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Activity Report 2016

Project-Team MEPHYSTO

Quantitative methods for stochastic models in physics

RESEARCH CENTER
Lille - Nord Europe

THEME
Numerical schemes and simulations

Table of contents

Project-Team MEPHYSTO

Creation of the Team: 2014 January 01, updated into Project-Team: 2016 July 01

Keywords:

Computer Science and Digital Science:

6. - Modeling, simulation and control
6.1. - Mathematical Modeling
6.1.1. - Continuous Modeling (PDE, ODE)
6.1.2. - Stochastic Modeling (SPDE, SDE)
6.1.4. - Multiscale modeling
6.2. - Scientific Computing, Numerical Analysis & Optimization
6.2.1. - Numerical analysis of PDE and ODE
6.2.2. - Numerical probability
6.2.3. - Probabilistic methods

Other Research Topics and Application Domains:

3.3.1. - Earth and subsoil
5.5. - Materials
9.4.2. - Mathematics
9.4.3. - Physics

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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 $A_{\rm hom}$ depending only on A (and not on f), such that u_ε behaves as $u_{\rm hom} \in H^1_0(D)$, the weak solution of

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

The homogenized coefficients $A_{\rm hom}$ 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 $u_{\rm hom}$ 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 $u_{\rm hom}$ 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 $u_{\rm hom}$. 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 ([75], [71]). The following natural question, asked more than thirty years ago, is whether one can develop an associated *quantitative* ergodic theory.

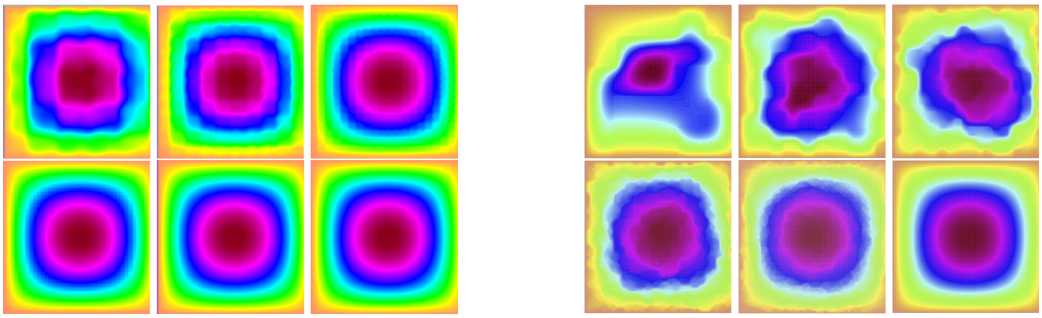

Figure 1. Solution u_ε for $\varepsilon = 1/5, 1/10, 1/20, 1/40, 1/80$ and solution $u_{\rm hom}$, periodic case (left) and random case (right)

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 $u_{\rm hom}$ 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 [76] and [43] 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 [76]. 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 [63]. 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 [77] 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 [55], [73] in the periodic setting, and [56] 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 [65] 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 $\langle|\nabla\phi_\xi|^2\rangle < \infty$, 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 [74], 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. [61].

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 [64] 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 [44]. 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 [58].

Another related and more general direction of research is the validity of *universality principle* of statistical physics, which states that the qualitative behaviour 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. Application Domains

4.1. Mechanics of heterogeneous media

The mechanics of heterogeneous materials aims at characterizing the macroscopic properties of heterogeneous materials using the properties of their constituents.

The homogenization theory is a natural tool for this task. In particular, for linear problems (linear conductivity or linear elasticity), the macroscopic properties are encoded into a single (conductivity or elasticity) homogenized tensor. The numerical approximation of this homogenized tensor is a typical objective of quantitative homogenization.

For nonlinear problems, such as rubber elasticity, the macroscopic properties are no longer characterized by a single tensor, but rather by a nonlinear energy density. 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. This endeavor is relevant both in science and technology. The rigorous derivation of rubber elasticity from polymer-physics was indeed emphasized by John Ball as an important open problem of nonlinear elasticity in his survey [50] on the field. Its solution could shed light on some aspects of polymer-physics. The associated ab initio derivation of constitutive laws (as an alternative to phenomenological laws) would also be of interest to computational mechanics and rubber industry.

For this application domain, we work in close collaboration with physicists (FranÃ§ois Lequeux, ESPCI) and researchers from mechanics and computational mechanics (Patrick Le Tallec, Ecole polytechnique).

4.2. Numerical simulation in heterogeneous media

Solving numerically PDEs in highly heterogeneous media is a problem encountered in many situations, such as the transport of pollutants or the design of oil extraction strategies in geological undergrounds. When such problems are discretized by standard numerical methods the number of degrees of freedom may become prohibitive in practice, whence the need for other strategies.

Numerical solution methods inspired by asymptotic analysis are among the very few feasible alternatives, and started fifteen years ago with the contributions of Hou and Wu [68] , Arbogast [47] etc. We refer to [62], [78],[2] for a recent state of the art. Numerical homogenization methods usually amount to looking for the solution of the problem (1) in the form $u_\varepsilon(x) \simeq u_0(x) + \varepsilon \nabla u_0(x) \cdot \Phi(x, \frac{x}{\varepsilon})$, where Φ is a proxy for the corrector field computed locally at point x (in particular, one does not use explicitly that the problem is periodic so that the method can be used for more general coefficients) and u_0 is a function which does not oscillate at scale.

Relying on our quantitative insight in stochastic homogenization, a first task consists in addressing the three following prototypical academic examples: periodic, quasi-periodic, and stationary ergodic coefficients with short range dependence, cf. [25]. The more ambitious challenge is to address more complex coefficients (of interest to practioners), and design adaptive and efficient algorithms for diffusion in heterogeneous media.

4.3. Laser physics

Our contribution to the analysis of models in laser physics is motivated by the LabEx CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions, a large eight-year research and training project approved by the French government in February 2012 as a "Laboratoire d'Excellence" and an initiative of mathematicians and physicists of the Université Lille 1). For this application domain, we work in close collaboration with physicists, which ensures our direct impact on these scientific issues. We focus on two applications: optical fibers and cold atoms.

In collaboration with physicists from the PhLAM laboratory in Lille, we aim at developping new techniques for the numerical integration of a family of 1D Schrödinger-like equations modelling the propagation of laser pulses in optical fibers. The questions arising are challenging since physicists would like to have fairly fast and cheap methods for their problems, with correct qualitative and quantitative behaviors. Another point is that they are interested in methods and codes that are able to handle different physical situations, hence different terms in the NLS equation. To meet these requirements, we will have to use numerical time-integration techniques such as splitting methods or exponential Runge-Kutta methods, space discretization techniques such as finite differences and fast Fourier transforms, and absorbent boundary conditions. Our goal, together with the physicists is to be able to reproduce numerically the results of the experiments they make in actual optical fibers, and then to be able to tune parameters numerically to get more insight into the appearance of rogue waves beyond the dispersive blowup phenomenon.

Recall that the Schrödinger equation also describes Bose-Einstein condensates. A second experimental team at PhLAM projects to study questions related to Anderson localization in such condensates. In fact, they will realize the "kicked rotor" (see [60]), which provides a paradigm for Anderson localization, in a Bose-Einstein condensate. We plan to collaborate with them on the theoretical underpinnings of their findings, which pose many challenging questions.

5. Highlights of the Year

5.1. Highlights of the Year

The team obtained two striking results in 2016:

- In collaboration with O. Blondel, T. Franco, and P. Gonçalves, M. Simon has made significant progress towards the *weak KPZ universality conjecture*, which states that a large class of one-dimensional weakly asymmetric conservative systems should converge to the KPZ equation, cf. [28], [7].
- In collaboration with F. Otto, M. Duerinckx and A. Gloria developed a complete theory of fluctuations in stochastic homogenization, cf. [39].

6. New Software and Platforms

6.1. MODULEF

FUNCTIONAL DESCRIPTION

The numerical method to approximate the constitutive laws for rubber elasticity derived from polymer physics are implemented in the Inria software Modulef.

It is based on : - algorithms from stochastic geometry to generate suitable polymer networks, - Delaunay tessellation algorithms to deal with steric effects (courtesy of the Inria project-team GAMMA2), - the introduction of 1-dimensional finite elements for the polymer-chains in Modulef.

- Participants: Marina Vidrascu and Antoine Gloria
- Contact: Marina Vidrascu
- URL: https://www.rocq.inria.fr/modulef/

7. New Results

7.1. Macroscopic behaviors of large interacting particle systems

7.1.1. Stochastic acceleration and approach to equilibrium

S. De Bièvre, Carlos Mejia-Monasterio (Madrid) and Paul E. Parris (Missouri) [57] studied thermal equilibration in a two-component Lorentz gas, in which the obstacles are modeled by rotating disks. They show that a mechanism of dynamical friction leads to a fluctuation-dissipation relation that is responsible for driving the system to equilibrium.

Stephan De Bièvre, Jeremy Faupin (Metz) and Schuble (Metz) [59] studied a related model quantum mechanically. Here a quantum particle moves through a field of quantized bose fields, modeling membranes that exchange energy and momentum with the particle. They establish a number of spectral properties of this model, that will be essential to study the time-asymptotic behavior of the system.

S. De Bièvre and collaborators analyse in [20] a multi-particle, kinetic version of a Hamiltonian model describing the interaction of a gas of particles with a vibrating medium. They prove existence results for weak solutions, and identify an asymptotic regime where the model, quite surprisingly, approaches the attractive Vlasov—Poisson system.

7.1.2. Towards the weak KPZ universality conjecture

One may start by considering the microscopic system in equilibrium (its measure is parametrized by the thermodynamical quantities under investigation). By removing the mean to the empirical measure and by scaling it properly, one would like to show that the random process, obtained by this rescaling, converges, as the size of the system is taken to infinity, to another random process which is a solution of some generalized stochastic PDE. Thanks to the remarkable recent result of M. Jara and P. Gonçalves [66], one has now all in hands to establish the latter result for a particular stochastic PDE known as the stochastic Burgers equation, and its companion, the Kardar-Parisi-Zhang (KPZ) equation. Indeed, in the latter 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 [28], M. Simon in collaboration with T. Franco and P. Gonçalves, investigate the case of a microscopic dynamics with local defects, which is much harder. More precisely, the microscopic particle system is locally perturbed, and depending on the type of perturbation, the macroscopic laws can hold different boundary conditions. Since the ideas of [66] do not apply to the model considered there, they propose a new way to estimate the error in the replacement performed in the Boltzmann-Gibbs principle.

In the same spirit, M. Simon in collaboration with O. Blondel and P. Gonçalves investigate in [7] the class of kinetically constrained lattice gases that have been introduced and intensively studied in the literature in the past few years. In these models, particles are subject to restrictive constraints that make both approaches of [66] and [28] not work, so that new mathematical tools are needed. The main technical difficulty is that their model exhibits configurations that do not evolve under the dynamics and are locally non-ergodic. Their proof does not impose any knowledge on the spectral gap for the microscopic models. Instead, it relies on the fact that, under the equilibrium measure, the probability to find a blocked configuration in a finite box is exponentially small in the size of the box.

With these two recent results, M. Simon and coauthors contribute towards the *weak KPZ universality conjecture*, which states that a large class of one-dimensional weakly asymmetric conservative systems should converge to the KPZ equation.

7.1.3. Diffusion and fractional diffusion of energy

The rigorous derivation of the heat equation from deterministic systems of Newtonian particles is one of the most fundamental questions in mathematical physics. The main issue is that the existence of conservation laws and the high number of degrees of freedom impose very poor ergodic properties to the associated dynamical systems. A possible way out of this lack of ergodicity is to introduce stochastic models, in such a way that in one hand ergodicity issues are solved by the stochastic dynamics and in the other hand the qualitative behaviour of the system is not modified by the randomness. In these models, one starts with a chain of oscillators with a Hamiltonian dynamics, and one adds a stochastic component in such a way that the fundamental conservation laws (energy, momentum and *stretch* in this case) are maintained, and the corresponding Gibbs measures become ergodic.

It was already proved in [51] that these stochastic chains model correctly the behaviour of the conductivity. In particular, it is prove that Fourier law holds in dimension $d \geq 3$ if energy and momentum are conserved, and in any dimension if only energy is conserved. Once the conductivity has been successfully understood, one investigates the existence of the *hydrodynamic limit*, which fully describes the macroscopic evolution of the *empirical profiles* associated to the conserved quantity. In [41], M. Simon in collaboration with T. Komorowski and S. Olla consider the unpinned harmonic chain where the velocities of particles can randomly change sign. The only conserved quantities of the dynamics are the energy and the elongation. Using a diffusive space-time scaling, the profile of elongation evolves independently of the energy and follows a linear diffusive equation.

The energy profile evolves following a non-linear diffusive equation involving the elongation. The presence of non-linearity makes the macroscopic limit non-trivial, and its mathematical proof requires very sophisticated arguments.

In [52] and [69] it has been previously shown that in the case of one-dimensional harmonic oscillators with noise that preserves the momentum, the scaling limit of the energy fluctuations is ruled by the *fractional* heat equation

$$\partial_t u = -(-\Delta)^{3/4} u.$$

This equation does not only predict the superdiffusivity of energy in momentum-conserving models, but it also predicts the speed at which it diverges. This result opens a way to a myriad of open problems. The main goal is to observe anomalous fractional superdiffusion type limit in the context of low dimensional asymmetric systems with several conserved quantities. In two recent papers by M. Simon in collaboration with C. Bernardin, P. Gonçalves, M. Jara, M. Sasada [53] & [32], they confirmed rigorously recent Spohn's predictions on the Lévy form of the energy fluctuations for a harmonic chain perturbed by an energy-volume conservative noise. In [32] they also showed the existence of a crossover between a normal diffusion regime and a fractional superdiffusion regime by tuning a parameter of a supplementary stochastic noise conserving the energy but not the volume.

7.2. Qualitative results in homogenization

7.2.1. Isotropy and loss of ellipticity in periodic homogenization

Since the seminal contribution of Geymonat, Müller, and Triantafyllidis, it is known that strong ellipticity is not necessarily conserved by homogenization in linear elasticity. This phenomenon is typically related to microscopic buckling of the composite material. In [24] G. Francfort and A. Gloria study the interplay between isotropy and strong ellipticity in the framework of periodic homogenization in linear elasticity. Mixtures of two isotropic phases may indeed lead to loss of strong ellipticity when arranged in a laminate manner. They show that if a matrix/inclusion type mixture of isotropic phases produces macroscopic isotropy, then strong ellipticity cannot be lost.

7.2.2. From polymer physics to nonlinear elasticity

OIn [23], M. Duerinckx and A. Gloria succeeded in relaxing one of the two unphysical assumptions made in [1] on the growth of the energy of polymer chains. In particular, [23] deals with the case when the energy of the polymer chain is allowed to blow up at finite deformation.

7.2.3. The Clausius-Mossotti formula

In the mid-nineteenth century, Clausis, Mossotti and Maxwell essentially gave a first order Taylor expansion for (what is now understood as) the homogenized coefficients associated with a constant background medium perturbed by diluted spherical inclusions. Such an approach was recently used and extended by the team MATHERIALS to reduce the variance in numerical approximations of the homogenized coefficients, cf. [46], [45], [72]. In [22], M. Duerinckx and A. Gloria gave the first rigorous proof of the Clausius-Mossotti formula and provided the theoretical background to analyze the methods introduced in [72].

7.3. Quantitative results in stochastic homogenization

7.3.1. Quantitative results for almost periodic coefficients

In [6], S. Armstrong, A. Gloria and T. Kuusi (Aalto University) obtained the first improvement over the thirty year-old result by Kozlov [70] on almost periodic homogenization. In particular they introduced a class of almost periodic coefficients which are not quasi-periodic (and thus strictly contains the Kozlov class) and for which almost periodic correctors exist. Their approach combines the regularity theory developed by S. Armstrong and C. Smart in [49] and adapted to the almost periodic setting by S. Armstrong and Z. Shen [48], a new quantification of almost-periodicity, and a sensitivity calculus in the spirit of [3].

7.3.2. Optimal stochastic integrability in stochastic homogenization

In [40] A. Gloria and F. Otto consider uniformly elliptic coefficient fields that are randomly distributed according to a stationary ensemble of a finite range of dependence. They show that the gradient and flux $(\nabla\phi, a(\nabla\phi + e))$ of the corrector ϕ, when spatially averaged over a scale $R \gg 1$ decay like the CLT scaling $R^{-d/2}$. They establish this optimal rate on the level of *sub-Gaussian* bounds in terms of the stochastic integrability, and also establish a suboptimal rate on the level of optimal Gaussian bounds in terms of the stochastic integrability. The proof unravels and exploits the self-averaging property of the associated semi-group, which provides a natural and convenient disintegration of scales, and culminates in a propagator estimate with strong stochastic integrability. As an application, they characterize the fluctuations of the homogenization commutator, and prove sharp bounds on the spatial growth of the corrector, a quantitative two-scale expansion, and several other estimates of interest in homogenization.

7.3.3. A theory of fluctuations in stochastic homogenization

In [39], M. Duerinckx, A. Gloria, and F. Otto establish a path-wise theory of fluctuations in stochastic homogenization of linear elliptic equations in divergence form. More precisely they consider the model problem of a discrete equation with independent and identically distributed conductances (as considered in [27]). They identify a single quantity, which they call the homogenization commutator, that drives the fluctuations in stochastic homogenization in the following sense. On the one hand, this tensor-valued stationary random field satisfies a functional central limit theorem, and (when suitably rescaled) converges to a Gaussian white noise. On the other hand, the fluctuations of the gradient of the corrector, the fluctuations of the flux of the corrector, and the fluctuations of any solution of the PDE with random coefficients and localized right-hand side are characterized at leading order by the fluctuations of this homogenization commutator in a path-wise sense. As a consequence, when properly rescaled, the solution satisfies a functional central limit theorem, the gradient of the corrector converges to the Helmholtz projection of a Gaussian white noise, and the flux of the corrector converges to the Leray projection of the same white noise. Compared to previous contributions, our approach, based on the homogenization commutator, unravels the complete structure of fluctuations. It holds in any dimension $d \geq 2$, yields the first path-wise results, quantifies the limit theorems in Wasserstein distance, and only relies on arguments that extend to the continuum setting and to the case of systems.

7.4. Numerical methods for evolution equations

In [36] G. Dujardin analyzes an exponential integrator applied to the nonlinear Schrödinger equation with white noise dispersion. This models appears in optic fibers. Together with his co-author, he proves that this explicit scheme applied to the sctochastic PDE is of mean-square order 1. He uses it to illustrate a conjecture on the well-posedness of the equation in some regimes of the nonlinearity. Comparisons with several other schemes of the litterature are proposed. A last, another new (implicit) exponential integrators is proposed, which preserves the L^2-norm of the solution and is compared with the explicit one introduced beforehand.

7.5. Schrödinger equations

7.5.1. Nonlinear optical fibers

S. Rota Nodari, G. Dujardin, S. De Bièvre and collaborators continued their previous work on periodically modulated optical fibers with the experimental physicists of PhLAM [19]. They show that the nonlinear stage of modulational instability induced by parametric driving in the *defocusing* nonlinear Schrödinger equation can be accurately described by combining mode truncation and averaging methods, valid in the strong driving regime. The resulting integrable oscillator reveals a complex hidden heteroclinic structure of the instability. A remarkable consequence, validated by the numerical integration of the original model, is the existence of breather solutions separating different Fermi-Pasta-Ulam recurrent regimes.

In [42] S. de Bièvre and G. Dujardin analyze the formation of the Kuznetsov-Ma soliton of the 1D Schrödinger equation in the presence of periodic modulation satisfying an integrability condition. They show that this particular soliton has several compression points, the number, position and shape of which are controlled by the amplitude and the frequency of the modulation. They analyze the interplay between the frenquency of the soliton and the frequency of the modulation. Moreover, they show that one can suppress any component of the output spectrum of the soliton by a suitable choice of the amplitude and frequency of the modulation.

These works are part of the activities developped in the LabEx CEMPI.

7.5.2. Nonlinear Schrödinger equations

In [54], D. Bonheure, J.-B. Casteras and R. Nascimento obtained new results on the existence and qualitative properties of waveguides for a mixed-diffusion NLS. In particular, they proved the first existence results for waveguides with fixed mass and provided several qualitative descriptions of these.

S. De Bièvre and S. Rota Nodari continued their work on orbital stability of relative equilibria of Hamiltonian dynamical systems on Banach spaces, with a second paper [37], dealing with the situation where multi-dimensional invariance groups are present in the systems considered. They 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 the plane waves of a system of two coupled nonlinear Schrödinger equations. They provide a comparison of their approach to the classical one by Grillakis-Shatah-Strauss.

7.6. Miscellaneous results

In [21] Mitia Duerinckx establishes the global well-posedness of a family of equations, which are obtained in certain regimes — in a joint work in preparation with Sylvia Serfaty — as the mean-field evolution of the supercurrent density in a (2D section of a) type-II superconductor with pinning and with imposed electric current. General vortex-sheet initial data are also considered, and the uniqueness and regularity properties of the solution are investigated.

In [33], [8], [11], [12], 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 [16], [17], [35], J.-B. Casteras and collaborators study different problems related to the existence of constant mean curvature hypersurfaces with prescribed asymptotic boundary on Cartan-Hadamard manifold. In particular, they obtained the first existence results for minimal graphs with prescribed asymptotic Dirichlet data under a pointwise pinching condition for sectionals curvatures.

S. De Bièvre and co-workers present in [67] a general approach to calculating the entanglement of formation for superpositions of two-mode coherent states, placed equidistantly on a circle in phase space. In the particular case of rotationally-invariant circular states the value of their entanglement is shown to be given by analytical expressions. They analyse the dependence of the entanglement on the radius of the circle and number of components in the superposition.

A. Benoit continues his analysis of hyperbolic equations in corner spaces. He addresses in [30] the rigorous construction of geometric optics expansions for weakly well-posed hyperbolic corner problems. He studies in [31] the semi-group stability for finite difference discretizations of hyperbolic systems of equations in corner domains, extending previous results of Coulombel & Gloria and Coulombel in the case of the halfspace.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. 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.

8.1.2. 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 Rennes.

Duration: October 2014 - October 2019.

8.1.3. 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 behaviour 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.

8.1.4. 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)

8.1.5. 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.

8.1.6. 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.

8.2. European Initiatives

8.2.1. FP7 & H2020 Projects

8.2.1.1. QUANTHOM

Title: Quantitative methods in stochastic homogenization

Programm: FP7

Duration: February 2014 - January 2019

Coordinator: Université Libre de Bruxelles (Belgium)

Partner: Inria

Inria contact: A. 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 I 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, I 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. I 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.'

8.2.2. Collaborations with Major European Organizations

Max Planck Institute for Mathematics in the Sciences (Germany)

Long-term collaboration with F. Otto on the development of a quantitative theory of stochastic homogenization of linear elliptic systems.

8.3. International Research Visitors

8.3.1. Visits of International Scientists

Milton Jara, Professor Adjunto, IMPA, Rio de Janeiro (Brazil), was an invited professor at Université Lille 1 funded by the LabeX CEMPI.

8.3.1.1. Internships

Pierre Mennuni, MA2 Université Lille 1, Internship, 3 months

8.3.1.2. Research Stays Abroad

M. Simon spent one month at Universidade Federal Fluminense (Niteroi, Brazil) in march 2016, sponsored by the "Réseau France-Brésil", as a guest of Freddy Hernandez.

S. De Bièvre visited C. Mejia-Monasterio at the Technical University of Madrid in June 2016.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

D. Bonheure was General chair of the committee of the BRUXELLES-TORINO TALKS IN PDE'S MAY 2-5 2016 UNIVERSITÀ DEGLI STUDI DI TORINO DIPARTIMENTO DI MATEMATICA "GIUSEPPE PEANO"

9.1.2. Journal

9.1.2.1. Member of the Editorial Boards

D. Bonheure is associate editor at the Bulletin of the Belgian Mathematical Society - Simon Stevin (http://projecteuclid.org/info/euclid.bbms)

A. Gloria is associated editor at the North-Western European Journal of Mathematics (http://math.univ-lille1.fr/~nwejm/).

9.1.3. Invited Talks

D. Bonheure was invited speaker at

- 02/12/2016, Recent progress in Partial Differential Equations, Université Aix-Marseille
- 03/10/2016 au 07/10/2016, New trends in Partial Differential Equations, Centro De Giorgi, SNS Pisa
- 28/09/2016 au 30/09/2016, 3rd Conference on Recent Trends in Nonlinear Phenomena, Perugia
- 12/09/2016 au 17/09/2016, Partial Differential Equations and Related Topics – On the occasion of Giorgio Talenti's 75th birthday , Alghero

Stephan De Bièvre was invited speaker at

- Université Fourier, Grenoble, Mathematical Physics Seminar, April 2016
- Université de Nantes, Mathematical Physics Seminar, May 2016
- Spectral and Scattering theories in QFT, IV, Porquerolles, May 2016
- 11th AIMS Conference on Dynamical systems, ODE, and Applications, Orlando, July 2016
- Conference "Coherent States and their Applications: A Contemporary Panorama", CIRM Marseille, November 2016

A. Gloria was invited speaker at

- ENS Rennes, January 2016
- GAMM conference, Paris, January 2016
- Winter school on stochastic homogenization, Augsburg, February 2016
- Bristish Mathematical Colloquium, Bristol, March 2016
- Courant Institute, NYU, New York, May 2016
- 15th European Mechanics of Materials Conference, Brussels, September 2016
- Probability seminar, Warwick, October 2016
- Workshop “Functional inequalities, heat kernels, and random processes”, Oberwolfach institute, December 2016

M. Simon was invited speaker at

- YEP XIII: Large Deviations for Interacting Particle Systems and Partial Differential Equations, Eindhoven (Netherlands)
- Workshop in Stochastic Analysis, Universidade Federal de Campinas, Brazil
- Tokyo University, Probability Seminar
- Workhsop "Large Scale Stochastic Dynamics", Oberwolfach institute, Germany

9.1.4. Leadership within the Scientific Community

D. Bonheure is member of the Executive board of the Belgian Mathematical Society.

S. De Bièvre is

- the scientific coordinator of the CEMPI (2012-2019),
- member of the drafting committee of the IDEX UDL, and of the delegation that presented the project to the jury in Paris (April 2015, January 2016),
- member of the Executive Committee of the International Association of Mathematical Physics (since 2012).

9.1.5. Scientific Expertise

D. Bonheure is a member of the ESF College of Expert Reviewers from 20 October 2016 to 19 October 2019

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence : Denis Bonheure, Integral and differential calculus, 46h, L1 (mathematics & physics), Université Libre de Bruxelles, Belgium

Licence : Denis Bonheure, Mathematics for management engineering, 30h, L1 (mathematics & physics), Université Libre de Bruxelles, Belgium

Licence : Guillaume Dujardin, Integral and differential calculus, 60h, L2 (mathematics & physics), Université Libre de Bruxelles, Belgium

Licence : Stephan De Bièvre, Probability, 15h, L2 (physics), Université Lille 1

Licence : Stephan De Bièvre, Probability, 50h, L3 (mathematics), Université Lille 1

Licence : Stephan De Bièvre, Financial mathematics, 30h, L1 (economics), Université Lille 1

Master : Denis Bonheure, Variational methods and PDEs, 30h, M2, Université Libre de Bruxelles, Belgium

Master : Antoine Gloria, Anderson localization, 30h, M2, Université Libre de Bruxelles, Belgium

Master : Antoine Gloria, Fluctuations in stochastic homogenization, 4h30, Doctoral course, YEP XIII, Eindhoven, Netherlands

9.2.2. Supervision

PhD in progress : Mitia Duerinckx, Topics in stochastic homogenization of PDEs, 01/10/2014, A. Gloria & S. Serfaty (NYU).

PhD in progress : Pierre Mennuni, Université Lille 1, 01/10/2016, S. De Bièvre, A. De Laire (Lille 1) & G. Dujardin

PhD in progress : Hussein Cheikh-Ali, Université Libre de Bruxelles and Université de Lorraine, D. Bonheure (ULB) & F. Robert (Nancy)

PhD in progress : Robson Alves do Nascimento Filho, Université Libre de Bruxelles, D. Bonheure (ULB)

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9.2.3. Juries

S. De Bièvre was in the jury of the PhD theses of A. Newman (Loughbourough, England), A. Vavasseur (Nice) and J.P. Miqueu (Rennes).

9.3. Popularization

M. Simon gave a talk at ESPE (Ecole Supérieure du Professorat et de l'Education) during the week "Semaine des mathématiques", about the mathematical properties of the official soccer ball. Marielle Simon is part of the program "MathenJeans".

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