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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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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 [28, 30, 31, 34] 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* [27] 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 [29] 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, [30], 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 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 [25] 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 [28].

Multiscale numerical methods for stochastic PDEs

AP schemes have been developed recently for kinetic equations with noise in the context of Uncertainty Quantification UQ [33]. 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 [37]- 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 [26]) 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 [34], 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 [35, 31]). 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 [36]). 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 an 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. [28]. 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 uniform 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 [32]). 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 [32]). 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 [37]), 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 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 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 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

Three members of team have been hired by a startup and left the team.

7 New software and platforms

We have two softwares developed and maintained in the team.

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

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.

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

8.1 Multiscale numerical schemes

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.

We present in [12] a general-purpose library called HOODESolver.jl written in Julia dedicated to the efficient resolution of highly oscillatory ODEs. In the documentation details are given to explain how to simulate highly oscillatory ODEs using a Uniformly Accurate (UA) method, i.e. 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 [15], 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 [18], 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 [19], 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.

8.2 Numerical schemes for Hamiltonian PDEs

In J. Bernier (FoCM(5), 2021), some exact splittings are proposed for inhomogeneous quadratic differential equations including, for example, transport equations, kinetic equations, and Schrödinger type equations with a rotation term. In [3], these exact splittings are combined with pseudo-spectral methods in space to illustrate their high accuracy and efficiency.

In [6], 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.

In [17], 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.

In [22], 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 [24], we define a class of discrete operators acting on infinite, finite or periodic sequences mimicking the standard properties of pseudo-differential operators. In particular we can define the notion of order and regularity, and we recover the fundamental property that the commutator of two discrete operators gains one order of regularity. We show that standard differential operators acting on periodic functions, finite difference operators and fully discrete pseudo-spectral methods fall into this class of discrete pseudo-differential operators. As examples of practical applications, we revisit standard error estimates for the convergence of splitting methods, obtaining in some Hamiltonian cases no loss of derivative in the error estimates, in particular for discretizations of general waves and/or water-waves equations. Moreover, we give an example of preconditioner constructions inspired by normal form analysis to deal with the similar question for more general cases.

8.2.1 Analysis of PDEs and SPDEs

In [4], we consider general classes of nonlinear Schrödinger equations on the circle with nontrivial cubic part and without external parameters. We construct a new type of normal forms, namely rational normal forms, on open sets surrounding the origin in high Sobolev regularity. With this new tool we prove that, given a large constant M and a sufficiently small parameter ε , for generic initial data of size ε , the flow is conjugated to an integrable flow up to an arbitrary small remainder of order ε^{M+1} . This implies that for such initial data $u(0)$, we control the Sobolev norm of the solution $u(t)$ for time of order ε^{-M} . Furthermore this property is locally stable: if $v(0)$ is sufficiently close to $u(0)$ (of order $\varepsilon^{3/2}$) then the solution $v(t)$ is also controlled for time of order ε^{-M} .

In [5], 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 [8], 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 [9], we consider the Nonlinear Schrödinger (NLS) equation and prove that the Gaussian measure with covariance $(1 - \partial_x^2)^{-\alpha}$ on $L^2(T)$ is quasi-invariant for the associated flow for $\alpha > 1/2$. This is sharp and improves a previous result obtained in a former work 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 former results in the literature. The arguments are general and can be used to other Hamiltonian equations.

In [10], we study the dynamics of perturbations around an inhomogeneous stationary state of the Vlasov-HMF (Hamiltonian Mean-Field) model, satisfying a linearized stability criterion (Penrose criterion). We consider solutions of the linearized equation around the steady state, and prove the algebraic decay in time of the Fourier modes of their density. We prove moreover that these solutions exhibit a scattering behavior to a modified state, implying a linear Landau damping effect with an algebraic rate of damping.

In [14], 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 $T_{k,n}$ of k -pull operations needed for all the n nodes to learn the rumor. We compute the expected value and the variance of $T_{k,n}$, 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 [21], we consider the logarithmic Schrödinger equations with damping, also called Schrödinger-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 [20], 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 [23], 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 [7], 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.

A biochemical network can be simulated by a set of ordinary differential equations (ODE) under well stirred reactor conditions, for large numbers of molecules, and frequent reactions. This is no longer a robust representation when some molecular species are in small numbers and reactions changing them are infrequent. In this case, discrete stochastic events trigger changes of the smooth deterministic dynamics of the biochemical network. Piecewise-deterministic Markov processes (PDMP) are well adapted for describing such situations. Although PDMP models are now well established in biology, these models remain computationally challenging. Previously we have introduced the push-forward method to compute how the probability measure is spread by the deterministic ODE flow of PDMPs, through the use of analytic expressions of the corresponding semigroup. In this paper [11], we provide a more general simulation algorithm that works also for non-integrable systems. The method can be used for biochemical simulations with applications in fundamental biology, biotechnology and biocomputing.

In [13], we analyse average-based distributed algorithms relying on simple and pairwise random interactions among a large and unknown number of anonymous agents. This allows the characterization of global properties emerging from these local interactions. Agents start with an initial integer value, and at each interaction keep the average integer part of both values as their new value. The convergence occurs when, with high probability, all the agents possess the same value which means that they all know a property of the global system. Using a well chosen stochastic coupling, we improve upon existing results by providing explicit and tight bounds of the convergence time. We apply these general results to both the proportion problem and the system size problem.

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.

- 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.

- 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 originally scheduled in 2019 but delayed due to the sanitary situation) or by organizing some *Semaine mathématiques et entreprises* (SEME) for student who work during one week on problems brought by some industrial companies. These SEME are essentially funded by **AMIES** and the next one will be in 2022, after many adjournements due to the sanitary condition.

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 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

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

10.1 International initiatives

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

- 2018-2022: associated team ANTIPODE with university of Wisconsin-Madison (US), headed by P. Chartier (2018-2021) and N. Crouseilles (2021-2022). 15000 euro per year.

The project focuses on the development of multi-scale numerical schemes for PDEs with uncertain data. The project is in partnership with university of Wisconsin-Madison and with Shanghai Jiao Tong University. Since the leader left Inria and due to the pandemia, this future of this project is a bit uncertain.

10.1.2 Participation in other International Programs

Simons project on wave turbulence

Wave turbulence

New York University, Princeton, ENS Lyon, ENS Paris

2019-2023

This project is 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 National initiatives

- 2019-2021: AdT (Aide au développement technologique) J-Plaff, headed by N. Crouseilles. 2 years engineer.
The goal was the development of libraries written in Julia on highly oscillatory ODEs and nonlinear transport equations, in partnership with the Fluminance group (Inria Rennes). Y. Mocquard has been hired and actively worked during 2 years to implement in Julia some numerical methods developed in the team.
- 2018-2023: participation IPL SURF headed by A. Vidard (Airsea team).
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.
- project funded by Fédération de Recherche Fusion par Confinement Magnétique, headed by N. Crouseilles. 5000 euros.
This project are focused on the design of numerical schemes for tokamak plasmas and involve 5 members (of the team but also colleagues from university of Nantes).
- 2019-2023: A. Debussche is the local coordinator of ANR project ADA, headed by J. Vovelle (ENS Lyon). 160000 euros
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.
- 2019-2021: International Actions project funded by university of Rennes 1, headed by N. Crouseilles. 3000 euros.
This project focused on multi-scale numerical schemes for collisional kinetic equations in partnership with university of Ferrare.
- 2019-2024 GdR TRAG on rough path theory. The goal of the TRAG GDR is to gather french mathematicians who work on the rough path theory. [GDR TRAG](#).

10.3 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 postdoc contract.
This project focuses on modelling and numerical schemes for spin plasmas in collaboration with physicists from university of Strasbourg.

11 Dissemination

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

11.1 Promoting scientific activities

11.1.1 Scientific events: organisation

- P. Navaro: Organization of "Action Nationale de Formation sur le langage Julia" for CNRS (Fréjus, France), 13-17 September.
- P. Navaro: Formation "Python pour le calcul scientifique" for IMT members (Rennes, France), 13-17 June.
- P. Navaro: Organisation of the mini-symposium "Julia, a langage for mathematicians" SMAI conference (la Grande Motte, France), 21-25 June.
- P. Navaro: Organisation of 6 webinars "Café Calcul".
- E. Faou: Organization of the semester **Hamiltonian Methods in Dispersive and Wave Evolution Equations**, ICERM, Brown University, USA. Fall 2021.
- E. Faou: Organization of the workshop *Numerics, Modeling, and Experiments in Wave Phenomena*, with D. Cordoba, E. Dormy, T. Sapsis and L. Vega, ICERM, Brown University, USA.

11.1.2 Journal

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 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 Annales de l'IHP Probabilité's et Statistiques (2020-)
- A. Debussche: Member of the editorial committee of the collection de monographie : Matheématiques and Applications, sous l'égide de la SMAI.
- M. Lemou: member of editorial board of CMS.
- P. Chartier: member of editorial board of M2AN.

Reviewer - reviewing activities

All the members review articles in the journal in which they publish.

11.1.3 Invited talks

- J. Massot: invitation to the working group CMAP Polytechnique (Palaiseau), 8 October.
- J. Massot: invitation: invitation to the Workshop Models and methods for kinetic equations (Bordeaux), 20 November.
- J. Massot: invitation to the seminar (Nantes), 9 November.
- A. Mouzard: invitation to "Colloque des Jeunes Probabilistes et Statisticiens" (Oléron, France), October.
- A. Mouzard: invitation to "Rough path techniques in stochastic analysis and mathematical probability" (Oslo, Norway), November.
- A. Mouzard: invitation to "Simons Collaboration on Wave Turbulence Annual Meeting 2021" (online with NYU and Lyon), December.
- A. Mouzard: invitation to Colloquium Singular and Random PDEs (Nancy, France), December.
- E. Faou: Paris-Moscow seminar "Dynamical systems and PDEs" managed by S. Kuksin and D. Treschev (online), September.
- E. Faou: Seminar at the University of Nantes, September.
- E. Faou: Wave turbulence seminar, New-York University. Online, January.
- E. Faou: lecture series on wave turbulence, New-York University. Online, January.
- N. Crouseilles: invited to the workshop "Numerical methods for kinetic equations" (CIRM Marseille, France), June

11.1.4 Scientific expertise

- A. Crestetto: member of the recruitment committee of maitre de conference, university of Nantes.
- A. Crestetto: member of the recruitment committee of maitre de conference, university of Nice.
- A. Crestetto: member of the CNU, section 26.
- A. Debussche: member of the EAB (External Advisory Board) of the Synergy ERC STUOD.
- A. Debussche: reviewer for ERC, Austrian Science Fund.
- N. Crouseilles: member of the Inria evaluation committee (and then jury for promotions DR, admissibility jury CR-Saclay, admission jury CR).
- E. Faou: Member of the ICIAM Maxwell Prize.
- N. Crouseilles: member of the recruitment committee of professor, university of Bordeaux.

11.1.5 Research administration

- A. Crestetto: member of the scientific council of UFR Sciences et Techniques University of Nantes.
- A. Crestetto: locale coordinator SMAI for mathematical laboratory of university of Nantes.
- A. Debussche: member of the scientific council of Fédération Denis Poisson (Orléans-Tours) (2012-).
- A. Debussche: vice-head of research at ENS Rennes.
- A. Debussche: member of the CA ENS Paris-Saclay.

- E. Faou: Director of the **Henri Lebesgue Center** (Excellence laboratory of the program *investissement d'avenir*).
- E. Faou: Member of the organization committee of the **Agence Lebesgue de Mathématiques pour l'innovation**.
- N. Crouseilles: member of the IRMAR laboratory council.
- N. Crouseilles: responsible for the university of Rennes 1 of the Federation de recherche pour la fusion confinement magnétique.

11.2 Teaching - Supervision - Juries

11.2.1 Teaching

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

- 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.
- P. Navaro (course Python-Fortran, Bordeaux). Cancelled.
- 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.
- E. Faou: Numerical transport, 24 hours, Master 2, University of Rennes.

11.2.2 Supervision

- E. Faou and N. Crouseilles: PhD of Y. Le Hénaff.
- E. Faou: PhD of Q. Chauleur (with R. Carles, CNRS IRMAR, Rennes).
- A. Debussche: PhD of G. Barrué (with A. de Bouard, Ecole Polytechnique).
- A. Debussche: PhD of B. Hug (with E. Mémin, Inria Rennes).
- A. Crestetto and N. Crouseilles: PhD of D. Prel.

11.2.3 Juries

- A. Crestetto: member of the PhD defense jury of Mme Rihab Daadaa, 13 December, University Lorraine.
- A. Crestetto: member of the PhD defense jury of J. Massot, University Rennes, December.
- A. Debussche: member of the PhD defense jury of A. Mouzard, 24 June, University Rennes.
- A. Debussche: member of the PhD defense jury of P. M. Boulevard, 5 May, University Paris.
- A. Debussche: member of the PhD defense jury of L. Li, 23 March, University Rennes.
- A. Debussche: member of the HDR defense jury of C.-E. Bréhier, 17 June, ENS Lyon.
- E. Castella: member of the PhD defense jury of L. Trémant, 8 December, University Rennes.
- E. Faou: reviewer for the PhD defense of P. Brun, University of Bordeaux, December.

- E. Faou: president of the HDR defense jury of C. Scheid, University of Nice, December.
- E. Faou: president of the HDR defense jury of V. Duchêne, University of Rennes, December.
- N. Crouseilles: president of the PhD defense jury of V. Pages, Sorbonne University, December.
- N. Crouseilles: member of the PhD defense jury of J. Massot, University Rennes, December.

11.3 Popularization

11.3.1 Interventions

- N. Crouseilles gave a conference for master students for University of Nantes and Ecole Centrale of Nantes to explain research opportunities at Inria, online, January.
- A. Crestetto: participation to the "fête de la science", Nantes.
- J. Massot: talk for the Nantes Society of Astronomy, 26 December.

12 Scientific production

12.1 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>.

12.2 Publications of the year

International journals

- [3] J. Bernier, N. Crouseilles and Y. Li. 'Exact splitting methods for kinetic and Schrödinger equations'. In: *Journal of Scientific Computing* 86.1 (2021). DOI: [10.1007/s10915-020-01369-9](https://doi.org/10.1007/s10915-020-01369-9). URL: <https://hal.archives-ouvertes.fr/hal-02425605>.
- [4] J. Bernier, E. Faou and B. Grebert. 'Rational normal forms and stability of small solutions to nonlinear Schrödinger equations'. In: *Annals of PDE* 6.2 (2021), pp. 1–53. DOI: [10.1007/s40818-020-00089-5](https://doi.org/10.1007/s40818-020-00089-5). URL: <https://hal.archives-ouvertes.fr/hal-01965082>.
- [5] Q. Chauleur. 'Dynamics of the Schrödinger-Langevin equation'. In: *Nonlinearity* 34.4 (2021), pp. 1943–1974. DOI: [10.1088/1361-6544/abd528](https://doi.org/10.1088/1361-6544/abd528). URL: <https://hal.archives-ouvertes.fr/hal-02541831>.
- [6] N. Crouseilles, P.-A. Hervieux, Y. Li, G. Manfredi and Y. Sun. 'Geometric Particle-in-Cell methods for the Vlasov-Maxwell equations with spin effects'. In: *Journal of Plasma Physics* 87.3 (28th May 2021), article n° 825870301. DOI: [10.1017/S0022377821000532](https://doi.org/10.1017/S0022377821000532). URL: <https://hal.inria.fr/hal-03148534>.
- [7] A. Debussche and M. J. Nguapedja Nankep. 'A Piecewise Deterministic Limit for a Multiscale Stochastic Spatial Gene Network'. In: *Applied Mathematics and Optimization* (2021). DOI: [10.1007/s00245-021-09809-0](https://doi.org/10.1007/s00245-021-09809-0). URL: <https://hal.archives-ouvertes.fr/hal-02894345>.
- [8] A. Debussche, A. Rosello and J. Vovelle. 'Diffusion-approximation for a kinetic spray-like system with markovian forcing'. In: *Discrete and Continuous Dynamical Systems - Series S* 14.8 (2021), pp. 2751–2803. DOI: [10.3934/dcdss.2021039](https://doi.org/10.3934/dcdss.2021039). URL: <https://hal.archives-ouvertes.fr/hal-02612572>.

- [9] A. Debussche and Y. Tsutsumi. ‘Quasi-Invariance of Gaussian Measures Transported by the Cubic NLS with Third-Order Dispersion on T ’. In: *Journal of Functional Analysis* 281.3 (2021), article n° 109032. DOI: [10.1016/j.jfa.2021.109032](https://doi.org/10.1016/j.jfa.2021.109032). URL: <https://hal.archives-ouvertes.fr/hal-02477109>.
- [10] E. Faou, R. Horsin and F. Rousset. ‘On Linear Damping around Inhomogeneous Stationary States of the Vlasov-HMF Model’. In: *Journal of Dynamics and Differential Equations* 33 - special issue.3 (2021), pp. 1531–1577. DOI: [10.1007/s10884-021-10044-y](https://doi.org/10.1007/s10884-021-10044-y). URL: <https://hal.inria.fr/hal-03218110>.
- [11] G. C. P. Innocentini, A. Hodgkinson, F. Antoneli, A. Debussche and O. Radulescu. ‘Push-forward method for piecewise deterministic biochemical simulations’. In: *Theoretical Computer Science* 893 (2021), pp. 17–40. DOI: [10.1016/j.tcs.2021.05.025](https://doi.org/10.1016/j.tcs.2021.05.025). URL: <https://hal.archives-ouvertes.fr/hal-03137189>.
- [12] Y. Mocquard, P. Navaro and N. Crouseilles. ‘HOODESolver.jl: A Julia package for highly oscillatory problems’. In: *Journal of Open Source Software* 6.61 (2021). DOI: [10.21105/joss.03077](https://doi.org/10.21105/joss.03077). URL: <https://hal.inria.fr/hal-03142594>.
- [13] Y. Mocquard, B. Sericola, F. Robin and E. Anceaume. ‘Stochastic Analysis of Average Based Distributed Algorithms’. In: *Journal of Applied Probability* 58.2 (21st June 2021), pp. 394–410. DOI: [10.1017/jpr.2020.97](https://doi.org/10.1017/jpr.2020.97). URL: <https://hal-cnrs.archives-ouvertes.fr/hal-02473856>.
- [14] F. Robin, B. Sericola, E. Anceaume and Y. Mocquard. ‘Stochastic analysis of rumor spreading with k -pull operations’. In: *Methodology and Computing in Applied Probability* (23rd Oct. 2021). URL: <https://hal.archives-ouvertes.fr/hal-03128118>.

Reports & preprints

- [15] I. Almuslimani, P. Chartier, M. Lemou and F. Méhats. *Uniformly accurate schemes for oscillatory stochastic differential equations*. 8th Oct. 2021. URL: <https://hal.inria.fr/hal-03371466>.
- [16] P. Alphonse and J. Bernier. *Polar decomposition of semigroups generated by non-selfadjoint quadratic differential operators and regularizing effects*. 29th Dec. 2021. URL: <https://hal.archives-ouvertes.fr/hal-02280971>.
- [17] F. Casas, P. Chartier, A. Escorihuela-Tomàs and Y. Zhang. *Compositions of pseudo-symmetric integrators with complex coefficients for the numerical integration of differential equations*. 15th Feb. 2021. URL: <https://hal.inria.fr/hal-03141166>.
- [18] P. Chartier, M. Lemou, F. Méhats and X. Zhao. *Derivative-free high-order uniformly accurate schemes for highly-oscillatory systems*. 15th Feb. 2021. URL: <https://hal.inria.fr/hal-03141156>.
- [19] P. Chartier, M. Lemou and L. Trémant. *A uniformly accurate numerical method for a class of dissipative systems*. 1st Apr. 2021. URL: <https://hal.inria.fr/hal-02619512>.
- [20] Q. Chauleur. *The isothermal limit for the compressible Euler equations with damping*. 8th Sept. 2021. URL: <https://hal.archives-ouvertes.fr/hal-03335294>.
- [21] Q. Chauleur and E. Faou. *Around plane waves solutions of the Schrödinger-Langevin equation*. 30th Oct. 2021. URL: <https://hal.archives-ouvertes.fr/hal-03409804>.
- [22] A. Crestetto, N. Crouseilles, Y. Li and J. Massot. *Comparison of high-order Eulerian methods for electron hybrid model*. 8th Nov. 2021. URL: <https://hal.inria.fr/hal-03418778>.
- [23] A. De Bouard, A. Debussche and R. Fukuizumi. *Two dimensional Gross-Pitaevskii equation with space-time white noise*. 15th Feb. 2021. URL: <https://hal.archives-ouvertes.fr/hal-03137755>.
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- [30] A. Debussche and J. Vovelle. ‘Diffusion limit for a stochastic kinetic problem’. In: *Commun. Pure Appl. Anal.* 11 (2012), pp. 2305–2326.
- [31] E. Faou and F. Rousset. ‘Landau damping in Sobolev spaces for the Vlasov-HMF model’. In: *Arch. Ration. Mech. Anal.* 219 (2016), pp. 887–902.
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- [33] S. Jin and H. Lu. ‘An Asymptotic-Preserving stochastic Galerkin method for the radiative heat transfer equations with random inputs and diffusive scalings’. In: *J. Comp. Phys.* 334 (2017), pp. 182–206.
- [34] M. Lemou, F. Méhats and P. Raphaël. ‘Orbital stability of spherical galactic models’. In: *Invent. Math.* 187 (2012), pp. 145–194.
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