Activity Report 2019

Team MEPHYSTO

Quantitative methods for stochastic models in physics

RESEARCH CENTER
Lille - Nord Europe

THEME
Numerical schemes and simulations

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Team MEPHYSTO

Creation of the Team: 2017 October 01

Keywords:

Computer Science and Digital Science:
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

Other Research Topics and Application Domains:
B9.5.2. - Mathematics

1. Team, Visitors, External Collaborators

Research Scientists
Guillaume Dujardin [Team leader, Inria, Researcher, HDR]
Marielle Simon [Inria, Researcher]

Faculty Members
Stephan de Bièvre [Université de Lille, Professor, HDR]
André de Laire [Université de Lille, Associate Professor]
Adrien Hardy [Université de Lille, Associate Professor]
Michele Triestino [Université de Bourgogne, Associate Professor, until Feb 2019]

PhD Students
Pierre Mennuni [Université de Lille, PhD Student, until Sep 2019]
Anthony Nahas [Université de Lille, PhD Student, from Oct 2019]

Technical staff
Alexandre Roget [Inria, Engineer, from Nov 2019]

Administrative Assistant
Karine Lewandowski [Inria]

2. Overall Objectives

2.1. Overall Objectives

The MEPHYSTO team is a follow up of the MEPHYSTO project-team. Since the former scientific leader, Antoine Gloria, left in September 2017, the scientific objectives have been modified.

The MEPHYSTO 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 focus on model derivation, study of stationary states and asymptotic behaviors, as well as links between different levels of description (e.g. micro and macro models) and numerical methods to simulate such models. Applications include nonlinear optics, thermodynamics and ferromagnetism.

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 nonlocal problems such as that of the Gross–Pitaevskii (GP) equation which arises in models of dipolar gases. These models, in general, also introduce nonzero 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 nonlocal problems.

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

Another typical example of problems 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 [37] and solitons in magnetic media are of particular interest as a mechanism for data storage or information transfer [38]. 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 done [36], [35]. In particular, the geometry of the target sphere imposes nonvanishing 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 work in this direction by the team. As a second step, similar models as the ones considered classically will be defined and analysed 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 [7]). 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 (FPME), a nonlinear variation of the fractional diffusion equation, involving the fractional Laplacian instead of the usual one. Its rigorous study carries out many mathematical difficulties in treating at the same time the nonlinearity and fractional diffusion. We want to make PDE theorists and probabilists work together, in order to take advantage of the analytical results which went far 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 nonlinear 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 nonlinear nonlocal 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. Highlights of the Year

4.1. Highlights of the Year

The team has almost completed the process of creation of a new project-team named Paradyse (for PARticles And DYnamical SystEms), between Inria and the Laboratoire Paul Painlevé of the Université de Lille in 2019.

In 2019, the Mephysto team has been granted an Action de Développement Technologique (ADT) by Inria. This allowed the team to hire Alexandre Roget as an engineer for 2 years. The goal of this ADT is to develop software using mathematical techniques developed in the team, to be used by theoretical and experimental physics communities.

In 2019, the team also had individual successes that can be highlighted. Amongst others, M. Simon submitted an ERC Starting Grant project which was ranked A, and S. De Bièvre became Associate Editor of the Journal of Mathematical Physics.

5. New Results

5.1. Traveling waves for some nonlocal 1D Gross-Pitaevskii equations with nonzero conditions at infinity

The nonlocal 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 nonlinearity is usually highly nonlocal. A. de Laire and P. Mennuni have considered a nonlocal family of Gross–Pitaevskii equations in dimension one, and they have provided in [27] conditions on the nonlocal interaction such that there is a branch of traveling waves solutions with nonvanishing conditions at infinity. Moreover, they showed that the branch is orbitally stable. In this manner, this result generalizes known properties for the contact interaction given by a Dirac delta function. Their proof relies on the minimization of the energy at fixed momentum.

5.2. Numerical simulation of traveling waves for some nonlocal Gross-Pitaevskii equations with nonzero conditions at infinity in dimensions 1 and 2

As a follow-up of the previous result, P. Mennuni and G. Dujardin carried out numerical simulations of traveling waves for some nonlocal nonlinear Gross-Pitaevskii equations with nonzero conditions at infinity in dimensions 1 and 2. Using a numerical analogue of the minimization of the energy at fixed momentum, they used gradient methods with nonuniform fast Fourier transforms (to deal with the nonlocal terms numerically) to carry out significant numerical simulations to illustrate numerically the theoretical results and to discuss the hypotheses numerically. These results can be found in P. Mennuni's PhD manuscript [10].

5.3. 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 [26] a rigorous justification to this observation. 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.

5.4. The Cauchy problem for the Landau–Lifshitz–Gilbert equation in BMO and self-similar solutions

A. de Laire and S. Gutierrez established in [22] a global well-posedness result for the Landau–Lifshitz equation with Gilbert damping, provided that the BMO semi-norm of the initial data is small. As a consequence, they deduced the existence of self-similar solutions in any dimension. Moreover, in the one-dimensional case, they characterized the self-similar solutions when the initial data is given by some step function and established their stability. They also showed the existence of multiple solutions if the damping is strong enough.

5.5. Microscopic derivation of moving interfaces problems

In [15], M. Simon and her coauthors derive the porous medium equation from an interacting particle system which belongs to the family of kinetically constrained lattice gases. It was already proved in the literature that the macroscopic density profile is governed by the porous medium equation for initial densities uniformly bounded away from 0 and 1. Here we consider the more general case where the density can take those extreme values. The solutions display a richer behavior, like moving interfaces, finite speed of propagation and breaking of regularity. Since standard techniques cannot be straightforwardly applied, we present a way to generalize the relative entropy method, by involving approximations of solutions to the hydrodynamic equation, instead of exact solutions.

In [16], M. Simon and her coauthors study the hydrodynamic limit for a similar one-dimensional exclusion process but with an even more restricting dynamical constraint: this process with degenerate jump rates admits transient states, which it eventually leaves to reach an ergodic component if the initial macroscopic density is larger than a critical value, or one of its absorbing states otherwise. They show that, for initial profiles smooth enough and uniformly larger than the critical density, the macroscopic density profile evolves under the diffusive time scaling according to a fast diffusion equation. The first step in the proof is to show that the system typically reaches an ergodic component in subdiffusive time.

These two macroscopic behaviors belong to the class of moving interfaces problems, which are particularly hard to derive from the microscopic point of view.

5.6. Towards the weak KPE universality conjecture

In [32], P. Gonçalves, N. Perkowski and M. Simon derive the KPZ equation with boundary conditions, from an interacting particle system in contact with stochastic reservoirs, and they legitimate the choice done at the macroscopic level for the KPZ equation from the microscopic description of the system. This is more subtle than expected, because the boundary conditions do not behave canonically. The main challenge is to clarify the link between the macroscopic boundary effects and their atomic description.

5.7. Joule effect in chains of oscillators

In physics, the rotor chain has been investigated as an example of a system with two conserved quantities (angular momentum and energy), for which the thermal conductivity is finite (and therefore energy diffuses). Numerics shows an unexpected behaviour of the chain when the latter is connected at the boundaries to two thermostats, and a mechanical force imposes an average angular momentum at one boundary: the stationary temperature profile coincides with the values of the thermostats, but in the middle of the chain it raises to a much higher value. This behaviour is related to the presence of two conserved quantities and is sometimes referred to as Joule effect. Since the rotor model is too difficult to be treated analytically, T. Komorowski, S. Olla and M. Simon investigate in [25] the harmonic chain of oscillators, perturbed with a stochastic noise, which makes the heat transport diffusive, namely: the noise destroys the conservation law of the total momentum, but keeps the other two conservation laws (energy and stretch) intact. The boundaries of the chain are connected to two Langevin thermostats and an external force acting on one boundary puts the system in a non-equilibrium stationary state. The authors rigorously derive the Joule effect for a particular value of the noise intensity.

5.8. Quantum optics

In [18], S. De Bièvre and his co-authors introduce a new measure of the nonclassicality of the quantum states of an optical field, the so-called “ordering sensitivity” of the state, that measures the fluctuations of its Wigner function. This work is prolonged in two subsequent papers. In [24], S. De Bièvre and the same co-authors investigate a new class of quantum states they call the “Thermal Difference States” that can be generated by parametric down conversion. They investigate in particular the degree to which such states are nonclassical. In [34], S. De Bièvre and his postdoc A. Hertz, re-interpret the ordering sensitivity in terms of another physical property of the quantum states of an optical field, namely their quadrature coherence scale. It is shown in particular that a large such coherence scale is responsible for very fast environmental decoherence of the state.

5.9. Orbital stability

In [19], S. De Bièvre and S. Rota Nodari consider the orbital stability of relative equilibria of Hamiltonian dynamical systems on Banach spaces, in the presence of a multi-dimensional invariance group for the dynamics. They prove a persistence result for such relative equilibria, present a generalization of the Vakhitov-Kolokolov slope condition to this higher dimensional setting, and show how it allows to prove the local coercivity of the Lyapunov function, which in turn implies orbital stability. The method is applied to study the orbital stability of relative equilibria of nonlinear Schrödinger and Manakov equations. A comparison of their approach to the one by Grillakis-Shatah-Strauss is provided.

5.10. Exponential time-decay for discrete Fokker–Planck equations

In the research direction exposed in Section 3.3, G. Dujardin and his coauthors proposed and studied in [21] several discrete versions of homogeneous and inhomogeneous one-dimensional Fokker-Planck equations. They proved in particular, for these discretizations of velocity and space, the exponential convergence to the equilibrium of the solutions, for time-continuous equations as well as for time-discrete equations. Their method uses new types of discrete Poincaré inequalities for a “two-direction” discretization of the derivative in velocity. For the inhomogeneous problem, they adapted for the very first time hypocoercive methods to the discrete level.

5.11. Energy preserving methods for nonlinear Schrödinger equations

G. Dujardin and his coauthors have revisited and extended relaxation methods for nonlinear Schrödinger equations (NLS). The classical relaxation method for NLS is an energy preserving method and a mass preserving method. Moreover, it is only linearly implicit. A first proof of the second order accuracy was achieved in [14]. Moreover, the method was extended to enable to treat noncubic nonlinearities, nonlocal nonlinearities, as well as rotation terms. The resulting methods are still energy preserving and mass 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.

5.12. High order linearly implicit methods for evolution problems

In [31], I. Lacroix and G. Dujardin have developed a new class of numerical integration methods for evolution problems. This class contains methods of arbitrarily high order that only require the solution of a linear system per time step. For evolution ODEs (Cauchy problems), they give a constructive proof of existence for such arbitrarily high order methods. For evolution PDEs, they demonstrate numerically that these new methods can outperform high order methods from the literature on several test cases.

5.13. CLT for Circular beta-Ensembles at High Temperature

In [33], A. Hardy and G. Lambert have obtained a central limit theorem for the 2D Coulomb gas particle system constrained on a circle in the high temperature regime. An interesting feature is that the limiting variance interpolates between the Lebesgue L^2 norm, corresponding to the infinite temperature setting, and the Sobolev $H^{1/2}$ seminorm, corresponding to the zero temperature regime.

5.14. DLR equations and rigidity for the Sine-β process

The work [20] by A. Hardy and his collaborators, recently accepted for publication in Communications on Pure and Applied Mathematics, provides a “statistical physics” description of the sine-β process by means of Dobroshin-Lanford-Ruelle (DLR) equations. This basically allows to give a meaning to “the natural infinite configurations process on the real line in the 2D Coulomb interaction”, provided there is a unique solution to the DLR equation which turns out to be true in this setting.

6. Partnerships and Cooperations

6.1. National Initiatives

6.1.1. ANR

A. de Laire is a member of the ANR ODA project.

Title: Dispersive and random waves

ANR reference: ANR-18-CE40-0020-01

Coordinator: Nikolay Tzvetkov, Université de Cergy-Pontoise

A. Hardy is a member of the ANR BoB project.

Title: Inférence bayésienne à ressources limitées - données massives et modèles coûteux

Programme ANR: (DS0705) 2016

ANR reference: ANR-16-CE23-0003

Coordinator: R. Bardenet, CNRS & Université de Lille

Duration: October 2016 - October 2020

M. Simon has been a member of the ANR EDNHS project.

Title: Diffusion de l'énergie dans des système hamiltoniens bruités
Type: Défi de tous les savoirs (DS10) 2014
ANR reference: ANR-14-CE25-0011
Coordinator: C. Bernardin, Université de Nice
Duration: October 2014 - October 2019

6.2. European Initiatives

6.2.1. FP7 & H2020 Projects

M. Simon is a collaborator of the ERC Starting Grant HyLEF project.

Title: Hydrodynamic Limits and Equilibrium Fluctuations: universality from stochastic systems
Duration: May 2017 - April 2022
Coordinator: P. Gonçalves, Instituto Superior Técnico, Lisbon, Portugal

7. Dissemination

7.1. Promoting Scientific Activities

7.1.1. Scientific Events: Organisation

7.1.1.1. Member of the Organizing Committees

A. de Laire co-organized the "Journée des Doctorants en Mathématiques du Nord-Pas-de-Calais".

7.1.2. Journal

7.1.2.1. Member of the Editorial Boards

S. De Bièvre is Associate Editor of the Journal of Mathematical Physics since January 2019.

7.1.2.2. Reviewer - Reviewing Activities

M. Simon is reviewer for the main international peer-reviewed journals in probability and statistical physics. In 2019, G. Dujardin served as a reviewer for the numerical analysis journals ESAIM:M2AN, Numerische Mathematik and IMA Journal of Numerical Analysis.

7.1.3. Invited Talks

M. Simon has been invited speaker at several conferences, among them:

- *Interactions PDEs/Probability: particle systems, hyperbolic conservation laws*, CIRM, Marseille
- *1st SFB International Workshop Taming Complexity in Partial Differential Systems*, University of Vienna, Austria

7.2. Teaching - Supervision - Juries

7.2.1. Teaching

Licence: A. de Laire, Mathématiques fondamentales 1, 54 TD, L1, Université de Lille

Licence: G. Dujardin, Calcul différentiel et intégral, 60h, BA2, Université Libre de Bruxelles, Belgium.

Master: A. de Laire, "Etude de Problèmes Elliptiques", 60h, M1, Université de Lille

Master: A. Hardy, "Probabilité, modèles et applications" 60h, M1, Université de Lille

Master: A. Hardy, "Séries temporelles", 30h, M1, Université de Lille

Master: M. Simon, "Introduction à la physique statistique", 56h, M2, Université de Lille

Master: M. Simon, "Markov Chains and Applications", Université de Lille and École Centrale Lille

In addition, A. de Laire is in charge of the Master 2 of Applied Mathematics at Université de Lille.

7.2.2. Supervision

PhD: P. Mennuni, “Ondes progressives de l’équation de Gross–Pitaevskii non locale : analyse et simulations”, Université de Lille, defended on the November 4, 2019; advisors: S. De Bièvre, A. de Laire, G. Dujardin.

7.3. Popularization

7.3.1. Interventions

M. Simon participated in the programs “Chercheurs itinérants” and “Fête de la Science”, and gave several lectures aimed at high-school students.

8. Bibliography

Major publications by the team in recent years

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Publications of the year

Doctoral Dissertations and Habilitation Theses

[10] P. MENNUNI. *Traveling waves of the nonlocal Gross-Pitaevskii equation: analysis and simulations*, Université de Lille, November 2019, https://hal.archives-ouvertes.fr/tel-02395234

[11] M. SIMON. *Microscopic derivation of degenerated diffusion phenomena*, Université de Lille, December 2019, Habilitation à diriger des recherches, https://hal.inria.fr/tel-02399713

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