RESEARCH CENTRE

Inria Center
at the University of Lille

IN PARTNERSHIP WITH:

Université de Lille, CNRS

2022
ACTIVITY REPORT

Project-Team

PARADYSE

PARticles And DYnamical SystEms

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

Contents

Project-Team PARADYSE

Creation of the Project-Team: 2020 March 01

Keywords

Computer sciences and digital sciences

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A6.1.4. – Multiscale modeling

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Other research topics and application domains

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B3.6.1. – Biodiversity

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B5.11. – Quantum systems

B6.2.4. – Optic technology

1 Team members, visitors, external collaborators

Research Scientists

- Guillaume Dujardin [Team leader, INRIA, Researcher, HDR]
- Clément Erignoux [INRIA, Researcher]
- Marielle Simon [INRIA, Researcher, until Aug 2022, HDR]

Faculty Members

- Stephan De Bièvre [UNIV LILLE, Professor, HDR]
- Olivier Goubet [UNIV LILLE, Professor, HDR]
- André de Laire [UNIV LILLE, Associate Professor, HDR]

Post-Doctoral Fellows

- Quentin Chauleur [UNIV LILLE, from Sep 2022]
- Lu Xu [INRIA, until Oct 2022]
- Linjie Zhao [INRIA, until Aug 2022]

PhD Students

- Christopher Langrenez [UNIV LILLE, from Sep 2022]
- Erwan Le Quiniou [UNIV LILLE, from Sep 2022]
- Anthony Nahas [UNIV LILLE, until Sep 2022]

Technical Staff

- Alexandre Roget [INRIA, Engineer]

Administrative Assistant

- Karine Lewandowski [INRIA]

2 Overall objectives

The PARADYSE team gathers mathematicians from different communities with the same motivation: to provide a better understanding of dynamical phenomena involving particles. These phenomena are described by fundamental models arising from several fields of physics. We shall focus on model derivation, study of stationary states and asymptotic behaviors, as well as links between different levels of description (from microscopic to macroscopic) and numerical methods to simulate such models. Applications include non-linear optics, thermodynamics and ferromagnetism. Research in this direction has a long history, that we shall only partially describe in the sequel. We are confident that the fact that we come from different mathematical communities (PDE theory, mathematical physics, probability theory and numerical analysis), as well as the fact that we have strong and effective collaborations with physicists, will bring new and efficient scientific approaches to the problems we plan to tackle and will make our team strong and unique in the scientific landscape. Our goal is to obtain original and important results on a restricted yet ambitious set of problems that we develop in this document.

3 Research program

3.1 Time asymptotics: Stationary states, solitons, and stability issues

The team investigates the existence of *solitons* and their link with the global dynamical behavior for non-local problems such as the Gross–Pitaevskii (GP) equation which arises in models of dipolar gases. These models, in general, also introduce non-zero boundary conditions which constitute an additional theoretical and numerical challenge. Numerous results are proved for local problems, and numerical simulations allow to verify and illustrate them, as well as making a link with physics. However, most fundamental questions are still open at the moment for non-local problems.

The non-linear Schrödinger (NLS) equation finds applications in numerous fields of physics. We concentrate, in a continued collaboration with our colleagues from the physics department (PhLAM) at Université de Lille (U-Lille), in the framework of the Laboratoire d'Excellence CEMPI, on its applications in non-linear optics and cold atom physics. Issues of orbital stability and modulational instability are central here (see Section 4.1 below).

Another typical example of problem that the team wishes to address concerns the Landau–Lifshitz (LL) equation, which describes the dynamics of the spin in ferromagnetic materials. This equation is a fundamental model in the magnetic recording industry [40] and solitons in magnetic media are of particular interest as a mechanism for data storage or information transfer [42]. It is a quasilinear PDE involving a function that takes values on the unit sphere $\mathbb{S}^2$ of $\mathbb{R}^3$. Using the stereographic projection, it can be seen as a quasilinear Schrödinger equation and the questions about the solitons, their dynamics and potential blow-up of solutions evoked above are also relevant in this context. This equation is less understood than the NLS equation: even the Cauchy theory is not completely understood [32, 39]. In particular, the geometry of the target sphere imposes non-vanishing boundary conditions; even in dimension one, there are kink-type solitons having different limits at $\pm\infty$.

3.2 Derivation of macroscopic laws from microscopic dynamics

The team investigates, from a microscopic viewpoint, the dynamical mechanism at play in the phenomenon of relaxation towards thermal equilibrium for large systems of interacting particles. For instance, a first step consists in giving a rigorous proof of the fact that a particle repeatedly scattered by random obstacles through a Hamiltonian scattering process will eventually reach thermal equilibrium, thereby completing previous works in this direction by the team. As a second step, similar models as the ones considered classically will be defined and analyzed in the quantum mechanical setting, and more particularly in the setting of quantum optics.

Another challenging problem is to understand the interaction of large systems with the boundaries, which is responsible for most energy exchanges (forcing and dissipation), even though it is concentrated in very thin layers. The presence of boundary conditions to evolution equations sometimes lacks understanding from a physical and mathematical point of view. In order to legitimate the choice done at the macroscopic level of the mathematical definition of the boundary conditions, we investigate systems of particles with different local interactions. We apply various techniques to understand how diffusive and driven systems interact with the boundaries.

Finally, we aim at obtaining results on the macroscopic behavior of large scale interacting particle systems subject to kinetic constraints. In particular, we study the behavior in one and two dimensions of the Facilitated Exclusion Process (FEP), on which several results have already been obtained. The latter is a very interesting prototype for kinetically constrained models because of its unique mathematical features (explicit stationary states, absence of mobile cluster to locally shuffle the configuration). There are very few mathematical results on the FEP, which was put forward by the physics community as a toy model for phase separation.

Our goal is to make PDE theorists and probabilists work together, in order to take advantage of the analytical results which went further ahead and are more advanced than the statistical physics theory.

3.3 Numerical methods: analysis and simulations

The team addresses both questions of precision and numerical cost of the schemes for the numerical integration of non-linear evolution PDEs, such as the NLS equation. In particular, we aim at developing, studying and implementing numerical schemes with high order that are more efficient for these problems. We also want to contribute to the design and analysis of schemes with appropriate qualitative properties. These properties may as well be “asymptotic-preserving” properties, energy-preserving properties, or convergence to an equilibrium properties. Other numerical goals of the team include the numerical simulation of standing waves of non-linear non-local GP equations. We also keep on developing numerical methods to efficiently simulate and illustrate theoretical results on instability, in particular in the context of the modulational instability in optical fibers, where we study the influence of randomness in the physical parameters of the fibers.

The team also designs simulation methods to estimate the accuracy of the physical description via microscopic systems, by computing precisely the rate of convergence as the system size goes to infinity. One method under investigation is related to cloning algorithms, which were introduced very recently and turn out to be essential in molecular simulation.

4 Application domains

4.1 Optical fibers

In the propagation of light in optical fibers, the combined effect of non-linearity and group velocity dispersion (GVD) may lead to the destabilization of the stationary states (plane or continuous waves). This phenomenon, known under the name of modulational instability (MI), consists in the exponential growth of small harmonic perturbations of a continuous wave. MI has been pioneered in the 60s in the context of fluid mechanics, electromagnetic waves as well as in plasmas, and it has been observed in non-linear fiber optics in the 80s. In uniform fibers, MI arises for anomalous (negative) GVD, but it may also appear for normal GVD if polarization, higher order modes or higher order dispersion are considered. A different kind of MI related to a parametric resonance mechanism emerges when the dispersion or the non-linearity of the fiber are periodically modulated.

As a follow-up of our work on MI in periodically modulated optical fibers, we investigate the effect of random modulations in the diameter of the fiber on its dynamics. It is expected on theoretical grounds that such random fluctuations can lead to MI and this has already been illustrated for some models of the randomness. We investigate precisely the conditions under which this phenomenon can be strong enough to be experimentally verified. For this purpose, we investigate different kinds of random processes describing the modulations, taking into account the manner in which such modulations can be created experimentally by our partners of the fiber facility of the PhLAM. This necessitates a careful modeling of the fiber and a precise numerical simulation of its behavior as well as a theoretical analysis of the statistics of the fiber dynamics.

This application domain involves in particular S. De Bièvre and G. Dujardin.

4.2 Ferromagnetism

The Landau–Lifshitz equation describes the dynamics of the spin in ferromagnetic materials. Depending on the properties of the material, the LL equation can include a dissipation term (the so-called Gilbert damping) and different types of anisotropic terms. The LL equation belongs to a larger class of non-linear PDEs which are often referred to as geometric PDEs, and some related models are the Schrödinger map equation and the harmonic heat flow. We focus on the following aspects of the LL equation.

Solitons In the absence of Gilbert damping, the LL equation is Hamiltonian. Moreover, it is integrable in the one-dimensional case and explicit formulas for solitons can be given. In the easy-plane case, the orbital and asymptotic stability of these solitons have been established. However, the stability in other cases, such as in biaxial ferromagnets, remains an open problem. In higher dimensional cases, the existence of solitons is more involved. In a previous work, a branch of semitopological solitons with different speeds has been obtained numerically in planar ferromagnets. A rigorous proof of the existence of such solitons is established using perturbation arguments, provided that the speed is small enough. However, the proof does not give information about their stability. We would like to propose a variational approach to study the existence of this branch of solitons, that would lead to the existence and stability of the whole branch of ground-state solitons as predicted. We also investigate numerically the existence of other types of localized solutions for the LL equation, such as excited states or vortices in rotation.

Approximate models An important physical conjecture is that the LL model is to a certain extent universal, so that the non-linear Schrödinger and Sine-Gordon equations can be obtained as its various limit cases. In a previous work, A. de Laire has proved a result in this direction and established an error estimate in Sobolev norms, in any dimension. A next step is to produce numerical simulations that will enlighten the situation and drive further developments in this direction.

Self-similar behavior Self-similar solutions have attracted a lot of attention in the study of non-linear PDEs because they can provide some important information about the dynamics of the equation. While self-similar expanders are related to non-uniqueness and long time description of solutions, self-similar shrinkers are related to a possible singularity formation. However, there is not much known about the self-similar solutions for the LL equation. A. de Laire and S. Gutierrez (University of Birmingham) have studied expander solutions and proved their existence and stability in the presence of Gilbert damping. We will investigate further results about these solutions, as well as the existence and properties of self-similar shrinkers.

This application domain involves in particular A. de Laire and G. Dujardin.

4.3 Cold atoms

The cold atoms team of the PhLAM Laboratory is reputed for having realized experimentally the so-called Quantum Kicked Rotor, which provides a model for the phenomenon of Anderson localization. The latter was predicted by Anderson in 1958, who received in 1977 a Nobel Prize for this work. Anderson localization is the absence of diffusion of quantum mechanical wave functions (and of waves in general) due to the presence of randomness in the medium in which they propagate. Its transposition to the Quantum Kicked Rotor goes as follows: a freely moving quantum particle periodically subjected to a “kick” will see its energy saturate at long times. In this sense, it “localizes” in momentum space since its momenta do not grow indefinitely, as one would expect on classical grounds. In its original form, Anderson localization applies to non-interacting quantum particles and the same is true for the saturation effect observed in the Quantum Kicked Rotor.

The challenge is now to understand the effects of interactions between the atoms on the localization phenomenon. Transposing this problem to the Quantum Kicked Rotor, this means describing the interactions between the particles with a Gross–Pitaevskii equation, which is a NLS equation with a local (typically cubic) non-linearity. So the particle’s wave function evolves between kicks following the Gross–Pitaevskii equation and not the linear Schrödinger equation, as is the case in the Quantum Kicked Rotor. Preliminary studies for the Anderson model have concluded that in that case the localization phenomenon gives way to a slow subdiffusive growth of the particle’s kinetic energy. A similar phenomenon is expected in the non-linear Quantum Kicked Rotor, but a precise understanding of the dynamical mechanisms at work, of the time scale at which the subdiffusive growth will occur and of the subdiffusive growth exponent is lacking. It is crucial to design and calibrate the experimental setup intended to observe the phenomenon. The analysis of these questions poses considerable theoretical and numerical challenges due to the difficulties involved in understanding and simulating the long term dynamics of the non-linear system. A collaboration of the team members with the PhLAM cold atoms group is currently under way.

This application domain involves in particular S. De Bièvre and G. Dujardin.

4.4 Qualitative and quantitative properties of numerical methods

Numerical simulation of multimode fibers The use of multimode fibers is a possible way to overcome the bandwidth crisis to come in our worldwide communication network consisting in singlemode fibers. Moreover, multimode fibers have applications in several other domains, such as high power fiber lasers and femtosecond-pulse fiber lasers which are useful for clinical applications of non-linear optical microscopy and precision materials processing. From the modeling point of view, the envelope equations are a system of non-linear non-local coupled Schrödinger equations. For a better understanding of several physical phenomena in multimode fibers (e.g. continuum generation, condensation) as well as for the design of physical experiments, numerical simulations are an adapted tool. However, the huge number of equations, the coupled non-linearities and the non-local effects are very difficult to handle numerically. Some attempts have been made to develop and make available efficient numerical codes for such simulations. However, there is room for improvement: one may want to go beyond MATLAB prototypes, and to develop an alternative parallelization to the existing ones, which could use the linearly implicit methods that we plan to develop and analyze. In link with the application domain 4.1, we develop in particular a code for the numerical simulation of the propagation of light in multimode fibers, using high-order efficient methods, that is to be used by the physics community.

This application domain involves in particular G. Dujardin and A. Roget.

Qualitative and long-time behavior of numerical methods We contribute to the design and analysis of schemes with good qualitative properties. These properties may as well be “asymptotic-preserving” properties, energy-preserving properties, decay properties, or convergence to an equilibrium properties. In particular, we contribute to the design and analysis of numerically hypocoercive methods for Fokker–Planck equations [37], as well as energy-preserving methods for hamiltonian problems [34].

This application domain involves in particular G. Dujardin.

High-order methods We contribute to the design of efficient numerical methods for the simulation of non-linear evolution problems. In particular, we focus on a class of linearly implicit high-order methods, that have been introduced for ODEs [13]. We wish both to extend their analysis to PDE contexts, and to analyze their qualitative properties in such contexts.

This application domain involves in particular G. Dujardin.

4.5 Modeling of the liquid-solid transition and interface propagation

Analogously to the so-called Kinetically Constrained Models (KCM) that have served as toy models for glassy transitions, stochastic particle systems on a lattice can be used as toy models for a variety of physical phenomena. Among them, the kinetically constrained lattice gases (KCLG) are models in which particles jump randomly on a lattice, but are only allowed to jump if a local constraint is satisfied by the system.

Because of the hard constraint, the typical local behavior of KCLGs will differ significantly depending on the value of local conserved fields (e.g. particle density), because the constraint will either be typically satisfied, in which case the system is locally diffusive (liquid phase), or not, in which case the system quickly freezes out (solid phase).

Such a toy model for liquid-solid transition is investigated by C. Erignoux, M. Simon and their co-authors in [3] and [35]. The focus of these articles is the so-called facilitated exclusion process, which is a terminology coined by physicists for a specific KCLG, in which particles can only jump on an empty neighbor if another neighboring site is occupied. They derive the macroscopic behavior of the model, and show that in dimension 1 the hydrodynamic limit displays a phase separated behavior where the liquid phase progressively invades the solid phase.

Both from a physical and mathematical point of view, much remains to be done regarding these challenging models: in particular, they present significant mathematical difficulties because of the way the local physical constraints put on the system distort the equilibrium and steady-states of the model. For this reason, C. Erignoux, A. Roget and M. Simon are currently working with A. Shapira (MAP5, Paris) to generate numerical results on generalizations of the facilitated exclusion process, in order to shine some light on the microscopic and macroscopic behavior of these difficult models.

This application domain involves in particular C. Erignoux, A. Roget and M. Simon.

4.6 Mathematical modeling for ecology

This application domain is at the interface of mathematical modeling and numerics. Its object of study is a set of concrete problems in ecology. The landscape of the south of the Hauts-de-France region is made of agricultural land, encompassing forest patches and ecological corridors such as hedges. The issues are

- the study of the invasive dynamics and the control of a population of beetles which damages the oaks and beeches of our forests;
- the study of native protected species (the purple wireworm and the pike-plum) which find refuge in certain forest species.

Running numerics on models co-constructed with ecologists is also at the heart of the project. The timescales of animals and plants are no different; the beetle larvae spend a few years in the earth before moving. As a by-product, the mathematical model may tackle other major issues such as the interplay between heterogeneity, diversity and invasibility.

The models use Markov chains at a mesoscopic scale and evolution advection-diffusion equations at a macroscopic scale.

This application domain involves O. Goubet. Interactions with PARADYSE members concerned with particle models and hydrodynamic limits are planned.

5 New software and platforms

5.1 New software

5.1.1 MM_Propagation

Name: MultiMode Propagation

Keywords: Optics, Numerical simulations, Computational electromagnetics

Functional Description: This C++ software, which is interfaced with MatLab, simulates the propagation of light in multimode optical fibers. It takes into account several physical effects such as dispersion, Kerr effect, Raman effect, coupling between the modes. It uses high order numerical methods that allow for precision at reasonable computational cost.

URL: https://github.com/alexandreroget/MM_Propagation

Contact: Alexandre Roget

6 New results

Participants: Quentin Chauleur, Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet, Marielle Simon, Lu Xu, Linjie Zhao.

Some of the results presented below overlap several of the main research themes presented in section 3. However, results presented in paragraphs 6.1-6.6 are mainly concerned with research axis 3.1, whereas paragraphs 6.7-6.16 mostly concern axis 3.2. Paragraphs 6.17-6.19 concern numerics-oriented results, and are encompassed in axis 3.3.

6.1 Crank-Nicolson scheme for logarithmic nonlinear Schrödinger equations with non standard dispersion

In [9], we consider a nonlinear Schrödinger equation with discontinuous modulation and logarithmic non linearity. We regularize the nonlinearity at 0 to avoid numerical problems; the regularization parameter is ε. We analyze the consistence of the classical Crank-Nicolson scheme and provide precise error estimates depending on the time step τ and on ε^{-1}.

6.2 Standing waves for nonlinear Schrödinger equations with non standard dispersion

In [14] and in the one dimensional case we study the existence of standing waves for a nonlinear Schrödinger equation whose dispersion is singular at $x = 0$. We overcome the difficulty that the problem is not invariant by space translations by introducing a suitable framework that takes into account the symetries of the problem.

6.3 Existence and decay of traveling waves for the non-local Gross–Pitaevskii equation

The non-local Gross–Pitaevskii equation is a model that appears naturally in several areas of quantum physics, for instance in the description of superfluids and in optics when dealing with thermo-optic materials because the thermal non-linearity is usually highly non-local. A. de Laire and S. López-Martínez considered a non-local family of Gross–Pitaevskii equations in dimension one, and they found in [16] general conditions on the interactions, for which there is existence of dark solitons for almost every subsonic speed. Moreover, they established properties of the solitons such as exponential decay at infinity and analyticity. This work improves on the results obtained in P. Mennuni's PhD thesis.

6.4 Recent results for the Landau–Lifshitz equation

In [15], A. de Laire surveys recent results concerning the Landau–Lifshitz equation, a fundamental non-linear PDE with a strong geometric content, describing the dynamics of the magnetization in ferromagnetic materials. He revisits the Cauchy problem for the anisotropic Landau–Lifshitz equation, without dissipation, for smooth solutions, and also in the energy space in dimension one. He also examines two approximations of the Landau–Lifshitz equation given by the sine–Gordon equation and the cubic Schrödinger equation, arising in certain singular limits of strong easy-plane and easy-axis anisotropy, respectively. Concerning localized solutions, he reviews the orbital and asymptotic stability problems for a sum of solitons in dimension one, exploiting the variational nature of the solitons in the hydrodynamical framework. Finally, he surveys results concerning the existence, uniqueness and stability of self-similar solutions (expanders and shrinkers) for the isotropic LL equation with Gilbert term.

6.5 Minimizing travelling waves for the Gross–Pitaevskii equation

In [27], A. de Laire, P. Gravejat and D. Smets study the 2D Gross–Pitaevskii equation with periodic conditions in one direction, or equivalently on the product space $\mathbb{R} \times \mathbb{T}_L$ where $L > 0$ and $\mathbb{T}_L = \mathbb{R}/L\mathbb{Z}$. They focus on the variational problem consisting in minimizing the Ginzburg–Landau energy under a fixed momentum constraint. They prove that there exists a threshold value for L below which minimizers are the one-dimensional dark solitons, and above which no minimizer can be one-dimensional.

6.6 Modulational instability in random fibers and stochastic Schrödinger equations

The team achieved an analysis of modulational instability in optical fibers with a normal dispersion perturbed with a coloured noise in [11]. The effect of coloured noise on the modulational instability was investigated in order to assess whether it can produce a larger modulational instability than periodic modulations or homogeneous fibers with anomalous dispersion. They found that generally this is not the case. In [19], randomly dispersion-managed fibers are on the contrary shown to be able to produce such large instabilities. This research was carried out with physicists from the PhLAM laboratory in Lille.

6.7 Large deviations principle for the SSEP with weak boundary interactions

Efficiently characterizing non-equilibrium stationary states (NESS) has been in recent years a central question in statistical physics. The Macroscopic Fluctuations Theory [33] developped by Bertini et al. has laid out a strong mathematical framework to understand NESS, however fully deriving and characterizing large deviations principles for NESS remains a challenging endeavour. In [20], C. Erignoux and his collaborators proved that a static large deviations principle holds for the NESS of the classical Symmetric Simple Exclusion Process (SSEP) in weak interaction with particles reservoirs. This result echoes a previous result by Derrida, Lebowitz and Speer [36], where the SSEP with strong boundary interactions was considered. In [20], it was also shown that the rate function can be characterized both by a variational formula involving the corresponding dynamical large deviations principle, and by the solution to a non-linear differential equation. The obtained differential equation is the same as in [36], with different boundary conditions corresponding to the different scales of boundary interaction.

6.8 Mapping hydrodynamics for the facilitated exclusion and zero-range processes

In [24], we derive the hydrodynamic limit for two degenerate lattice gases, the facilitated exclusion process (FEP) and the facilitated zero-range process (FZRP), both in the symmetric and the asymmetric case. For both processes, the hydrodynamic limit in the symmetric case takes the form of a diffusive Stefan problem, whereas the asymmetric case is characterized by a hyperbolic Stefan problem. Although the FZRP is attractive, a property that we extensively use to derive its hydrodynamic limits in both cases, the FEP is not. To derive the hydrodynamic limit for the latter, we exploit that of the zero-range process, together with a classical mapping between exclusion and zero-range processes, both at the microscopic and macroscopic level. Due to the degeneracy of both processes, the asymmetric case is a new result, but our work also provides a simpler proof than the one that was previously proposed for the FEP in the symmetric case in [35].

6.9 Equilibrium perturbations for stochastic interacting systems

In [28], we consider the equilibrium perturbations for two stochastic systems: the d-dimensional generalized exclusion process and the one-dimensional chain of anharmonic oscillators. We add a perturbation of order $N^{-\alpha}$ to the equilibrium profile, and speed up the process by $N^{1+\kappa}$ for parameters $0 < \kappa \le \alpha$. Under some additional constraints on κ and α, we show the perturbed quantities evolve according to the Burgers equation in the exclusion process, and to two decoupled Burgers equations in the anharmonic chain, both in the smooth regime.

6.10 Moderate deviations for the current and tagged particle in symmetric simple exclusion processes

In [29], we prove moderate deviation principles for the tagged particle position and current in one dimensional symmetric simple exclusion processes. There is at most one particle per site. A particle jumps to one of its two neighbors at rate $1/2$, and the jump is suppressed if there is already one at the target site. We distinguish one particular particle which is called the tagged particle. We first establish a variational formula for the moderate deviation rate functions of the tagged particle positions based on moderate deviation principles from hydrodynamic limit proved by Gao and Quastel [38] Then we construct a minimizer of the variational formula and obtain explicit expressions for the moderate deviation rate functions.

6.11 The voter model with a slow membrane

In [30], we introduce the voter model on the infinite lattice with a slow membrane and investigate its hydrodynamic behavior. The model is defined as follows: a voter adopts one of its neighbors' opinion at rate one except for neighbors crossing the hyperplane $\{x : x_1 = 1/2\}$, where the rate is $\alpha N^{-\beta}$. Above, $\alpha > 0, \beta \ge 0$ are two parameters and N is the scaling parameter. The hydrodynamic equation turns out to be heat equation with various boundary conditions depending on the value of β. The proof is based on duality method.

6.12 Long-time behavior of SSEP with slow boundary

In [17], we consider the symmetric simple exclusion process with slow boundary first introduced in [31]. We prove a law of large number for the empirical measure of the process under a longer time scaling instead of the usual diffusive time scaling.

6.13 Hydrodynamics for one-dimensional ASEP in contact with a class of reservoirs

In [41], we study the hydrodynamic behaviour of the asymmetric simple exclusion process (ASEP) on the lattice of size n, in contact with a type of slow boundary reservoirs. A scalar conservation law with boundary-trace conditions is obtained as the hydrodynamic limit in the Euler space-time scale.

6.14 A Microscopic Derivation of Coupled SPDE's with a KPZ Flavor

In [10], we consider an interacting particle system driven by a Hamiltonian dynamics and perturbed by a conservative stochastic noise so that the full system conserves two quantities: energy and volume. The Hamiltonian part is regulated by a scaling parameter vanishing in the limit. We study the form of the fluctuations of these quantities at equilibrium and derive coupled stochastic partial differential equations with a KPZ flavor.

6.15 Mathematical modeling for ecology

The team had an important contribution to multi-scale ecosystem modeling. O. Goubet and his collaborators computed in [12] the large population limit of a stochastic process that models the evolution of a complex forest ecosystem to an evolution convection-diffusion equation that is more suitable for concrete computations. Then, they proved on the limit equation that the existence of exchange of population between forest patches slows down the extinction of species.

6.16 Quantum optics and quantum information

Given two orthonormal bases in a d-dimensional Hilbert space, one may associate to each state its Kirkwood–Dirac (KD) quasi-probability distribution. KD-non-classical states – those for which the KD-distribution takes on negative and/or non-real values – have been shown to provide a quantum advantage in quantum metrology and information, raising the question of their identification. Under suitable conditions of incompatibility between the two bases, S. De Bièvre provided sharp lower bounds on the support uncertainty of states that guarantee their KD-non-classicality in [4] and [22]. In particular, when the bases are completely incompatible, a new notion introduced in this work, states whose support uncertainty is not equal to its minimal value d+1 are necessarily KD-non-classical. The implications of these general results for various commonly used bases, including the mutually unbiased ones, and their perturbations, are detailed.

In quantum optics, the notion of classical state is different than in the discrete value systems described above. In that case one requires the Glauber-Sudarshan P-function to be positive. Characterizing the classical states is a longstanding problem in this context as well. In [25], S. De Bièvre and collaborators establish an interferometric protocol allowing to determine a recently introduced nonclassicality measure, known as the quadrature coherence scale (QCS) [7]. A detailed study of the QCS of photon-added/subtracted states is provided in [26].

6.17 Linearly implicit high-order numerical methods for evolution problems

G. Dujardin and his collaborator derived in [13] a new class of numerical methods for the time integration of evolution equations set as Cauchy problems of ODEs or PDEs, in the research direction detailed in Section 3.3. The systematic design of these methods mixes the Runge–Kutta collocation formalism with collocation techniques, in such a way that the methods are linearly implicit and have high order. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods are expected to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so.

6.18 Numerical simulation of multispecies Bose–Einstein condensates

In [23], G. Dujardin, A. Nahas and I. Lacroix-Violet proposed a new numerical method for the simulation of multicomponent Bose–Einstein condensates in dimension 2. They implemented their method and demonstrated its efficiency compared to existing methods from the literature, in several physically relevant regimes (vortex nucleation, vortex sheets, giant holes, etc were obtained numerically). They verified numerically several theoretical results known for the minimizers in strong confinment regimes. They also supported numerically theoretical conjectures in other physically relevant contexts. In addition, they developped post-processing algorithms for the automatic detection of vortex structures (simple vortices, vortex sheets, etc), as well as for the numerical computation of indices.

6.19 Discrete quantum harmonic oscillator and Kravchuk transform

We consider in [21] 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.

7 Partnerships and cooperations

Participants: Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet, Marielle Simon.

7.1 International initiatives

Projet LISA IEA CNRS Lille-Santiago

Participants: André de Laire, Olivier Goubet.

Title: LISA

Partner Institution(s): Laboratoire Paul Painlevé, Lille, CNRS, and CMM, UMI CNRS, Santiago du Chili

Date/Duration: 2020-2022

Nature of the initiative: International Emerging Action (IEA) CNRS

Budget: 4000 €/year

Objective: Study of dispersive equations

7.2 International research visitors

7.2.1 Visits of international scientists

Claudio Muñoz

Status Researcher

Institution of origin: University of Chile

Country: Chile

Dates: Dec. 8-9, 2022

Context of the visit: projet LISA IEA CNRS Lille-Santiago

Mobility program/type of mobility: research stay

7.2.2 Visits to international teams

André de Laire

Visited institution: University of Birmingham

Country: United Kingdom

Dates: Oct. 6-12, 2022

Context of the visit: Research projet with Susana Gutiérrez

Mobility program/type of mobility: research stay

Guillaume Dujardin

Visited institution: University of Gothenburg (Chalmers)

Country: Sweden

Dates: Dec. 5-9, 2022

Context of the visit: Research projet with David Cohen and Andre Berg

Mobility program/type of mobility: research stay

Clément Erignoux

Visited institution: Instituto Superior Técnico

Country: Portugal

Dates: May 2-6, 2022

Context of the visit: Research projet with Patricia Gonçalves and Gabriel Nahum

Mobility program/type of mobility: research stay

Clément Erignoux

Visited institution: Cambridge University

Country: UK

Dates: May 16-18, 2022

Context of the visit: Research projet with Maria Bruna, Robert Jack and James Mason

Mobility program/type of mobility: research stay

7.3 European initiatives

Clément Erignoux and Marielle Simon are part of a franco-portuguese Pessoa project

- Title: "Kinetic theory, particle systems and their hydrodynamic limits".
- Grant 2022: 2400€

7.4 National initiatives

7.4.1 ANR MICMOV

Marielle Simon is the PI of the ANR MICMOV project

- Title: “Microscopic description of moving interfaces”
- Link to the website
- ANR Reference: ANR-19-CE40-0012
- Members: M. Simon (PI, Inria Lille), G. Barraquand (LPTENS Paris), O. Blondel (Université de Lyon), C. Cancès (Inria Lille), C. Erignoux (Inria Lille), M. Herda (Inria Lille), L. Zhao (Inria Lille)
- Total amount of the grant: 132 000 euros
- Duration: March 2020 – October 2024

7.4.2 LabEx CEMPI

Through their affiliation to the Laboratoire Paul Painlevé of Université de Lille, PARADYSE team members benefit from the support of the Labex CEMPI. In addition, the LabEx CEMPI is funding the postdoc of Quentin Chauleur in the team, in an interdisciplinary initiative between PhLAM and LPP.

Title: Centre Européen pour les Mathématiques, la Physique et leurs Interactions

Partners: Laboratoire Paul Painlevé (LPP) and Laser Physics department (PhLAM), Université de Lille

ANR reference: 11-LABX-0007

Duration: February 2012 - December 2024 (the project has been renewed in 2019)

Budget: 6 960 395 euros

Coordinator: Emmanuel Fricain (LPP, Université de Lille)

The "Laboratoire d’Excellence" CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions), a project of the Laboratoire de mathématiques Paul Painlevé (LPP) and the laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), was created in the context of the "Programme d’Investissements d’Avenir" in February 2012. The association Painlevé-PhLAM creates in Lille a research unit for fundamental and applied research and for training and technological development that covers a wide spectrum of knowledge stretching from pure and applied mathematics to experimental and applied physics. The CEMPI research is at the interface between mathematics and physics. It is concerned with key problems coming from the study of complex behaviors in cold atoms physics and nonlinear optics, in particular fiber optics. It deals with fields of mathematics such as algebraic geometry, modular forms, operator algebras, harmonic analysis, and quantum groups, that have promising interactions with several branches of theoretical physics.

7.5 Regional initiatives

The PARADYSE project-team was granted the SIMPAPH “Action de Développement Technologique”, which allowed to hire Alexandre Roget as an engineer in the project-team from 2019 to 2021. We obtained extensions of the contract of A. Roget, which was a team-member in 2022 as well. This ADT SIMPAPH’s goals were originally threefold:

- develop a software for the simulation of the propagation of light in *multimode* optical fibers for the optical physics community;
- simulate large systems of random particles such as two-dimensional constrained lattice gases;
- simulate the dynamics of 3D Bose–Einstein condensates.

8 Dissemination

Participants: Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet, Marielle Simon.

8.1 Promoting scientific activities

8.1.1 Scientific events: organisation

Workshop "Asymetry in interacting particle systems", held at INRIA Lille on October 3-5 2022.

- Organizers: G. Barraquand, O. Blondel, C. Erignoux, P. Illien, M. Simon

"Journée de rentrée de l'équipe probas-stats", held at Lille university on September 22 2022.

- Organizers: C. Baey, S. Dabo, D. Dereudre, C. Duval, C. Erignoux, B. Thiam

"Journée Analyse Appliquée Hauts-de France" 10 novembre 2022.

- Organizers: C. Calgaro, O. Goubet, M. Herda

"Journée des Doctorants en Mathématiques de la région Hauts-de-France", held at Université Polytechnique Hauts-de-France on September 9, 2022.

- Organizers: S. Biard, M. Davila, A. de Laire, A. El Mazouni, R. Ernst, B. Testud

8.1.2 Journal

Member of the editorial boards: S. De Bièvre is associate editor of the Journal of Mathematical Physics (since January 2019). O. Goubet is the editor in chief of the North-Western European Journal of Mathematics. O. Goubet is associate editor of ANONA (Advances in Nonlinear Analysis) O. Goubet is associate editor of the Journal of Math. Study.

Reviewer - reviewing activities: All permanent members of the PARADYSE team work as referees for many of the main scientific publications in analysis, probability and statistical physics, depending on their respective fields of expertise.

8.1.3 Invited talks

All PARADYSE team members take active part in numerous scientific conferences, workshops and seminars, and in particular give frequent talks both in France and abroad.

8.1.4 Research administration

- S. De Bièvre and A. de Laire are both members of the "Conseil de Laboratoire Paul Painlevé" at Université de Lille.
- S. De Bièvre is member of the executive committee of the LabEx CEMPI.
- A. de Laire is member of the "Fédération de Recherche Mathématique des Hauts-de-France".
- G. Dujardin is a member of the Executive Committee of the CPER Wavetech.
- O. Goubet is member of the "conseil de département de mathématiques" at Université de Lille.
- O. Goubet is member of "bureau du HUB numérique" de I-Site U-Lille
- O. Goubet is the president of SMAI (Société de Mathématiques Appliquées et Industrielles)
- C. Erignoux is a member of the LNE Inria research center's "Comité de Centre".

8.2 Teaching - Supervision - Juries

8.2.1 Teaching

The PARADYSE team teaches various undergraduate level courses in several partner universities and *Grandes Écoles*. We only make explicit mention here of the Master courses (level M1-M2) and the doctoral courses.

- Master: O. Goubet and A. de Laire, "Modélisation et Approximation par Différences Finies", M1 (Université de Lille, 54h).
- Master: O. Goubet, "Etude de problèmes elliptiques et paraboliques", M1 (Université de Lille, 24h).
- Master: A. de Laire, "Analyse numérique pour les EDP", M1 (Université de Lille, 60h).
- Master: C. Erignoux and L. Xu, "Advanced probabilites", M2 (Université de Lille, 24h).
- Master : G. Dujardin, "Condensats de Bose–Einstein : théorie et simulation numérique" (Université de Lille, 24h).
- Doctoral School: M. Simon, "Harmonic chain of oscillators with random flips of velocities" (GSSI Institute, L'Aquila, Italy, 12h).
- Doctoral School: S. De Bièvre, "Quantum information" (Université de Lille, 24h).

S. De Bièvre has represented (2018-2021) the department of Mathematics in the organization of the newly created Master of Data Science of EC Lille, Université de Lille and IMT. This role has since been taken over by O. Goubet.

8.2.2 Supervision

- C. Erignoux and M. Simon supervised Adel Assakaf, M2 - Maths internship, "Effet de dynamiques de bord sur le FEP". (10 weeks)
- C. Erignoux supervised Hugo Dorfsman, M1 - Calcul scientifique internship, "Comportement microscopique et macroscopique du SSEP en interaction faible avec des reservoirs". (10 weeks)
- C. Erignoux supervised Fael Rebei, L3 - ENS internship, "Limite hydrodynamique et grandes deviations pour le SSEP". (6 weeks)
- S. De Bièvre supervised C. Langrenez, M2-maths internship, "KD nonclassicality." (12 weeks)
- S. De Bièvre is supervising V. Niaussat, M2-maths internship, "Quantum random sampling." (12 weeks)
- S. De Bièvre is supervising the PhD thesis of C. Langrenez on "KD nonclassicality". 2022-2024.
- G. Dujardin supervised Charbel Ghosn, M2-maths internship, "High order numerical methods for high dimensional systems of ODEs". (12 weeks)
- G. Dujardin supervised (with I. Lacroix-Violet) the PhD thesis [18] of Anthony Nahas, entitled "Simulation numérique de condensats de Bose–Einstein", which was successfully defended in October 2022.
- A. de Laire and O. Goubet supervised Erwan Le Quiniou, M2 - Maths internship, "Solitons for a quasilinear Gross-Pitaevskii equation". (12 weeks)
- A. de Laire and O. Goubet are supervising the PhD thesis of Erwan Le Quiniou, "Solitons for the Landau–Lifshitz equation". 2022-2025.

8.2.3 Juries

- G. Dujardin served as reviewer for the PhD thesis of Martino Lovisetto (University of Nice, May 10th, 2022), entitled "Theoretical and numerical study of the Schrödinger-Newton equation with application to nonlinear optics and experimental observation of violent relaxation", supervised by Dider Clamond and Bruno Marcos.
- G. Dujardin served as reviewer for the PhD thesis of Grégoire Barrué (ÉNS de Rennes, July 7th, 2022), entitled "Approximation diffusion pour des équations dispersives", supervised by Arnaud Debussche and Anne De Bouard.

8.3 Popularization

8.3.1 Articles and contents

A. de Laire made a contribution to the "Book Summaries" section of the magazine Matapli N°127 by SMAI (Society of Applied and Industrial Mathematics).

8.3.2 Interventions

A. de Laire participed to the meeting Declics 2022 (Dialogue Between Researchers and High School Students to Engage them in the Construction of Knowledge) at Lycée Faidherbe, Lille

9 Scientific production

9.1 Major publications

[1] R. Ahmed, C. Bernardin, P. Gonçalves and M. Simon. 'A Microscopic Derivation of Coupled SPDE's with a KPZ Flavor'. In: *Annales de l'Institut Henri Poincaré* 58.2 (2022). DOI: 10.1214/21-AIHP1196. URL: https://hal.archives-ouvertes.fr/hal-02307963.

[2] C. Besse, S. Descombes, G. Dujardin and I. Lacroix-Violet. 'Energy preserving methods for nonlinear Schrödinger equations'. In: *IMA Journal of Numerical Analysis* 41.1 (Jan. 2021), pp. 618–653. DOI: 10.1093/imanum/drz067. URL: https://hal.archives-ouvertes.fr/hal-01951527.

[3] O. Blondel, C. Erignoux and M. Simon. 'Stefan problem for a non-ergodic facilitated exclusion process'. In: *Probability and Mathematical Physics* 2.1 (2021). DOI: 10.2140/pmp.2021.2.127. URL: https://hal.inria.fr/hal-02482922.

[4] S. De Bièvre. 'Complete Incompatibility, Support Uncertainty, and Kirkwood-Dirac Nonclassicality'. In: *Physical Review Letters* (2021). DOI: 10.1103/PhysRevLett.127.190404. URL: https://hal.archives-ouvertes.fr/hal-03464950.

[5] S. Dumont, O. Goubet and Y. Mammeri. 'Decay of solutions to one dimensional nonlinear Schrödinger equations with white noise dispersion'. In: *Discrete and Continuous Dynamical Systems - Series S* 14.8 (2021), pp. 2877–2891. DOI: 10.3934/dcdss.2020456. URL: https://hal.archives-ouvertes.fr/hal-02944262.

[6] C. Erignoux. 'Hydrodynamic limit for an active exclusion process'. In: *Mémoires de la Société Mathématique de France* 169 (May 2021). URL: https://hal.archives-ouvertes.fr/hal-01350532.

[7] A. Hertz and S. de Bièvre. 'Quadrature coherence scale driven fast decoherence of bosonic quantum field states'. In: *Physical Review Letters* (5th Mar. 2020). DOI: 10.1103/PhysRevLett.124.090402. URL: https://hal.archives-ouvertes.fr/hal-02394344.

[8] A. de Laire and S. López-Martínez. 'Existence and decay of traveling waves for the nonlocal Gross-Pitaevskii equation'. In: *Communications in Partial Differential Equations* 47.9 (2022), pp. 1732–1794. DOI: 10.1080/03605302.2022.2070853. URL: https://hal.archives-ouvertes.fr/hal-03422447.

9.2 Publications of the year

International journals

[9] M. Abidi, V. Martin and O. Goubet. 'Crank-Nicolson scheme for a logarithmic Schrödinger equation'. In: *North-Western European Journal of Mathematics* (2022). URL: https://hal.science/hal-03906217.

[10] R. Ahmed, C. Bernardin, P. Gonçalves and M. Simon. 'A Microscopic Derivation of Coupled SPDE's with a KPZ Flavor'. In: *Annales de l'Institut Henri Poincaré* 58.2 (2022). DOI: 10.1214/21-AIHP1196. URL: https://hal.science/hal-02307963.

[11] A. Armaroli, G. Dujardin, A. Kudlinski, A. Mussot, S. Trillo, S. De Bièvre and M. Conforti. 'Stochastic modulational instability in the nonlinear Schrödinger equation with colored random dispersion'. In: *Physical Review A* (7th Jan. 2022). DOI: 10.1103/PhysRevA.105.013511. URL: https://hal.science/hal-03456422.

[12] G. Delvoye, O. Goubet and F. Paccaut. 'Comparison principles and applications to mathematical modelling of vegetal meta-communities'. In: *Mathematics in Engineering* 4.5 (2022), pp. 1–17. DOI: 10.3934/mine.2022035. URL: https://hal.science/hal-03588659.

[13] G. Dujardin and I. Lacroix-Violet. 'High order linearly implicit methods for evolution equations: How to solve an ODE by inverting only linear systems'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* (25th Apr. 2022). DOI: 10.1051/m2an/2022018. URL: https://hal.inria.fr/hal-02361814.

[14] O. Goubet and I. Manoubi. 'Standing waves for semilinear Schrödinger equations with discontinuous dispersion'. In: *Rendiconti del Circolo Matematico di Palermo* 71.3 (Dec. 2022), pp. 1159–1171. DOI: 10.1007/s12215-022-00782-3. URL: https://hal.science/hal-03906178.

[15] A. de Laire. 'Recent results for the Landau-Lifshitz equation'. In: *SeMA Journal: Boletin de la Sociedad Española de Matemática Aplicada* 79.2 (2022), pp. 253–295. DOI: 10.1007/s40324-021-00254-1. URL: https://hal.science/hal-03209958.

[16] A. de Laire and S. López-Martínez. 'Existence and decay of traveling waves for the nonlocal Gross-Pitaevskii equation'. In: *Communications in Partial Differential Equations* 47.9 (2022), pp. 1732–1794. DOI: 10.1080/03605302.2022.2070853. URL: https://hal.science/hal-03422447.

[17] L. Zhao. 'Long-time behavior of SSEP with slow boundary'. In: *Statistics and Probability Letters* (2022). DOI: 10.1016/j.spl.2022.109452. URL: https://hal.science/hal-03510977.

Doctoral dissertations and habilitation theses

[18] A. Nahas. 'Numerical simulation of Bose-Einstein condensates'. Université de Lille, 11th Oct. 2022. URL: https://hal.science/tel-03992001.

Reports & preprints

[19] A. Armaroli, G. Dujardin, A. Kudlinski, A. Mussot, S. De Bièvre and M. Conforti. *Modulational instability in randomly dispersion-managed fiber links.* 22nd Dec. 2022. URL: https://hal.science/hal-03911304.

[20] A. Bouley, C. Erignoux and C. Landim. *Steady state large deviations for one-dimensional, symmetric exclusion processes in weak contact with reservoirs.* 13th Dec. 2022. URL: https://hal.science/hal-03897408.

[21] Q. Chauleur and E. Faou. *Discrete quantum harmonic oscillator and kravchuk transform.* 5th Dec. 2022. URL: https://hal.science/hal-03885282.

[22] S. De Bièvre. *Relating incompatibility, noncommutativity, uncertainty and Kirkwood-Dirac nonclassicality.* 22nd Dec. 2022. URL: https://hal.science/hal-03911322.

[23] G. Dujardin, I. Lacroix-Violet and A. Nahas. *A numerical study of vortex nucleation in 2D rotating Bose-Einstein condensates.* 3rd Nov. 2022. URL: https://hal.science/hal-03818063.

[24] C. Erignoux, M. Simon and L. Zhao. *Mapping hydrodynamics for the facilitated exclusion and zero-range processes*. 8th Dec. 2022. URL: https://hal.science/hal-03889620.

[25] C. Griffet, M. Arnhem, S. De Bièvre and N. J. Cerf. *Interferometric measurement of the quadrature coherence scale using two replicas of a quantum optical state*. 22nd Dec. 2022. URL: https://hal.science/hal-03911306.

[26] A. Hertz and S. De Bièvre. *Nonclassicality gain/loss through photon-addition/subtraction on multi-mode Gaussian states*. 22nd Dec. 2022. URL: https://hal.science/hal-03911324.

[27] A. de Laire, P. Gravejat and D. Smets. *Minimizing travelling waves for the Gross-Pitaevskii equation on* $\mathbb{R}\times\mathbb{T}$. 19th Jan. 2022. URL: https://hal.science/hal-03586112.

[28] L. Xu and L. Zhao. *Equilibrium perturbations for stochastic interacting systems*. 4th June 2022. URL: https://hal.science/hal-03688419.

[29] X. Xue and L. Zhao. *Moderate deviations for the current and tagged particle in symmetric simple exclusion processes*. 25th Mar. 2022. URL: https://hal.science/hal-03619413.

[30] X. Xue and L. Zhao. *The voter model with a slow membrane*. 25th Mar. 2022. URL: https://hal.science/hal-03619411.

9.3 Cited publications

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