Activity Report 2014

Team MEPHYSTO

Quantitative methods for stochastic models in physics

RESEARCH CENTER
Lille - Nord Europe

THEME
Numerical schemes and simulations

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Team MEPHYSTO

Keywords: Homogenization, Stochastic Models, Multiscale Analysis, Numerical Methods, Statistical Physics

Creation of the Team: 2014 January 01.

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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. A. Gloria spends one day a week in Lille, G. Dujardin spends one day a week in Brussels, and S. Armstrong visits both Brussels and Lille on a monthly basis.

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 ([54], [50]). The following natural question, asked more than thirty years ago, is whether one can develop an associated *quantitative* ergodic theory.

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 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.

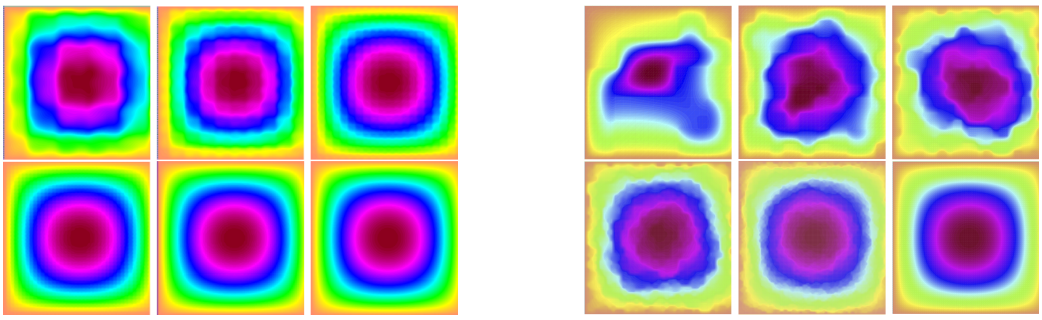

Figure 1. Solution u_ε for $\varepsilon = 1/5, 1/10, 1/20, 1/40, 1/80$ and solution u_{hom}, periodic case (left) and random case (right)

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 [55] and [35] 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 [55]. 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 [46]. 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 [56] 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 [41], [52] in the periodic setting, and [42] 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 [6]. With P. Le Tallec (Mechanics department, Ecole polytechnique, France), M. Vidrascu (project-team REO, Inria Paris-Rocquencourt), and A. Gloria introduced and tested in [15] 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 [4]. 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 [4], [5] 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 [53], 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. [44].

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 [47] 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. Dynamical localization and kicked rotors

The kicked rotor is a unitary discrete time dynamics proposed in the seventies in the context of studies on quantum chaos, and used recently as a "quantum simulator" for the Anderson model. It is a quantum equivalent of the standard map and is obtained by integrating a time-dependent linear Schrödinger equation with a time-periodic, very singular (delta comb) potential. It continues to pose considerable mathematical challenges, in particular the so-called "quantum suppression of classical chaos" in the presence of a strong potential, which remains an open problem from the mathematical point of view. It can be rephrased as follows: show that the H^1 norm of the solution is uniformly bounded in time (see [36] for more background). In more recent years, the question has arisen how the behavior of this system would change in the presence of a nonlinear term in the Schrödinger equation.

This problem displays both numerical and analytical challenges, in particular because of the difficulty to obtain long time simulations of the system and because of the presence of instabilities due to the nonlinearity. Preliminary theoretical results motivate some conjectures on the behavior of these systems, that we plan to validate empirically in a first step. Indeed, reliable long-time simulations of the system should allow us to get more insight into the behavior of the exact solutions in the unstable cases. One of the main difficulties for the numerical simulation is the intrinsic instability of the system, which magnifies quite rapidly the numerical error due to machine precision. This requires the use of multiprecision techniques in order to handle reasonably long times, even for moderate nonlinearities, and of the transparent boundary conditions recently introduced by members of the former SIMPAF project-team.

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 [40] 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 (François 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 [49], Arbogast [37] etc. We refer to [45], [57],[3] 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 $\Phi(x, \cdot)$ is a proxy for the corrector field computed locally at point $x \in D$ (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 ε.

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. 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 [43]), 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. New Software and Platforms

5.1. Platforms

5.1.1. Modulef

The numerical method to approximate the constitutive laws for rubber elasticity derived from polymer physics (as used in [15], [25]) are implemented in the Inria software Modulef (joint work of M. Vidrascu, projetc-team REO, and A. Gloria).

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.

5.1.2. CMA-ES

To solve the inverse problem for the reconstruction of an explicit constitutive law from in silico experiments in [25], we relied on the Covariance Matrix Adaptation Evolution Strategy developed in the project-team TAO.

https://www.lri.fr/~hansen/cmaesintro.html

5.1.3. FreeFEM++

The numerical methods proposed in [14] for the approximation of homogenized coefficients were implemented in FreeFEM++, a user-friendly PDE-solver.

http://www.freefem.org/ff++/

6. New Results

6.1. Highlights of the Year

A. Gloria, S. Neukamm, and F. Otto published their recent contribution [17] on quantitative homogenization in Inventiones Mathematicae.

As a plenary speaker of the World Congress of Computational Mechanics in Barcelone in July 2014, P. Le Tallec (Ecole polytechnique) presented our joint results [15], [25].

6.2. Quantitative stochastic homogenization

A. Gloria, S. Neukamm (Univ. Dresden), and F. Otto (MPI for mathematics in the sciences, Leipzig) developed in [17] a general approach to quantify ergodicity in stochastic homogenization of discrete elliptic equations. Using a parabolic approach, they obtained optimal estimates on the time-decay of the so-called environment seen from the particle. This allowed them to prove optimal bounds on the corrector gradient and the corrector itself in any dimension (thus improving on [4]). They also obtained the first error analysis of the popular periodization method to approximate the homogenized coefficients.

In [32], A. Gloria and F. Otto extended their results [4], [5] on discrete elliptic equations to the continuum setting. They treated in addition the case of non-symmetric coefficients, and obtained optimal estimates in all dimensions by the elliptic approach (whereas [4], [5] were suboptimal for $d = 2$).

In [28], A. Gloria and D. Marahrens (MPI for mathematics in the sciences, Leipzig) extended the annealed results [51] on the discrete Green function by D. Marahrens and F. Otto to the continuum setting. As a by-product of their result, they obtained new results in uncertainty quantification by estimating optimally the variance of the solution of an elliptic PDE whose coefficients are perturbed by some noise with short range of dependence.

In their recent work [29], A. Gloria, S. Neukamm, and F. Otto developed a regularity theory for random elliptic operators inspired by the contributions of Avellaneda and Lin [39] in the periodic setting and of our visitor S. Armstrong with C. Smart [38]. This allowed them to consider coefficients with arbitrarily slow decaying correlations in the form of a family of correlated Gaussian fields.

In [30], A. Gloria and J. Nolen (Duke Univ.) proved a quantitative central limit theorem for the effective conductance on the discrete torus. In particular, they quantified the Wasserstein distance between a normal random variable and the CLT-like rescaling of the difference between the approximation of the effective conductance by periodization and the effective conductance. Their estimate is sharp and shows that the Wasserstein distance goes to zero (up to logarithmic factors) as if the energy density of the corrector was iid (which it is not). This completes and settles the analysis started in [17] on the approximation of homogenized coefficients by periodization by characterizing the limiting law in addition to the scaling.

6.3. Derivation of nonlinear elasticity from polymer-physics

In [15], A. Gloria, P. Le Tallec (Mechanics department, Ecole polytechnique), and M. Vidrascu (Project-team REO, Inria) numerically investigated the nonlinear elasticity model obtained in [1] by discrete stochastic homogenization, and compared it to the standard measurements by Treloar on natural rubber. The implementation was realized in the Modulef software. These results are in rather good agreement, which shows that the approach seems to be promising.

In [25], M. de Buhan (CNRS, Univ. Paris Descartes), A. Gloria, P. Le Tallec and M. Vidrascu proposed a numerical method to produce analytical approximations (that can be used in practical nonlinear elasticity softwares) of the numerical approximations obtained in [15] of the discrete-to-continuum energy density derived theoretically in [1]. This numerical method is based on the parametrization of the set of polyconvex Ogden laws and on the combination of a least square method and a genetic algorithm (cf. CMA-ES).

6.4. Numerical homogenization

Inspired by the quantitative analysis of [17] and [48], Z. Habibi (former SIMPAF post-doctoral fellow) and A. Gloria introduced in [14] a general method to reduce the so-called resonance error in numerical homogenization, both at the levels of the approximation of the homogenized coefficients and of the correctors. This method significantly extends [2]. The method relies on the introduction of a massive term in the corrector equation and of a systematic use of Richardson extrapolation. In the three academic examples of heterogeneous coefficients (periodic, quasiperiodic, and Poisson random inclusions), the method yields optimal theoretical and empirical convergence rates, and outperforms most of the other existing methods.

6.5. Nonlinear Schrödinger equation

S. De Bièvre, S. Rota Nodari (CEMPI postdoc 2013-2015) and F. Genoud (CEMPI visitor, September 2013) have explained the geometry underlying the so-called energy-momentum method for proving orbital stability in infinite dimensional Hamiltonian systems. Applications include the orbital stability of solitons of the NLS and Manakov equations. This work is to appear as a chapter (120p) in the first volume of the CEMPI Lecture Notes in Mathematics, cf. [24].

6.6. Kicked rotors

S. De Bièvre and his PhD student E. Soret rigorously proved the growth rate of the energy in a Markovian model for stochastic acceleration of a particle in a random medium, cf. [34].

6.7. Time integration of Hamiltonian system with noise

G. Dujardin introduced an energy preserving method for Hamiltonian dynamics perturbed by a multiplicative noise, cf. [11].

6.8. Miscellaneous results

The MEPHYSTO team is currently hosting former members of the project-team SIMPAF who focus on numerical methods for dissipative systems:

- corrosion models [19], [23],
- fluid mechanics [9], [21], [27], [10],
- numerical analysis for asymptotic preserving properties [8], [7],
- a posteriori estimates [20].

T. Gallouët also made contributions in optimal transport [22], [26].

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

The team (C. Chainais and A. Gloria) has had its third bilateral contract with ANDRA (French nuclear waste storage agency) from December 2012 to June 2014. The post-doctoral position of T. Gallouët was funded by this contract.

This collaboration concerned mathematical and numerical issues on a corrosion model, and in particular the identification of steady-states and the design of asymptotic-preserving schemes for a free interface problem.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR BECASIM

G. Dujardin and I. Lacroix are members 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 2016.

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

8.1.2. 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.

8.2. European Initiatives

8.2.1. FP7 & H2020 Projects

8.2.1.1. QUANTHOM

Type: FP7
Instrument: ERC Starting Grant
Duration: February 2014 - January 2019
Coordinator: Antoine Gloria
Partner: Département de mathématique, Université Libre de Bruxelles (Belgium)
Inria contact: Antoine Gloria
Abstract: Quantitative methods in stochastic homogenization

8.2.2. Collaborations with Major European Organizations

Max Planck Institute for Mathematics in the Sciences (Germany).
Development of a quantitative theory of stochastic homogenization.

8.3. International Initiatives

8.3.1. Inria International Partners

8.3.1.1. Informal International Partners

The activity around quantitative stochastic homogenization was developed in collaboration with F. Otto, director of the Max Planck Institute for Mathematics in the Sciences, Leipzig (Germany).

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- Daniel Marahrens (MPIMS, Leipzig): one week in March (A. Gloria), annealed estimates on Green's functions.
- Felix Otto (MPIMS, Leipzig): one week in April (A. Gloria), quantitative stochastic homogenization.
- Gilbert Reinisch (physicist at University of Reykjavik): from May 12th 2014 to May 28th 2014 (G. Dujardin and M. Gazeau), numerical simulations of several differential systems modelling the evolution of quantum dots. This visit was cofounded by Inria and the LabEx CEMPI. This work is a follow up of the paper [18].
- Marco Cicalese (Univ. Munich): one week in May (A. Gloria), derivation of nonlinear elasticity from polymer-physics.
- Jean-Christophe Mourrat (ENS Lyon): 10 days in May (A. Gloria), quantitative stochastic homogenization.
- Stefan Neukamm (Weierstrass Institute, Berlin, now at Univ. Dresden): 10 days in May (A. Gloria), quantitative stochastic homogenization.
- Ansgar Jüngel (Univ. Vienna): one week in July (C. Chainais and I. Lacroix-Violet), discrete functional inequalities for asymptotic preserving schemes.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific events organisation

9.1.1.1. General chair, scientific chair

S. De Bièvre is the scientific coordinator of CEMPI

9.1.1.2. Member of the organizing committee

D. Bonheure and A. Gloria organize a PDE and analysis seminar at Brussels (http://homepages.ulb.ac.be/~dbonheur/seminaire-ANEDP.html).

G. Dujardin and I. Lacroix are in charge of the PDE and numerical analysis seminar of the Paul Painlevé mathematics department in Lille (http://math.univ-lille1.fr/d7/sanedp).

G. Francfort (Paris 13), A. Gloria, and M. Kruzik organized a workshop "Relaxation, homogenization and dimensional reduction in hyperelasticity" at Université Paris-Nord, March 25-27, 2014 (http://staff.utia.cas.cz/kruzik/workshop/).

9.1.2. Journal

9.1.2.1. Member of the editorial board

D. Bonheure is associate editor at the Bulletin of the Belgian Mathematical Society - Simon Stevin (http://projecteuclid.org/DPubS?service=UI&version=1.0&verb=Display&handle=euclid.bbms), the Journal of calculus of variations (http://www.hindawi.com/journals/jcv/), and International Scholarly Research Notices (http://www.hindawi.com/journals/isrn/).

C. Chainais and A. Gloria are associate editors at the North-Western European Journal of Mathematics (http://math.univ-lille1.fr/~nwejm/), a new journal launched by the mathematical departments of the French region Nord-Pas-De-Calais.

9.1.2.2. Reviewer

The members of the team reviewed numerous papers for numerous international journals.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

The members of the team are mainly academics. We teach at the licence and master levels at the Université Lille 1 and ULB.

9.2.2. Supervision

PhD in progress: P.-L. Colin, Theoretical and numerical study of some corrosion models, since October 2012, advised by C. Chainais and I. Lacroix-Violet.

PhD in progress: M. Duerinckx, Problems in stochastic homogenization, since October 2014, advised by A. Gloria and S. Serfaty (UPMC).

PhD in progress: E. Soret, Stochastic acceleration and thermalization, since October 2011, advised by S. De Bièvre and T. Simon (Lille 1).

9.3. Popularization

C. Calgaro is the organizer of the action "Mathématiques itinérantes" (http://mathematiques.univ-lille1.fr/Ouvertures/Mathematiques-itinerantes/), which promotes mathematics among young people (conferences in highschools, "journées de la science", etc.). Members of the team regularly participate in these actions.

10. Bibliography

Major publications by the team in recent years

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