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Activity Report 2017

Project-Team MEPHYSTO

Quantitative methods for stochastic models in physics

RESEARCH CENTER
Lille - Nord Europe

THEME
Numerical schemes and simulations

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Project-Team MEPHYSTO

Creation of the Team: 2014 January 01, updated into Project-Team: 2016 July 01, end of the Project-Team: 2017 September 30

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1. Personnel

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2. Overall Objectives

2.1. Presentation and overall objectives

In the context of the construction of the European landscape of research, Inria and ULB (Université Libre de Bruxelles) signed in 2013 an agreement to foster joint research teams on topics of mutual interests. The team MEPHYSTO, a joint project of Inria, the Université Lille 1 and CNRS, and the Université Libre de Bruxelles, is the first such collaboration, in applied mathematics. It operates in two locations: Lille and Brussels.

The main objective of the team is to develop mathematical and numerical tools to study in a quantitative way some specific physical models which display random and/or multiscale features. The emphasis is put on the interplay between analysis, probability, and numerics.

We focus our efforts on two prototypical examples: stochastic homogenization and the Schrödinger equations.

2.2. Scientific context

Whereas many models in physics involve randomness, they behave deterministically in suitable asymptotic regimes when stochastic effects average out. The qualitative and quantitative understanding of this deterministic behavior is the main challenge of this project.

From a mathematical point of view, our main fields of interest are stochastic homogenization of PDEs and random or deterministic one-dimensional nonlinear Schrödinger equations. These topics involve two challenges identified in the strategic plan of Inria “Objectif 2020": randomness and multiscale modeling.

From a physical point of view, the problems we shall consider find their origin in

- the statistical physics of random polymer-chain networks;
- light propagation in optical fibers.

Stochastic homogenization

Homogenization is a theory which deals with oscillations in PDEs. Let D be a smooth bounded domain of $\mathbb{R}^d$. The starting point is the fact that for linear elliptic equations, the oscillations of the weak solution $u_\varepsilon \in H^1_0(D)$ of

$$-\nabla \cdot A_\varepsilon \nabla u_\varepsilon \;=\; f \tag{1}$$

for some suitable r. h. s. f are a (nonlinear) function of the oscillations of A_ε. In particular, if A_ε oscillates at scale $\varepsilon > 0$, one expects u_ε to display oscillations at scale ε, and to be close to some function which does not oscillate if in addition $\varepsilon \ll 1$. This is the case when A_ε is the ε-rescaled version of a periodic function A. Then A_ε is ε-periodic, and there exists some fixed matrix A_{hom} depending only on A (and not on f), such that u_ε behaves as $u_{\text{hom}} \in H^1_0(D)$, the weak solution of

$$-\nabla \cdot A_{\text{hom}} \nabla u_{\text{hom}} \;=\; f. \tag{2}$$

The homogenized coefficients A_{hom} are characterized by the so-called correctors ϕ_ξ in direction $\xi \in \mathbb{R}^d$, distributional solutions in $\mathbb{R}^d$ of

$$-\nabla \cdot A(\xi + \nabla \phi_\xi) \;=\; 0. \tag{3}$$

In the periodic case, these correctors are well-behaved by standard PDE theory. The convergence of u_ε to u_{hom} is illustrated on Figure 1 (periodic checkerboard on the left, random checkerboard on the right), where the isolines of the solutions to (1) and (2) (with $f \equiv 1$ on the unit square) are plotted for several values of ε — the convergence of u_ε to u_{hom} is weak in $H^1(D)$. Yet, naturally-occuring structures are rarely periodic. If instead of considering some periodic A, we consider some random A, the story is different, cf. Figure 1 for results on the random checkerboard. In the early period of stochastic homogenization, in the seventies, it was not clear if just the ergodicity and stationarity of the coefficients and ellipticity were enough to prove convergence of u_ε almost surely and identify the limit u_{hom}. The meaning to give to (3) was indeed quite unclear (the equation is posed on the whole space). It was a surprise, therefore, that this was possible with random coefficients, and that stochastic homogenization was indeed a new type of *qualitative* ergodic theory ([50], [47]). The following natural question, asked more than thirty years ago, is whether one can develop an associated *quantitative* ergodic theory.

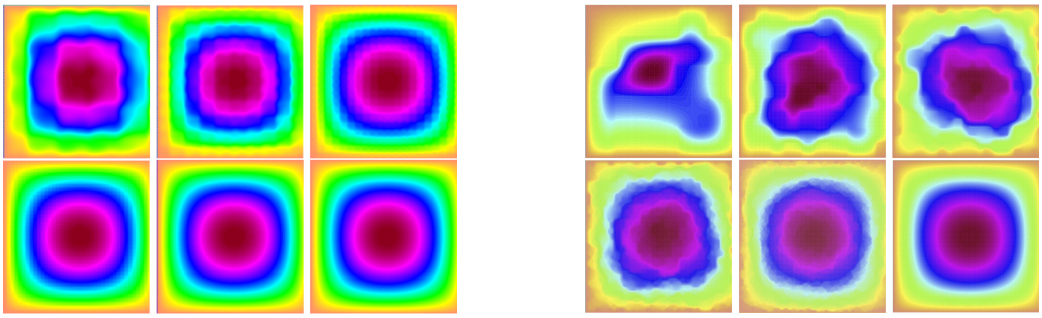

Figure 1. Solution u_ε for $\varepsilon = 1/5, 1/10, 1/20, 1/40, 1/80$ and solution u_{hom}, periodic case (left) and random case (right)

One of our initial motivations to develop a quantitative stochastic homogenization theory is the derivation of nonlinear elasticity from polymer physics, which is presented in the research program and application section. We plan to develop a complete quantitative theory of stochastic homogenization of elliptic equations. In particular we aim at quantifying how well u_{hom} approximates u_ε, and at identifying the asymptotic law of the solution u_ε in function of the law of A.

Schrödinger equations

The linear Schrödinger equation, with an appropriate choice of geometry and boundary conditions, has been central to the description of all non-relativistic quantum mechanical systems for almost a century now. In addition, its nonlinear variant arises in the mean field description of Bose-Einstein condensates, where it is known as the Gross-Pitaevskii equation, but also in nonlinear classical optics, and in particular in fiber optics. The quantitative and qualitative description of its solutions (for both the evolution and the stationary equations), their time-asymptotic behavior, their stability or instability in terms of the parameters of the initial conditions and/or the potentials and boundary conditions continue to pose numerous physical and mathematical problems (see [53] and [33] for general references).

In view of our collaboration with the Lille laser physics laboratory PhLAM, we will focus more particularly on the one-dimensional nonlinear Schrödinger equation (NLS). Indeed, (NLS) drives the envelope of the propagation of a laser pulse in a Kerr medium, such as an optical fiber [53]. Many phenomena on (NLS) (and variants thereof, with higher order derivatives, various types of initial conditions, external fields, etc.) are put in evidence by physical experiments at PhLAM, are not fully understood, and raise exciting questions from the numerical and analytical perspectives.

The same type of equation also describes Bose-Einstein condensates, for which questions related to Anderson localization are also of interest theoretically and experimentally at PhLAM.

3. Research Program

3.1. From statistical physics to continuum mechanics

Whereas numerical methods in nonlinear elasticity are well-developed and reliable, constitutive laws used for rubber in practice are phenomenological and generally not very precise. On the contrary, at the scale of the polymer-chain network, the physics of rubber is very precisely described by statistical physics. The main challenge in this field is to understand how to derive macroscopic constitutive laws for rubber-like materials from statistical physics.

At the continuum level, rubber is modelled by an energy E defined as the integral over a domain D of $\mathbb{R}^d$ of some energy density W depending only locally on the gradient of the deformation u: $E(u) = \int_D W(\nabla u(x))dx$. At the microscopic level (say 100nm), rubber is a network of cross-linked and entangled polymer chains (each chain is made of a sequence of monomers). At this scale the physics of polymer chains is well-understood in terms of statistical mechanics: monomers thermally fluctuate according to the Boltzmann distribution [42]. The associated Hamiltonian of a network is typically given by a contribution of the polymer chains (using self-avoiding random bridges) and a contribution due to steric effects (rubber is packed and monomers are surrounded by an excluded volume). The main challenge is to understand how this statistical physics picture yields rubber elasticity. Treloar assumed in [54] that for a piece of rubber undergoing some macroscopic deformation, the cross-links do not fluctuate and follow the macroscopic deformation, whereas between two cross-links, the chains fluctuate. This is the so-called affine assumption. Treloar's model is in rather good agreement with mechanical experiments in small deformation. In large deformation however, it overestimates the stress. A natural possibility to relax Treloar's model consists in relaxing the affine assumption while keeping the network description, which allows one to distinguish between different rubbers. This can be done by assuming that the deformation of the cross-links minimizes the free energy of the polymer chains, the deformation being fixed at the boundary of the macroscopic domain D. This gives rise to a "variational model". The analysis of the asymptotic behavior of this model as the typical length of a polymer chain vanishes has the same flavor as the homogenization theory of integral functionals in nonlinear elasticity (see [37], [48] in the periodic setting, and [39] in the random setting).

Our aim is to relate qualitatively and quantitatively the (precise but unpractical) statistical physics picture to explicit macroscopic constitutive laws that can be used for practical purposes.

In collaboration with R. Alicandro (Univ. Cassino, Italy) and M. Cicalese (Univ. Munich, Germany), A. Gloria analyzed in [1] the (asymptotic) Γ-convergence of the variational model for rubber, in the case when the polymer chain network is represented by some ergodic random graph. The easiest such graph is the Delaunay tessellation of a point set generated as follows: random hard spheres of some given radius ρ are picked randomly until the domain is jammed (the so-called random parking measure of intensity ρ). With M. Penrose (Univ. Bath, UK), A. Gloria studied this random graph in this framework [5]. With P. Le Tallec (Mechanics department, Ecole polytechnique, France), M. Vidrascu (project-team REO, Inria Paris-Rocquencourt), and A. Gloria introduced and tested in [44] a numerical algorithm to approximate the homogenized energy density, and observed that this model compares well to rubber elasticity qualitatively.

These preliminary results show that the variational model has the potential to explain qualitatively and quantitatively how rubber elasticity emerges from polymer physics. In order to go further and obtain more quantitative results and rigorously justify the model, we have to address several questions of analysis, modelling, scientific computing, inverse problems, and physics.

3.2. Quantitative stochastic homogenization

Whereas the approximation of homogenized coefficients is an easy task in periodic homogenization, this is a highly nontrivial task for stochastic coefficients. This is in order to analyze numerical approximation methods of the homogenized coefficients that F. Otto (MPI for mathematics in the sciences, Leipzig, Germany) and A. Gloria obtained the first quantitative results in stochastic homogenization [3]. The development of a complete stochastic homogenization theory seems to be ripe for the analysis and constitutes the second major objective of this section.

In order to develop a quantitative theory of stochastic homogenization, one needs to quantitatively understand the corrector equation (3). Provided A is stationary and ergodic, it is known that there exists a unique random field ϕ_ξ which is a distributional solution of (3) almost surely, such that $\nabla\phi_\xi$ is a stationary random field with bounded second moment $\left\langle|\nabla\phi_\xi|^2\right\rangle < \infty$, and with $\phi(0) = 0$. Soft arguments do not allow to prove that ϕ_ξ may be chosen stationary (this is wrong in dimension $d = 1$). In [3], [4] F. Otto and A. Gloria proved that, in the case of discrete elliptic equations with iid conductances, there exists a unique stationary corrector ϕ_ξ with vanishing expectation in dimension $d > 2$. Although it cannot be bounded, it has bounded finite moments of any order:

$$\langle|\phi_\xi|^q\rangle < \infty \text{ for all } q \geq 1. \tag{4}$$

They also proved that the variance of spatial averages of the energy density $(\xi + \nabla\phi_\xi) \cdot A(\xi + \nabla\phi_\xi)$ on balls of radius R decays at the rate R^{-d} of the central limit theorem. These are the *first optimal quantitative results* in stochastic homogenization.

The proof of these results, which is inspired by [49], is based on the insight that coefficients such as the Poisson random inclusions are special in the sense that the associated probability measure satisfies a spectral gap estimate. Combined with elliptic regularity theory, this spectral gap estimate quantifies ergodicity in stochastic homogenization. This systematic use of tools from statistical physics has opened the way to the quantitative study of stochastic homogenization problems, which we plan to fully develop.

3.3. Nonlinear Schrödinger equations

As well known, the (non)linear Schrödinger equation

$$\partial_t\varphi(t,x) = -\Delta\varphi(t,x) + \lambda V(x)\varphi(t,x) + g|\varphi|^2\varphi(t,x), \quad \varphi(0,x) = \varphi_0(x) \tag{5}$$

with coupling constants $g \in \mathbb{R}, \lambda \in \mathbb{R}_+$ and real potential V (possibly depending also on time) models many phenomena of physics.

When in the equation (5) above one sets $\lambda = 0, g \neq 0$, one obtains the nonlinear (focusing of defocusing) Schrödinger equation. It is used to model light propagation in optical fibers. In fact, it then takes the following form:

$$i\partial_z\varphi(t,z) = -\beta(z)\partial_t^2\varphi(t,z) + \gamma(z)|\varphi(t,z)|^2\varphi(z,t), \tag{6}$$

where β and γ are functions that characterize the physical properties of the fiber, t is time and z the position along the fiber. Several issues are of importance here. Two that will be investigated within the MEPHYSTO project are: the influence of a periodic modulation of the fiber parameters β and γ and the generation of so-called “rogue waves” (which are solutions of unusually high amplitude) in such systems.

If $g = 0, \lambda \neq 0$, V is a random potential, and φ_0 is deterministic, this is the standard random Schrödinger equation describing for example the motion of an electron in a random medium. The main issue in this setting is the determination of the regime of Anderson localization, a property characterized by the boundedness in time of the second moment $\int x^2 |\varphi(t,x)|^2 dx$ of the solution. If this second moment remains bounded in time, the solution is said to be localized. Whereas it is known that the solution is localized in one dimension for all (suitable) initial data, both localized and delocalized solutions exist in dimension 3 and it remains a major open problem today to prove this, cf. [41].

If now $g \neq 0, \lambda \neq 0$ and V is still random, but $|g| \ll \lambda$, a natural question is whether, and in which regime, one-dimensional Anderson localization perdures. Indeed, Anderson localization can be affected by the presence of the nonlinearity, which corresponds to an interaction between the electrons or atoms. Much numerical and some analytical work has been done on this issue (see for example [43] for a recent work at PhLAM, Laser physics department, Univ. Lille 1), but many questions remain, notably on the dependence of the result on the initial conditions, which, in a nonlinear system, may be very complex. The cold atoms team of PhLAM (Garreau-Szriftgiser) is currently setting up an experiment to analyze the effect of the interactions in a Bose-Einstein condensate on a closely related localization phenomenon called "dynamical localization", in the kicked rotor, see below.

3.4. Processes in random environment

In the course of developing a quantitative theory of stochastic homogenization of discrete elliptic equations, we have introduced new tools to quantify ergodicity in partial differential equations. These tools are however not limited to PDEs, and could also have an impact in other fields where an evolution takes place in a (possibly dynamic) random environment and an averaging process occurs. The goal is then to understand the asymptotics of the motion of the particle/process.

For a random walker in a random environment, the Kipnis-Varadhan theorem ensures that the expected squared-position of the random walker after time t is of order t (the prefactor depends on the homogenized coefficients). If instead of a random walk among random conductances we consider a particle with some initial velocity evolving in a random *potential* field according to the Newton law, the averaged squared-position at time t is expected to follow the scaling law t^2, see [34]. This is called stochastic acceleration.

Similar questions arise when the medium is reactive (that is, when the potential is modified by the particle itself). The approach to equilibrium in such systems was observed numerically and explained theoretically, but not completely proven, in [40].

Another related and more general direction of research is the validity of *universality principle* of statistical physics, which states that the qualitative behavior of physical systems depend on the microscopic details of the system only through some large-scale variables (the thermodynamic variables). Therefore, it is a natural problem in the field of interacting particle systems to obtain the macroscopic laws of the relevant thermodynamical quantities, using an underlying microscopic dynamics, namely particles that move according to some prescribed stochastic law. Probabilistically speaking, these systems are continuous time Markov processes.

4. New Results

4.1. Long-time homogenization of the wave equation

In a joint work [36], A. Benoit and A. Gloria considered an elliptic operator in divergence form with symmetric coefficients. If the diffusion coefficients are periodic, the Bloch theorem allows one to diagonalize the elliptic operator, which is key to the spectral properties of the elliptic operator and the usual starting point for the study of its long-time homogenization. When the coefficients are not periodic (say, quasi-periodic, almost periodic, or random with decaying correlations at infinity), the Bloch theorem does not hold and both the spectral properties and the long-time behavior of the associated operator are unclear. At low frequencies, we may however consider a formal Taylor expansion of Bloch waves (whether they exist or not) based on correctors in elliptic homogenization. The associated Taylor-Bloch waves diagonalize the elliptic operator up to an error term (an “eigendefect”), which we express with the help of a new family of extended correctors. We use the Taylor-Bloch waves with eigendefects to quantify the transport properties and homogenization error over large times for the wave equation in terms of the spatial growth of these extended correctors. On the one hand, this quantifies the validity of homogenization over large times (both for the standard homogenized equation and higher-order versions). On the other hand, this allows us to prove asymptotic ballistic transport of classical waves at low energies for almost periodic and random operators.

4.2. Weighted functional inequalities

Functional inequalities like spectral gap, covariance, or logarithmic Sobolev inequalities are powerful tools to prove nonlinear concentration of measure properties and central limit theorem scalings. Besides their well-known applications in mathematical physics (e.g. for the study of interacting particle systems like the Ising model or for interface models), such inequalities were recently used by the team to establish quantitative stochastic homogenization results.

These functional inequalities have nevertheless two main limitations for stochastic homogenization. On the one hand, whereas only few examples are known to satisfy them (besides product measures, Gaussian measures, and more general Gibbs measures with nicely behaved Hamiltonians), these inequalities are not robust with respect to various simple constructions: for instance, a Poisson point process satisfies a spectral gap, but the random field corresponding to the Voronoi tessellation of a Poisson point process does not. On the other hand, these functional inequalities require random fields to have an integrable covariance, which prevents one to consider fields with heavier tails.

In the series of work [26], [27], [28], M. Duerinckx and A. Gloria introduced weaker versions of these functional inequalities in the form of weighted inequalities. The interest of such inequalities is twofold: first, as their unweighted counterpart they ensure strong concentration properties; second, they hold for a large class of statistics of interest to homogenization (which is shown using a constructive approach).

4.3. Macroscopic behaviors of large interacting particle systems

A vast amount of physical phenomena were first described at the macroscopic scale, in terms of the classical partial differential equations (PDEs) of mathematical physics. Over the last decades the scientific community has pursued part of its research towards the following *universality principle*, which is well known in statistical physics: “the qualitative behavior of physical systems depend on the microscopic details of the system only through some large-scale variables”. Typically, the microscopic systems are composed of a huge number of atoms and one looks at a very large time scale with respect to the typical frequency of atom vibrations. Mathematically, this corresponds to a space-time scaling limit procedure.

The macroscopic laws that can arise from microscopic systems can either be partial differential equations (PDEs) or stochastic PDEs (SPDEs) depending on whether one is looking at the convergence to the mean or at the fluctuations around that mean. Therefore, it is a natural problem in the field of interacting particle systems to obtain the macroscopic laws of the relevant thermodynamical quantities, using an underlying microscopic dynamics, namely particles that move according to some prescribed stochastic law. Probabilistically speaking, these systems are continuous time Markov processes.

4.3.1. Anomalous diffusion

First, one can imagine that at the *microscopic* scale, the population is well modeled by stochastic differential equations (SDEs). Then, the *macroscopic* description of the population densities is provided by partial differential equations (PDEs), which can be of different types. All these systems may characterize the collective behavior of individuals in biology models, but also agents in economics and finance. In [14] M. Simon in collaboration with C. Olivera has obtained a limit process which belongs to the family of non-local PDEs, and is related to anomalous diffusions. More precisely, they study the asymptotic behavior of a system of particles which interact *moderately*, i.e. an intermediate situation between weak and strong interaction, and which are submitted to random scattering. They prove a law of large numbers for the empirical density process, which in the macroscopic limit follows a fractional conservation law. The latter is a generalization of convection-diffusion equations, and can appear in physical models (e.g. over-driven detonation in gases [38], or semiconductor growth [55]), but also in areas like hydrodynamics and molecular biology.

Another approach which aims at understanding this abnormally diffusive phenomena is to start from deterministic system of Newtonian particles, and then perturb this system with a stochastic component which will provide enough ergodicity to the dynamics. It is already well known that these stochastic chains model correctly the behavior of the conductivity [35]. In two published papers [18][32], and another submitted one [19], M. Simon with her coauthors C. Bernardin, P. Gonçalves, M. Jara, T. Komorowski, S. Olla and M. Sasada have observed both behaviors, normal and anomalous diffusion, in the context of low dimensional asymmetric systems. They manage to describe the microscopic phenomena at play which are responsible for each one of these phenomena, and they go beyond the predictions that have recently been done in [51], [52].

4.3.2. *Towards the weak KPZ universality conjecture*

Among the classical SPDEs is the Kardar-Parisi-Zhang (KPZ) equation which has been first introduced more than thirty years ago in [46] as the *universal* law describing the fluctuations of randomly growing interfaces of one-dimensional stochastic dynamics close to a stationary state (as for example, models of bacterial growth, or fire propagation). In particular, the *weak KPZ universality conjecture* [52] states that the fluctuations of a large class of one-dimensional microscopic interface growth models are ruled at the macroscopic scale by solutions of the *KPZ equation*. Thanks to the recent result of M. Jara and P. Gonçalves [45], one has now all in hands to establish that conjecture. In their paper, the authors introduce a new tool, called the second order Boltzmann-Gibbs principle, which permits to replace certain additive functionals of the dynamics by similar functionals given in terms of the density of the particles. In [13], M. Simon in collaboration with P. Gonçalves and M. Jara give a new proof of that principle, which does not impose the knowledge on the spectral gap inequality for the underlying model and relies on a proper decomposition of the antisymmetric part of the current of the system in terms of polynomial functions. In addition, they fully derive the convergence of the equilibrium fluctuations towards (1) a trivial process in case of super-diffusive systems, (2) an Ornstein-Uhlenbeck process or the unique *energy solution* of the stochastic Burgers equation (SBE) (and its companion, the KPZ equation), in case of weakly asymmetric diffusive systems. Examples and applications are presented for weakly and partial asymmetric exclusion processes, weakly asymmetric speed change exclusion processes and Hamiltonian systems with exponential interactions.

In [30], M. Simon together with P. Gonçalves and N. Perkowski go beyond the weak KPZ universality conjecture to derive a new SPDE, namely, the KPZ equation with boundary conditions, from an interacting particle system in contact with stochastic reservoirs. They legitimate the choice done at the macroscopic level for the KPZ/SBE equation from the microscopic description of the system. For that purpose, they prove two main theorems: first, they extend the notion of energy solutions to the stochastic Burgers equation by adding Dirichlet boundary conditions. Second, they construct a microscopic model (based on weakly asymmetric exclusion processes) from which the energy solution naturally emerges as the macroscopic limit of its stationary density fluctuations. This gives a physical justification for the Dirichlet boundary conditions the SBE equation. They also prove existence and uniqueness of energy solutions to two related SPDEs: the KPZ equation with Neumann boundary conditions and the SHE with Robin boundary conditions, and they rigorously establish the formal links between the equations. This is more subtle than expected, because the boundary conditions do not behave canonically. Finally, they associate an interface growth model to the microscopic model, roughly speaking by integrating it in the space variable, and show that it converges to the energy solution of the KPZ equation, thereby giving a physical justification of the Neumann boundary conditions.

4.4. High order exponential integrators for nonlinear Schrödinger equations with application to rotating Bose–Einstein condensates

In a recent work with C. Besse and I. Violet [6], Guillaume Dujardin has proposed and analyzed new methods for the time integration of the nonlinear Schrödinger equation in the context of rotating Bose–Einstein condensates. In particular, he has proposed a systematic way to design high-order in time implicit exponential methods, given sufficient conditions to ensure mass preservation by the methods and proved high order in several physically relevant situations. He has compared those methods to several other popular methods from the literature and provided several numerical experiments.

4.5. Periodic modulations controlling Kuznetsov-Ma soliton formation in nonlinear Schrödinger equations

Together with colleages from the Physics department of the Université de Lille, S. de Bièvre and G. Dujardin have analyzed the exact Kuznetsov–Ma soliton solution of the one-dimensional nonlinear Schrödinger equation in the presence of periodic modulations satisfying an integrability condition [15]. They showed that, in contrast to the case without modulation, the Kuznetsov–Ma soliton develops multiple compression points whose number, shape and position are controlled both by the intensity of the modulation and by its frequency. In addition, when this modulation frequency is a rational multiple of the natural frequency of the Kutzetsov–Ma soliton, a scenario similar to a nonlinear resonance is obtained: in this case the spatial oscillations of the Kuznetsov–Ma soliton's intensity are periodic. When the ratio of the two frequencies is irrational, the soliton's intensity is a quasiperiodic function. A striking and important result of this analysis is the possibility to suppress any component of the output spectrum of the Kuznetsov–Ma soliton by a judicious choice of the amplitude and frequency of the modulation.

4.6. Exponential integrators for nonlinear Schrödinger equations with white noise dispersion

Together with D. Cohen, G. Dujardin has proposed several exponential numerical methods for the time integration of the nonlinear Schrödinger equation with power law nonlinearity and random dispersion [11]. In particular, he introduced a new explicit exponential integrator for this purpose that integrates the noisy part of the equation exactly. He prove that this scheme is of mean-square order 1 and he drew consequences of this fact. He compared the exponential integrator with several other numerical methods from the literature. Finally, he proposed a second exponential integrator, which is implicit and symmetric and, in contrast to the first one, preserves the L^2-norm of the solution.

4.7. New results on waveguides with mixed diffusion

In [21], [8], [22], D. Bonheure, J.-B. Casteras and collaborators obtained new results on the existence and qualitative properties of waveguides for a mixed-diffusion NLS equation. In particular, they proved the first existence results for waveguides with fixed mass and provided several qualitative descriptions of these. They also showed that the ground-state solutions are instable by finite (or infinite) time blow-up improving a recent result of Boulenger and Lenzmann and answering a conjecture of Baruch and Fibich.

4.8. New result on the Boltzmann scenario

Boltzmann provided a scenario to explain why individual macroscopic systems inevitably approach a unique macroscopic state of thermodynamic equilibrium, and why after having done so, they remain in that state, apparently forever. In [12], new rigorous results are provided that mathematically prove the basic features of Boltzmann's scenario for two classical models: a simple boundary-free model for the spatial homogenization of a non-interacting gas of point particles, and the well-known Kac ring model.

4.9. Other new results

In [9], [20], D. Bonheure, J.-B. Casteras and collaborators made bifurcation analysis and constructed multi-layer solutions of the Lin-Ni-Takagi and Keller-Segel equations, which come from the Keller-Segel system of chemotaxis in specific cases. A remarkable feature of the results is that the layers do not accumulate to the boundary of the domain but satisfy an optimal partition problem contrary to the previous type of solutions constructed for these models.

In [10], [23], J.-B. Casteras and collaborators study different problems related to the existence of A-harmonic functions with prescribed asymptotic boundary on Cartan-Hadamard manifold. In particular, they obtained a sharp lower bound on the section curvature for the existence of minimal graphic functions with prescribed asymptotic boundary.

In [25], a kinetic equation of the Vlasov-Wave type is studied, which arises in the description of the behavior of a large number of particles interacting weakly with an environment. Variational techniques are used to establish the existence of large families of stationary states for this system, and analyze their stability.

5. Partnerships and Cooperations

5.1. National Initiatives

5.1.1. ANR BECASIM

G. Dujardin is a member of the ANR BECASIM project (http://becasim.math.cnrs.fr/). This ANR project gathers mathematicians with theoretical and numerical backgrounds together with engineers. The objective is to develop numerical methods to accurately simulate the behavior of Bose-Einstein condensates.

Title: Simulation numérique avancée pour les condensats de Bose-Einstein.

Type: Modèles Numériques - 2012.

ANR reference: ANR-12-MONU-0007.

Coordinator: Ionut DANAILA, Université de Rouen.

Duration: January 2013 - December 2017.

Partners: Université Lille 1, UPMC, Ecole des Ponts ParisTech, Inria-Nancy Grand-Est, Université Montpellier 2, Université Toulouse 3.

5.1.2. ANR EDNHS

M. Simon is 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: Cédric Bernardin, Université de Nice.

Duration: October 2014 - October 2019.

5.1.3. Labex CEMPI

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

Coordinator: Stephan De Bièvre.

Duration: January 2012 - December 2019.

Partners: Laboratoire Paul Painlevé and Laser physics department (PhLAM), Université Lille 1.

The “Laboratoire d'Excellence” Centre Européen pour les Mathématiques, la Physique et leurs interactions (CEMPI), a project of the Laboratoire de Mathématiques Paul Painlevé 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.

One of the three focus areas of CEMPI research is the interface between mathematics and physics. This focus area encompasses three themes. The first is concerned with key problems of a mathematical, physical and technological nature coming from the study of complex behavior in cold atoms physics and non-linear optics, in particular fibre optics. The two other themes deal 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.

5.1.4. PEPS "Jeunes Chercheurs"

M. Simon obtained a CNRS grant "PEPS Jeunes Chercheurs" for a project in collaboration with Oriane Blondel (Université Lyon 1), Clément Erignoux (IMPA, Rio de Janeiro) and Makiko Sasada (Tokyo University).

5.1.5. MIS

Incentive Grant for Scientific Research (MIS) of the Fonds National de la Recherche Scientifique (Belgium).

Title: Patterns, Phase Transitions, 4NLS & BIon.

Coordinator: D. Bonheure.

Duration: January 2014 - December 2016.

Partner: Université libre de Bruxelles.

5.1.6. PDR

Research Project (PDR) of the Fonds National de la Recherche Scientifique (Belgium).

D. Bonheure is co-investigator of this PDR.

Title: Asymptotic properties of semilinear systems.

Coordinator: Christophe Troestler (UMons).

Duration: July 2014 - June 2018.

Partner: Université de Mons, Université catholique de Louvain, Université libre de Bruxelles.

5.2. European Initiatives

5.2.1. FP7 & H2020 Projects

5.2.1.1. QUANTHOM

Title: Quantitative methods in stochastic homogenization.

Programm: FP7.

Duration: February 2014 - August 2017.

Coordinator: Inria.

Partner: Département de mathématique, Université Libre de Bruxelles (Belgium).

Inria contact: Antoine Gloria.

This proposal deals with the development of quantitative tools in stochastic homogenization, and their applications to materials science. Three main challenges will be addressed. First, a complete quantitative theory of stochastic homogenization of linear elliptic equations will be developed starting from results we recently obtained on the subject combining tools originally introduced for statistical physics, such as spectral gap and logarithmic Sobolev inequalities, with elliptic regularity theory. The ultimate goal is to prove a central limit theorem for solutions to elliptic PDEs with random coefficients. The second challenge consists in developing an adaptive multiscale numerical method for diffusion in inhomogeneous media. Many powerful numerical methods were introduced in the last few years, and analyzed in the case of periodic coefficients. Relying on my recent results on quantitative stochastic homogenization, we have made a sharp numerical analysis of these methods, and introduced more efficient variants, so that the three academic examples of periodic, quasi-periodic, and random stationary diffusion coefficients can be dealt with efficiently. The emphasis of this challenge is put on the adaptivity with respect to the local structure of the diffusion coefficients, in order to deal with more complex examples of interest to practitioners. The last and larger objective is to make a rigorous connection between the continuum theory of nonlinear elastic materials and polymer-chain physics through stochastic homogenization of nonlinear problems and random graphs. Analytic and numerical preliminary results show the potential of this approach. We plan to derive explicit constitutive laws for rubber from polymer chain properties, using the insight of the first two challenges. This requires a good understanding of polymer physics in addition to qualitative and quantitative stochastic homogenization.

5.2.2. HyLEF

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

- Title: Hydrodynamic Limits and Equilibrium Fluctuations: universality from stochastic systems.
- Duration: May 2017 - April 2022.
- Coordinator: P. Gonçalves, Instituto Superior Técnico, Lisbon.
- A classical problem in the field of interacting particle systems (IPS) is to derive the macroscopic laws of the thermodynamical quantities of a physical system by considering an underlying microscopic dynamics which is composed of particles that move according to some prescribed stochastic, or deterministic, law. The macroscopic laws can be partial differential equations (PDE) or stochastic PDE (SPDE) depending on whether one is looking at the convergence to the mean or to the fluctuations around that mean.

  One of the purposes of this research project is to give a mathematically rigorous description of the derivation of SPDE from different IPS. We will focus on the derivation of the stochastic Burgers equation (SBE) and its integrated counterpart, namely, the KPZ equation, as well as their fractional versions. The KPZ equation is conjectured to be a universal SPDE describing the fluctuations of randomly growing interfaces of 1d stochastic dynamics close to a stationary state. With this study we want to characterize what is known as the KPZ universality class: the weak and strong conjectures. The latter states that there exists a universal process, namely the KPZ fixed point, which is a fixed point of the renormalization group operator of spacetime scaling 1:2:3, for which the KPZ is also invariant. The former states that the fluctuations of a large class of 1d conservative microscopic dynamics are ruled by stationary solutions of the KPZ.

  Our goal is threefold: first, to derive the KPZ equation from general weakly asymmetric systems, showing its universality; second, to derive new SPDE, which are less studied in the literature, as the fractional KPZ from IPS which allow long jumps, the KPZ with boundary conditions from IPS in contact with reservoirs or with defects, and coupled KPZ from IPS with more than one conserved quantity. Finally, we will analyze the fluctuations of purely strong asymmetric systems, which are conjectured to be given by the KPZ fixed point.

5.3. International Initiatives

5.3.1. Inria International Partners

5.3.1.1. Informal International Partners

Max Planck Institute for Mathematics in the Sciences: long-term collaboration with Felix Otto on stochastic homogenization.
University of Umea: long-time collaboration with David Cohen on numerical methods for the numerical integration of stochastic evolution problems.

5.4. International Research Visitors

5.4.1. Research Stays Abroad

M. Simon spent three weeks in Berkeley University, visiting Pr. Alan Hammond (July 2017).

M. Simon spent two weeks at Braga University, as a guest of P. Gonçalves (September 2017).

6. Dissemination

6.1. Promoting Scientific Activities

6.1.1. Scientific Events Organisation

6.1.1.1. Member of the Organizing Committees

M. Simon was a member of the Organizing Committee for the *Journée de la Fédération de Recherche Mathématique du Nord Pas de Calais 2017* (place: Villeneuve d'Ascq, duration: one day).

M. Simon was a member of the Organizing Committee for the *Semaine d'Études Maths-Entreprises Hauts de France 2018* (place: Villeneuve d'Ascq, duration: one week). For that aim, she got a subvention by Inria.

6.1.2. Journal

6.1.2.1. Member of the Editorial Boards

Antoine Gloria is editor at NWJM.

6.1.2.2. Reviewer - Reviewing Activities

G. Dujardin is reviewer for M2AN.

6.1.3. Invited Talks

M. Simon was an invited speaker at:

- *Collège de France*, for the physics seminar (January 2017).
- the congress *Stochastic Analysis and its Applications*, taking place in Bedlewo Center (Poland) in june 2017.

6.2. Teaching - Supervision - Juries

6.2.1. Supervision

PhD: M. Duerinckx, PhD at Université Libre de Bruxelles, defended on 19th December 2017 (A. Gloria).

PhD in progress: P. Mennuni, PhD at Université de Lille 1 (S. De Bièvre and G. Dujardin).

6.3. Popularization

M. Simon participated in the diffusion program *MathenJeans*, in Lille. She followed a group of 4 children (aged 10–11), who presented a project to the national competition named *CGénial*.

7. Bibliography

Major publications by the team in recent years

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