications of the year

#### International journals

 I. Almuslimani, P. Chartier, M. Lemou and F. Méhats. 'Uniformly accurate schemes for driftoscillatory stochastic differential equations'. In: *Applied Numerical Mathematics* 468-482 (2022), pp. 468–482. DOI: 10.1016/j.apnum.2022.07.001. URL: https://hal.inria.fr/hal-03371 466.

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#### **Reports & preprints**

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