RESEARCH CENTRE

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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

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Keywords

Computer sciences and digital sciences

A6.1.1. – Continuous Modeling (PDE, ODE)

A6.1.2. – Stochastic Modeling

A6.1.4. – Multiscale modeling

A6.2.1. – Numerical analysis of PDE and ODE

A6.2.3. – Probabilistic methods

A6.5. – Mathematical modeling for physical sciences

Other research topics and application domains

B3.6. – Ecology

B3.6.1. – Biodiversity

B5.3. – Nanotechnology

B5.5. – Materials

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, Starting Faculty Position]
- Marielle Simon [Inria, Researcher, HDR]

Faculty Members

- Stephan De Bièvre [Université de Lille, Professor, HDR]
- Olivier Goubet [Université de Lille, Professor, HDR]
- André de Laire [Université de Lille, Associate Professor, HDR]

Post-Doctoral Fellows

- Salvador López Martínez [Inria, until Aug 2021]
- Linjie Zhao [Inria]

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- Alexandre Roget [Inria, Engineer]

Interns and Apprentices

- Hugues Moyart [Ecole normale supérieure Paris-Saclay, from Apr 2021 until Jul 2021]

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 [39] and solitons in magnetic media are of particular interest as a mechanism for data storage or information transfer [41]. 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 [28, 35]. 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 atoms (precisely chains of oscillators) with different local microscopic defects. We apply our recent techniques to understand how anomalous (in particular fractional) diffusive systems interact with the boundaries. For instance, the powerful tool given by Wigner functions that we already used has been successfully applied to the derivation of anomalous behaviors in open systems (for instance in [34]). The next step consists in developing an extension of that tool to deal with bounded systems provided with fixed boundaries. We also intend to derive anomalous diffusion by adding long-range interactions to diffusive models. There are very few rigorous results in this direction.

Finally, we aim at obtaining from a microscopic description the fractional porous medium equation (FPM), a non-linear variation of the fractional diffusion equation, involving the fractional Laplacian instead of the usual one. Its rigorous study carries many mathematical difficulties in treating at the same time the non-linearity and fractional diffusion. We want 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 [33], as well as energy-preserving methods for hamiltonian problems [2].

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 [23]. 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 [31]. 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 trying to work 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 results

Participants: Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet, Salvador López-Martínez, Marielle Simon, Linjie Zhao.

Some of the results presented below overlap several of the main research themes presented in section 3. However, results presented in paragraphs 5.1-5.5 are mainly concerned with research axis 3.1, whereas paragraphs 5.6-5.13 mostly concern axis 3.2. Paragraphs 5.14-5.16 concern numerics-oriented results, and are encompassed in axis 3.3.

5.1 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 [26] 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 by A. de Laire and P. Mennuni in [38].

5.2 The cubic Schrödinger regime of the Landau–Lifshitz equation with a strong easy-axis anisotropy

It is well-known that the dynamics of biaxial ferromagnets with a strong easy-axis anisotropy is essentially governed by the cubic Schrödinger equation. A. de Laire and P. Gravejat provided in [7] a rigorous justification to this observation, continuing with the work started in [37]. More precisely, they showed the convergence of the solutions to the Landau–Lifshitz equation for biaxial ferromagnets towards the solutions to the cubic Schrödinger equation in the regime of an easy-axis anisotropy. This result holds for solutions to the Landau–Lifshitz equation in high-order Sobolev spaces. By introducing high-order energy quantities with good symmetrization properties, they derived the convergence from the consistency of the Landau–Lifshitz equation with the sine-Gordon equation by using well-tailored energy estimates.

In this regime, they additionally classified the one-dimensional solitons of the Landau–Lifshitz equation and quantified their convergence towards the solitons of the one-dimensional cubic Schrödinger equation.

5.3 Recent results for the Landau–Lifshitz equation

In [16], 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.

5.4 Modulational instability in random fibers and stochastic Schrödinger equations

The team achieved an analysis of modulational instability in optical fibers with randomly kicked normal dispersion in [12] as well as with a normal dispersion perturbed with a coloured noise in [20]. S. De Bièvre, G. Dujardin and collaborators developed and analyzed in [12] a physically realistic model of optical fibers with randomly kicked normal dispersion. They analyzed the modulational instability generated in such fibers through the associated gain, both theoretically and numerically. In [20] the effect of coloured noise on the modulational instability was investigated in order to assess whether it can produce a larger modulational instability. We found that generally this is not the case. This research was carried out with physicists from the PhLAM laboratory in Lille.

Another important result of the team in this direction is [5], where O. Goubet et al. established the decay rate of solutions to a non-linear Schrödinger equation with stochastic modulation. The result of [5] is the first result concerning the long time behavior of solutions for non-linear Schrödinger equations with white noise modulation. The final result is that the decay rate towards equilibrium for the non-linear Schödinger equation is twice slower with white noise modulation than in the deterministic case.

5.5 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]. 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.

5.6 Hydrodynamic limit for a chain with thermal and mechanical boundary forces

In a collaboration with T. Komorowski and S. Olla [15], M. Simon proved the hydrodynamic limit for an harmonic chain with a random exchange of momentum that conserves the kinetic energy but not the momentum. The system is open and subject to two thermostats at the boundaries and to external tension. Under a diffusive scaling of space-time, the authors proved that the empirical profiles of the two locally conserved quantities, the volume stretch and the energy, converge to the solution of a non-linear diffusive system of conservative partial differential equations.

5.7 Stefan problem for a non-ergodic facilitated exclusion process

In [3], O. Blondel, C. Erignoux and M. Simon investigated the general hydrodynamics for the *facilitated exclusion process* whose supercritical phase's hydrodynamics had been previously investigated in [31]. This process is similar to the celebrated *symmetric simple exclusion process*, except that a particle is only allowed to jump to a neighboring site if its other neighbor is occupied by a particle. This hard constraint on the particle's motion has a number of consequences on the microscopic and macroscopic behavior of the system. In particular, under the critical density $\rho_c = 1/2$, the system quickly freezes out and particles stop moving.

The purpose of this work was to investigate the macroscopic invasion of the frozen phase by the ergodic phase, and the authors were able to prove that starting from a profile with both supercritical and subcritical regions, the hydrodynamics for the facilitated exclusion process is given by a Stefan problem: the diffusive supercritical phase progressively invades the subcritical phase via flat interfaces, until either one of the phases disappears.

5.8 Hydrodynamic limit for an active exclusion process

In [6], C. Erignoux investigated the scaling limit of an active exclusion process, which is a microscopic dynamics put forward to model self-organization as observed in various animal species (e.g. school of fish, flock of birds). Active models can exhibit rich phenomenology, such as Motility Induced Phase Separation (MIPS), and the formation of spontaneous collective dynamics, as in Viszek's celebrated model. However, because of the exclusion rule between particles (two particles cannot occupy the same site of the lattice), the model is non-gradient, resulting in a complex, non-explicit, cross-diffusive hydrodynamic equation.

In [24], C. Erignoux builds on previous work [6], [36] and explores various aspects of modeling individual-based active matter models. In particular, [24] describes general aspects of the mathematical theory of hydrodynamic limits, and basic principles to conjecture the hydrodynamic equation given the underlying microscopic system. One of the objectives of the article is to provide members of the physics community interested in active matter with tools to navigate and use mathematical theory for hydrodynamic limits. The article also conjectures the so-called non-equilibrium fluctuating hydrodynamics for active lattice gases. The long term goal is to derive in a mathematically satisfying way the two phenomena described above (MIPS and collective dynamics), for which the hydrodynamic equation yields some information, but the fluctuating hydrodynamics is necessary to fully understand the underlying mechanisms.

5.9 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 [30] 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 [27], 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 [32], where the SSEP with strong boundary interactions was considered. In [27], 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 [32], with different boundary conditions corresponding to the different scales of boundary interaction.

5.10 Asymmetric attractive zero-range process with destruction at the origin

In [25], C. Erignoux, M. Simon and L. Zhao considered the effect of boundary interactions on the one-dimensional asymmetric zero-range process on the full line. More precisely, particles are destroyed at the origin of the system at rate αN^{β}, and they showed that depending on the value of β, different behaviors can be derived for the macroscopic limit of the system: for negative β, particle destructions do not have a macroscopic effect, and the system macroscopically behaves as the asymmetric zero-range process without destruction. For $\beta = 0$, a proportion (depending on α) of particles is destroyed, and the right-hand side $x > 0$ behaves as a zero-range process with a boundary condition at the origin which is a function of the density on the left of the origin. For $\beta > 0$, finally, most particles are destroyed while they go through the origin, so that no mass crosses through the origin at the macroscopic level.

5.11 SSEP with a slow bond and site boundary

In [18], L. Zhao and his coauthor considered the one-dimensional symmetric simple exclusion process with a slow bond. In this model, particles cross each bond at rate N^2, except one particular bond, the slow bond, where the rate is N. Above, N is the scaling parameter. This model has been considered in the context of hydrodynamic limits, fluctuations and large deviations. They investigated moderate deviations from hydrodynamics and obtained a moderate deviations principle.

5.12 Non-equilibrium fluctuations of the weakly asymmetric normalized binary contact path process

In [19], X. Xue and L. Zhao further investigated the problem studied in [40], where the authors proved a law of large numbers for the empirical measure of the weakly asymmetric normalized binary contact path process on $\mathbb{Z}^d$, $d \geq 3$, and then conjectured that a central limit theorem should hold under a non-equilibrium initial condition. They proved that the said conjecture is true when the dimension d of the underlying lattice and the infection rate λ of the process are sufficiently large.

5.13 Mathematical modeling for ecology

The team had an important contribution to the multi-scale ecosystem modeling. O. Goubet and his collaborators computed in [22] 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.

In [21] O. Goubet and his collaboraters addressed the initial value problem for a shallow water system of equations with a Coriolis force term. This result is non-standard due to the Coriolis term.

5.14 Numerical integration of the stochastic Manakov system

The stochastic Manakov system is a dispersive non-linear system of PDEs that models the propagation of light in an optical fiber with randomly varying birefringence.

In [29], G. Dujardin and his collaborators introduced a linearly implicit scheme for the time integration of the stochastic Manakov system, that they analyzed and compared to the existing methods from the literature. In particular, they proved that the strong order of the numerical approximation is $1/2$ if the non-linear term in the system is globally Lipschitz-continuous. They also proved that this numerical method converges with order $1/2$ in probability and with order $1/2^-$ almost surely, in the case of the cubic non-linear coupling which is relevant in optical fibers. They also proposed a modification of their method to obtain a mass-preserving scheme.

In [8], G. Dujardin and his collaborators developed, analyzed and implemented a numerical method based on the Lie–Trotter formula for the integration of the stochastic Manakov system. In particular, they proved that the strong order of the numerical approximation is $1/2$ if the non-linear term in the system is globally Lipschitz. They also proved that this splitting scheme converges with order $1/2$ in probability, and converges almost surely with order $1/2^-$ as well. They provided numerical experiments to compare the efficiency of this scheme with existing methods from the literature, and they investigated numerically the possible blow-up in finite time of solutions to this SPDE system.

5.15 Linearly implicit high-order numerical methods for evolution problems

G. Dujardin and his collaborator derived in [23] 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.

5.16 Energy-preserving methods for non-linear Schrödinger equations

G. Dujardin and his co-authors revisited and extended relaxation methods for non-linear Schrödinger equations (NLS). The classical relaxation method for NLS is a mass- and energy-preserving method. Moreover, it is only linearly implicit. A first proof of the second-order accuracy was achieved in [2]. Moreover, the method was extended to enable to treat non-cubic non-linearities, non-local non-linearities, as well as rotation terms. The resulting methods are still mass-preserving and energy-preserving. Moreover, they are shown to have second-order accuracy numerically. These new methods are compared with fully implicit, mass- and energy-preserving methods of Crank and Nicolson.

6 Partnerships and cooperations

Participants: André de Laire, Olivier Goubet, Marielle Simon.

6.1 International initiatives

André de Laire and Olivier Goubet got a support from CNRS to develop a collaboration on the study of travelling wave solutions with the CMM of Santiago in Chile (with the team of Claudio Muñoz).

- Title: "LISA (LIlle-Santiago)"
- Members: A. de Laire, O. Goubet
- Total amount of the grant: 4 000 euros/year
- Duration: 2021-2022

6.2 European initiatives

Marielle Simon is the PI of the MATMOVIN project cofunded by the European Union together with the "Fonds de Développement Régional".

- Title: "Description microscopique des transitions de phase et interfaces mobiles : avancées mathématiques"
- Type: Post-doc grant of 2 years
- Duration: September 2020 – August 2022
- Research group: M. Simon (PI, Inria Lille), A. Roget (Inria Lille), L. Zhao (Inria Lille)

6.3 National initiatives

6.3.1 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

6.3.2 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.

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.

6.3.3 ADT SIMPAPH

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. 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.

6.4 Regional initiatives

Olivier Goubet (PI) got a support from Région Hauts-de-France (grant STIMULE STIR) to initiate a research program involving applied mathematicians in Amiens, Calais, Lille and Valenciennes.

- Title: "Super QUantum fluids and shAllow Water equations"
- Members: C. Calgaro, O. Goubet, T. Rey (U-Lille), J.-P. Chehab, V. Desveaux, Y. Mammeri, V. Martin, H. Le Meur (UPJV), A. Benoit, C. Bourel, C. Rosier, L. Rosier (ULCO), E. Creusé (UPHF)
- Total amount of the grant: 14 400 euros
- Duration: November 2021–April 2023

7 Dissemination

Participants: Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet, Salvador López-Martínez, Marielle Simon, Linjie Zhao.

7.1 Promoting scientific activities

7.1.1 Scientific events: organisation

- A. de Laire co-organized the “Journée des Doctorants en Mathématiques de la région Hauts-de-France”, on October 1st, 2021, held at the Universtié Picardie Jules Verne, Amiens. Event’s webpage.
- C. Erignoux co-organized the “Journée de rentrée du Laboratoire Paul Painlevé”, on November 25th, 2021, held at "La Piscine de Roubaix". Event’s webpage.
- O. Goubet co-organized the "Conférence en l’honneur de Serge Nicaise", from November 2nd to 5th, 2021, held at the University of Valenciennes. Event’s webpage.
- M. Simon co-organized the "Online junior conference on random graphs and interacting particle systems", from September 6th to 10th, 2021, held online. Event’s webpage.

7.1.2 Journal

Member of the editorial boards: O. Goubet was the guest co-editor of the special issue of Discrete & Continuous Dynamical Systems - A (DCDS-A) Vol. 14, no. 8 of August 2021.

S. De Bièvre is associate editor of the Journal of Mathematical Physics (since January 2019).

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.

7.1.3 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.

7.1.4 Leadership within the scientific community

O. Goubet is the president of the Société de Mathématiques Appliquées et Industrielles (SMAI).

7.1.5 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.
- C. Erignoux is a member of the LNE Inria research center’s "Comité de Centre".
- M. Simon is member of the CNU (Conseil National des Universités), Section 26.

7.2 Teaching - Supervision - Juries

7.2.1 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).
- 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 represents (since 2018) the department of Mathematics in the organization of the newly created Master of Data Science of EC Lille, Université de Lille and IMT.

7.2.2 Supervision

- A. de Laire supervised the post-doc of S. López-Martínez, which ended in August 2021.
- G. Dujardin co-advises (with I. Lacroix-Violet) the PhD thesis of Anthony Nahas. Title: "Simulation of rotating multi-species Bose–Einstein condensates".
- C. Erignoux and M. Simon co-supervise the post-doc of Linjie Zhao.
- C. Erignoux supervised the first year of master's internship of Hugues Moyart from March to August 2021. Title: "Duality and influence of thermostats on the macroscopic limit of the symmetric simple exclusion process".
- O. Goubet co-advises (with B. Alouini, B. Dehman and V. Martin) the PhD thesis of Mariem Abidi. Title: "Logarithmic Schrödinger equations".
- O. Goubet co-advises (with V. Desveaux) the PhD thesis of Alice Masset. Title: "Shallow water equations with Coriolis forcing and temperature".
- O. Goubet co-advises (with G. Decocq) the PhD thesis of Clément Carlier. Title: "Models for metapopulations in forest ecology".
- M. Simon co-advises (with P. Gonçalves) the PhD thesis of Gabriel Nahum. Title: "Non-linear Problems in Interacting Particle Systems".

7.2.3 Juries

- A. de Laire was referee and member of the jury of the PhD thesis of J. Alhelou (Université de Toulouse III, November 2021). Title: "Mathematical and numerical analysis for a Gross–Clark–Schrödinger system".
- A. de Laire was referee and member of the jury of the PhD thesis of X. Yuan (École polytechnique, Paris, June 2021). Title: "Long time dynamics for non-linear wave-type equations with or without damping".
- O. Goubet was the referee and member of the jury of the PhD thesis of S. Bahrouni (University of Monastir, Tunisia, July 2021). Title: "Orlicz–Sobolev fractional spaces and applications to non-linear problems".

- O. Goubet was president of the jury of the PhD thesis of M. Handa (Unheld iverstié Picardie Jules Verne, Amiens, July 2021). Title: "Modelisation, optimisation and simulation of power distribution networks".
- O. Goubet was member of the jury of the Habilitation of B. Alouini (University of Monastir, Tunisia, July 2021). Title: "Study of non-linear anisotropic Bose–Einstein and Shrödinger equations".
- M. Simon was member of the jury of the PhD thesis of B. Dagallier (École polytechnique, Paris, September 2021). Title: "Large deviations in interacting particle systems: out of equilibrium correlations and interface dynamics".
- M. Simon was member of the jury of the PhD thesis of A. Ertul (Université Lyon 1, December 2021). Title: "Diffusion and relaxation for particle systems with kinetic constraints".
- M. Simon was member of the jury of the PhD thesis of A. Hannani (Université PSL Dauphine, Paris, December 2021). Title: "Random perturbation of certain interacting particle systems related to quantum mechanics".

7.3 Popularization

A. de Laire participated in Declics 2021, a scientific speed meeting with high school students at Lycée Faidherbe, on December 7th 2021, Lille.

S. De Bièvre published a series of three articles in Images des Mathématiques on quantum cryptography.

8 Scientific production

8.1 Major publications

[1] C. Bernardin, P. Gonçalves, M. Jara and M. Simon. 'Interpolation process between standard diffusion and fractional diffusion'. In: *Annales de l'Institut Henri Poincaré (B) Probabilités et Statistiques* 54.3 (2018), pp. 1731–1757. DOI: 10.1214/17-AIHP853. URL: https://hal.archives-ouvertes.fr/hal-01348503.

[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. de Laire and P. Gravejat. 'The cubic Schrödinger regime of the Landau-Lifshitz equation with a strong easy-axis anisotropy'. In: *Revista Matemática Iberoamericana* 37.1 (2021), pp. 95–128. DOI: 10.4171/rmi/1202. URL: https://hal.archives-ouvertes.fr/hal-01954762.

8.2 Publications of the year

International journals

[8] A. Berg, D. Cohen and G. Dujardin. 'Lie-Trotter Splitting for the Nonlinear Stochastic Manakov System'. In: *Journal of Scientific Computing* 88.6 (22nd May 2021). DOI: 10.1007/s10915-021-01514-y. URL: https://hal.inria.fr/hal-02975684.

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[10] 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.

[11] 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.

[12] G. Dujardin, A. Armaroli, S. R. Nodari, A. Mussot, A. Kudlinski, S. Trillo, M. Conforti and S. De Bièvre. 'Modulational instability in optical fibers with randomly-kicked normal dispersion'. In: *Physical Review A* 103.5 (24th May 2021), p. 053521. DOI: 10.1103/PhysRevA.103.053521. URL: https://hal.archives-ouvertes.fr/hal-03157350.

[13] 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.

[14] 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.

[15] T. Komorowski, S. Olla and M. Simon. 'Hydrodynamic limit for a chain with thermal and mechanical boundary forces'. In: *Electronic Journal of Probability* 26 (2021). DOI: 10.1214/21-EJP581. URL: https://hal.inria.fr/hal-02538469.

[16] A. de Laire. 'Recent results for the Landau-Lifshitz equation'. In: *SeMA Journal: Boletin de la Sociedad Española de Matemática Aplicada* (2021). DOI: 10.1007/s40324-021-00254-1. URL: https://hal.archives-ouvertes.fr/hal-03209958.

[17] A. de Laire and P. Gravejat. 'The cubic Schrödinger regime of the Landau-Lifshitz equation with a strong easy-axis anisotropy'. In: *Revista Matemática Iberoamericana* 37.1 (2021), pp. 95–128. DOI: 10.4171/rmi/1202. URL: https://hal.archives-ouvertes.fr/hal-01954762.

[18] X. Xue and L. Zhao. 'Moderate Deviations for the SSEP with a Slow Bond'. In: *Journal of Statistical Physics* (Feb. 2021). URL: https://hal.archives-ouvertes.fr/hal-03145320.

[19] X. Xue and L. Zhao. 'Non-equilibrium Fluctuations of the Weakly Asymmetric Normalized Binary Contact Path Process'. In: *Stochastic Processes and their Applications* (2021). URL: https://hal.archives-ouvertes.fr/hal-03103489.

Reports & preprints

[20] A. Armaroli, G. Dujardin, A. Kudlinski, A. Mussot, S. Trillo, S. De Bièvre and M. Conforti. *Stochastic modulational instability in the nonlinear Schr\"odinger equation with colored random dispersion*. 30th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03456422.

[21] N. Bedjaoui, V. Desveaux, O. Goubet and A. Masset. *Initial value problem for one-dimensional rotating shallow water equations*. 8th Mar. 2021. URL: https://hal.archives-ouvertes.fr/hal-03162689.

[22] G. Delvoye, O. Goubet and F. Paccaut. *Comparison principles and applications to mathematical modelling of vegetal meta-communities*. 16th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03431483.

[23] G. Dujardin and I. Lacroix-Violet. *High order linearly implicit methods for evolution equations: How to solve an ODE by inverting only linear systems*. 17th Nov. 2021. URL: https://hal.inria.fr/hal-02361814.

[24] C. Erignoux. *On the hydrodynamics of active matter models on a lattice*. 16th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03431146.

[25] C. Erignoux, L. Zhao and M. Simon. *Asymmetric attractive zero-range processes with particle destruction at the origin*. 16th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03431141.

[26] A. de Laire and S. López-Martínez. *Existence and decay of traveling waves for the nonlocal Gross-Pitaevskii equation*. 9th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03422447.

[27] C. Landim, A. Bouley and C. Erignoux. *Steady state large deviations for one-dimensional, symmetric exclusion processes in weak contact with reservoirs*. 15th Nov. 2021. URL: https://hal.archives-ouvertes.fr/hal-03428271.

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