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Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization

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Abstract. The workshop has brought together experts in the broad field of partial differential equations with highly heterogeneous coefficients. Analysts and computational and applied mathematicians have shared results and ideas on a topic of considerable interest both from the theoretical and applied viewpoints. A characteristic feature of the workshop has been to encourage discussions on the theoretical as well as numerical challenges in the field, both from the point of view of deterministic as well as stochastic modeling of the heterogeneities.

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Introduction by the Organisers

Multiscale problems are ubiquitous in modern science and engineering. Applications are many: materials science, underground flows, wave propagation, etc. Indeed, materials that seem to be a continuum are made up of atoms. Geological media have many scales ranging from very small (atomistic), to an order of magnitude larger (pore and crack sizes), and to even much larger sizes of tectonic plates. Composite materials that are critical for modern technology are typically multiscale (e.g., small filling particles of different sizes in a sample of much larger size or layers of various thickness in a laminate composite).

Many, though not all, of the models involve random modeling. Mathematics evidently plays a major role in this area. It covers the whole spectrum from theory

(with homogenization theory, variational calculus, etc) to scientific computing, via numerical analysis (with the development of adequate, multiscale, finite element methods and related approaches). Statistics-based methods are also employed. While modeling at each specific fundamental scale (e.g., molecular dynamics at atomistic scales, continuum PDEs at much larger scales) has been quite successful, the coupling between different scales is not well understood mathematically.

The workshop has been an opportunity to make a state-of-the art review of the mathematical knowledge in a broad sense, to draw up a list of the challenges to overcome in the near future. It was a unique opportunity to bring together experts from all the areas involved. Approximately 45 scientists with very different backgrounds attended. Many delivered a talk, presenting their recent contributions in the light of their own perspectives. The quite compact schedule we had did not prevent many informal interactions to take place over coffee breaks, meals and lively evenings.

On the theoretical side, we heard about recent theoretical achievements on quantitative rates of convergence in stochastic homogenization, on the Einstein relation, or on derivations of models for rough boundaries. Several contributions presented novel results on homogenization in the presence of large random potentials and on the derivation of macroscopic models to understand the energy density and phase information of waves propagating in highly heterogeneous media. Several discussions focused on the relatively uncharted territory of understanding the propagation of uncertainty from the coefficients in an equation to the solution of said equation.

Many numerical analysis talks were devoted to novel numerical methods for approximating the solution space of PDEs with rough coefficients and possibly with non-separated scales. This generated intense discussion among the participants. Common features and differences between the approaches were discussed in terms of robustness, cost, assumptions made, generality, ease of implementation, mathematical rigor and optimality. While there is a variety of heuristic numerical schemes, the mathematical understanding of such problems remains relatively underdeveloped. The workshop helped fill that gap through such discussions.

Techniques using polynomial chaos expansion were also a topic of choice. Variance reduction issues, and more general aspects of Monte-Carlo methods, were the topic of several talks. Applications as varied as transport processes through membranes, wave propagation phenomena, underground flows in porous media, nanotechnologies, colloid dynamics, optimal design of trussed materials, modeling of composite materials used in the aerospace industry, were addressed. Based on the feedback already received from participants, we consider the organization of such a workshop equally beneficial for scientists interested in theoretical issues, applied mathematicians developing numerical techniques, and mechanical engineers in contact with practical problems. The mixing of experts at deterministic and stochastic techniques was extremely rewarding for both camps. We hope other workshops in the same spirit will be organized in the near future.

Workshop: Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization

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Abstracts

Coupling reduced basis and numerical homogenization methods for solving quasilinear elliptic problems

Assyr Abdulle

We study finite element (FE) discretizations of quasilinear second-order elliptic problems of the form

$$-\nabla \cdot (a^\varepsilon(x, u^\varepsilon(x))\nabla u^\varepsilon(x)) = f(x) \text{ in } \Omega, \qquad u^\varepsilon(x) = 0 \text{ on } \partial\Omega, \tag{1}$$

where Ω is a bounded convex polyhedron in $\mathbb{R}^d$ with $d \leq 3$. The $d \times d$ tensor $a^\varepsilon(x, s)$, assumed to be uniformly elliptic and bounded, is allowed to vary on a very small spatial scale denoted by ε. We note that the homogenization of this problem has been studied in [8],[9], where it is shown that the homogenized equation is of the same quasilinear type as the original equation, with $a^\varepsilon(x, u^\varepsilon(x))$ replaced by a homogenized tensor $a^0(x, u^0(x))$ depending nonlinearly on a homogenized solution u^0. We are interested in the following two problems:

- derive an efficient numerical homogenization of (1) (i.e., a numerical method that approximate the homogenized solution u^0 without the a priori knowledge of $a^0(x, u^0(x))$),
- control the error of the approximation process, i.e., derive an a priori error analysis.

Notations. We consider a macro finite element (FE) space $S_0^\ell(\Omega, \mathcal{T}_H)$ made of piecewise polynomial of degree ℓ defined on a family of (macro) partition $\mathcal{T}_H$ of Ω in simplicial or quadrilateral elements K of diameter H_K ($H \gg \varepsilon$ is allowed). We then define a quadrature formula (QF) $\{x_{K_j}, \omega_{K_j}\}_{j=1}^J$ on each $K \in \mathcal{T}_H$ given by an affine transformation of a QF from a reference element $\hat{K}$. For each $K \in \mathcal{T}_H$ and $x_{K_j} \in K$, $j = 1, \ldots, J$, we define a sampling domain $K_{\delta_j} = x_{K_j} + (-\delta, \delta)^d$, ($\delta \geq \varepsilon$) and we consider a micro FE space $S^q(K_{\delta_j}, \mathcal{T}_h) \subset W(K_{\delta_j})$ with simplicial or quadrilateral FEs and piecewise polynomial of degree q ($\mathcal{T}_h$ is a conformal and shape regular family of triangulation $\mathcal{T}_h$). The space $W(K_{\delta_j})$ is either the Sobolev space $W(K_{\delta_j}) = W^1_{per}(K_{\delta_j}) = \{z \in H^1_{per}(K_{\delta_j});\ \int_{K_{\delta_j}} z dx = 0\}$ or $W(K_{\delta_j}) = H^1_0(K_{\delta_j})$.

The numerical homogenization method. We work in the framework of the finite element heterogeneous multiscale method (FE-HMM) [1, 10, 4] and consider the following micro-macro FEM [5]: Find $u^H \in S_0^\ell(\Omega, \mathcal{T}_H)$ such that

$$B_H(u^H; u^H, w^H) = F(w^H), \qquad \forall w^H \in S_0^\ell(\Omega, \mathcal{T}_H),$$

where

$$B_H(u^H; v^H, w^H) = \sum_{K \in \mathcal{T}_H} \sum_{j=1}^J \frac{\omega_{j,K}}{|K_{\delta_j}|} \int_{K_{\delta_j}} a^\varepsilon(x, u^H_{K_j}) \nabla v^h_{K_j}(u^H_{K_j}) \cdot \nabla w^h_{K_j}(u^H_{K_j}) dx,$$

and $v^h_{K_j}(s)$ is sol. of the micro pblm $v^h_{K_j}(s) - v^H_{lin} \in S_h(K_{\delta_j}, \mathcal{T}_h)$

$$\int_{K_{\delta_j}} a^\varepsilon(x,s)\nabla v^h_{K_j}(s)\cdot\nabla z^h dx = 0 \quad \forall z^h \in S_h(K_{\delta_j},\mathcal{T}_h),$$

and similarly for $w^h_{K_j}(s)$). Here we use the short-hand notation $u^H_{K_j} = u^H(x_{K_j})$.

The Newton method. A practical computation of a macroscopic numerical solution relies on a Newton method: consider a sequence $\{u^H_k\}$ such that

$$\partial B_H(u^H_k; u^H_{k+1} - u^H_k, w^H) = F_H(w^H) - B_H(u^H_k; u^H_k, w^H)\ \forall w^H \in S^\ell_0(\Omega,\mathcal{T}_H),$$

where the Fréchet derivative ∂B_H is given by

$$\partial B_H(z^H; v^H, w^H) := B_H(z^H; v^H, w^H)$$
$$+ \quad \sum_{K\in\mathcal{T}_H}\sum_{j=1}^{J} \omega_{K_j}\frac{d}{ds}a^0_{K_j}(s)|_{s=z^H(x_{K_j})} v^H(x_{K_j})\nabla z^H(x_{K_j})\cdot\nabla w^H(x_{K_j}).$$

For the implementation we consider $z^H_k = \sum_{i=1}^{M_{macro}} U^i_k \phi^H_i$, $U_k = (U^1_k, \dots, U^{M_{macro}}_k)^T$

$$\big(B(z^H_k) + B'(z^H_k)\big)(U_{k+1} - U_k) = -B(z^H_k)U_k + F.$$

The local contribution to the stiffness matrix relies on the matrices $B_K(z^H_k)$ and $B'_K(z^H_k)$. This latter matrix involves the computation of $\frac{\partial}{\partial s}(B_{K,j}(s))$ that can be approximated by $\frac{\partial}{\partial s}(B_{K,j}(s)) \approx \frac{B_{K,j}(s+\sqrt{eps})-B_{K,j}(s)}{\sqrt{eps}}$. Hence, at each iteration of the Newton method, we have to solve $\mathcal{O}(M_{mac})$ micro problems, where M_{mac} represents the macroscopic degrees of freedom (DOF). Furthermore the a-priori estimates given in [5] indicate that the DOF in each micro problem have to increase as M_{mac} increases.

Reduced basis FE-HMM. In order to reduce the computational complexity of the FE-HMM, we suggest a reduced basis (RB) FE-HMM. The use of RB for numerical homogenization problems has first been proposed in [12] and analyzed for the FE-HMM for a class of linear elliptic problems in [3],[6]. The RB-FE-HMM method is based on offline and online stages. In the offline procedure, accurate micro solutions for the original problem on sampling domains are selected and computed. Theses micro problems are parametrized by the location of the cell problem in the domain Ω and (for nonlinear problems) by the value of the macroscopic solution at this location. We consider a compact subspace $\mathcal{D}$ of $\Omega\times\mathbb{R}$ ($\mathcal{D}$ should be chosen such that $T_\delta \subset \Omega$, for all $(x_\tau, s) \in \mathcal{D}$). For any randomly chosen parameter we define the map G_{x_τ} from the physical sampling domain $T_\delta = x_\tau + (-\delta/2, \delta/2)^d$ centered at x_τ to the reference domain Y. A greedy algorithm allows to choose an optimal basis of micro functions

$$\hat{S}_N(Y) = \mathrm{span}\{\hat{\xi}_{\mathcal{N},n}(y),\ n = 1,..,N\}$$

that is computed with high accuracy for selected values of the parameters.

We note that a crucial ingredient for the Greedy algorithm are appropriate a posteriori error estimates for the construction of the basis of $\hat{S}_N(Y)$. As the pre-computed microscopic functions depend nonlinearly on the macroscopic solution,

we introduce a new a posteriori error estimator for the Greedy algorithm that guarantees the convergence of the online Newton method and the uniqueness of the method.

In the online stage, the micro problems are then computed in the sampling domains K_{δ_j} as defined above using the reduced basis space (a shifted and scaled version of $\hat{S}_N(Y)$). If one has an "affine" representation of the tensor $a^\varepsilon(x,s) = a(x,x/\varepsilon,s) = \sum_{q=1}^{Q} \Theta_q(x,s) a_q(x/\varepsilon)$ then the online micro problems can be computed by solving a small $N \times N$ linear system (essentially pre-assembled in the onfline stage), where N is the dimension of $\hat{S}_N(Y)$ (N is usually small when the RB strategy applies). When the affine representation is not available an interpolation method [11] can be used to approximate the tensor in an affine form.

A priori error estimates in terms of macro, micro, modeling and reduced basis errors have been derived for the RB-FE-HMM applied to quasilinear homogenization problems have been derived in [7], generalizing results for quasilinear problems previously obtained for the FEM [2] and the FE-HMM [5].

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How to construct a corrector when the homogenization limit may not exist due to non-separated scales.

Leonid Berlyand
(joint work with Houman Owhadi and Lei Zhang)

The homogenization of PDEs with periodic or random ergodic coefficients and well-separated scales is well understood. In particular, one of the central issues is the construction of the *corrector* that provides an approximation in the H^1 norm.

In this talk we present an overview of three subsequent constructions of a generalized corrector (GC) for the most general case of arbitrary L^∞ coefficients for linear problems, which may contain infinitely many scales that are not necessarily well-separated or ergodic. The key issue here is a proper generalization of the periodic cell problem. For stationary & ergodic coefficients such a generalization was obtained by S. Kozlov in his seminal work on random homogenization.

First, we present results of a joint work with H. Owhadi [1] when GC is constructed from globally supported solutions of "cell problems" (basis functions). This construction required an introduction of novel notions of the *flux norm* and the *transfer property*. While allowing for the optimal constant in the error estimate that does not depend on the contrast, the numerical implementation is rather costly due to the global support of the basis functions. This motivated a subsequent work by H. Owhadi and L. Zhang [2], where localized basis functions with support $\sqrt{h}\log 1/h$ were developed. We next present the results of this work and the main ideas of the proof that is based on the Caccioppoli inequality and exponential decay of the Green's function for an auxiliary problem. Finally, we briefly mention the most recent joint work with H. Owhadi and L. Zhang [3], described in the talk by L. Zhang, where GC is constructed from a variational polyharmonic nodal basis with support $h\log 1/h$.

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Some variants of stochastic homogenization

Xavier Blanc
(joint work with C. Le Bris, P.-L. Lions)

We review works in which the setting for stochastic homogenization is seen as a perturbation of the periodic setting. In the case when this perturbation is small, simplifications are possible for computing the homogenized coefficient.

1. The classical setting

In [5, 6], the following stochastic setting was introduced: the group $(\mathbb{Z}^d;+)$ acts on the probability space $(\Omega,\mathcal{F},\mathbb{P})$, this action is assumed to preserve the measure $\mathbb{P}$:

$$\forall y\in\mathbb{Z}^d,\forall B\in\mathcal{F},\quad \mathbb{P}(\tau_y B)=\mathbb{P}(B), \tag{1}$$

and is assumed to be ergodic:

$$\forall B\in\mathcal{F},\quad \big(\forall y\in\mathbb{Z}^d,\quad \tau_y B=B\big)\Rightarrow(\mathbb{P}(A)=0\quad\text{or}\quad 1). \tag{2}$$

A function $F\in L^1_{\mathrm{loc}}\left(\mathbb{R}^d,L^1(\Omega)\right)$ is *stationary* if

$$\forall k\in\mathbb{Z}^d,\quad F(x+k,\omega)=F(x,\tau_k\omega)\ \text{almost everywhere in } x,\ \text{almost surely.} \tag{3}$$

In this setting, the ergodic theorem can be stated as follows:

Theorem 1 (Ergodic theorem, [7, 8])**.** *Let $F\in L^\infty\left(\mathbb{R}^d,L^1(\Omega)\right)$ be a stationary random variable in the sense of (3). Then*

$$F\left(\frac{x}{\varepsilon},\omega\right)\xrightarrow[\varepsilon\to 0]{*}\mathbb{E}\left(\int_Q F(x,\cdot)dx\right)\quad \textit{in } L^\infty(\mathbb{R}^d),\ \textit{almost surely.} \tag{4}$$

This allows to derive a homogenization theory for linear elliptic operator, defining a homogenized equation with the help of a corrector, which is the solution to an elliptic stationary equation posed on the whole space $\mathbb{R}^d$. Note that in the classical works [9, 10], the group acting on Ω is $\mathbb{R}^d$ rather than $\mathbb{Z}^d$, which is a different setting. The present one allows to recover the periodic case by simply assuming that F in (3) is deterministic.

2. Deformation of a periodic structure

In the works [2, 3], we have introduced a slightly different setting which make it more explicit the fact that the random coefficients of our equation are close to a periodic reference configuration. This setting is the following: We fix some $\mathbb{Z}^d$-periodic matrix A_{per} which is uniformly elliptic and bounded, and define

$$A_\varepsilon(x,\omega)=A_{per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right). \tag{5}$$

We consider the following homogenization problem:

$$\begin{cases} -\mathrm{div}\left(A_{per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right)\nabla u\right)=f\quad\text{in}\quad\mathcal{D},\\[2ex] u=0\quad\text{on}\quad\partial\mathcal{D}, \end{cases} \tag{6}$$

where the function $\Phi(\cdot,\omega)$ is assumed to be a diffeomorphism from $\mathbb{R}^d$ to $\mathbb{R}^d$ $\mathbb{P}$-almost surely. The diffeomorphism is assumed to additionally satisfy

$$\operatorname*{EssInf}_{\omega\in\Omega,\,x\in\mathbb{R}^d}\left[\det(\nabla\Phi(x,\omega))\right]=\nu>0, \tag{7}$$

$$\operatorname*{EssSup}_{\omega\in\Omega,\,x\in\mathbb{R}^d}\left(|\nabla\Phi(x,\omega)|\right)=M<\infty, \tag{8}$$

$$\nabla\Phi(x,\omega)\quad\text{is stationary in the sense of (3).} \tag{9}$$

Such a Φ will be called a *random stationary diffeomorphism.*

We proved in [2] the following results:

Theorem 2. *Let $A_{\rm per}$ be a square matrix which is $\mathbb{Z}^d$-periodic, bounded and uniformly elliptic, and Φ a random stationary diffeomorphism satisfying hypotheses (7)-(8)-(9). Then for any $p \in \mathbb{R}^d$, the system*

(10)
$$\begin{cases} -\mathrm{div}\left[A_{per}\left(\Phi^{-1}(y,\omega)\right)(p+\nabla w_p)\right] = 0, \\ \\ w_p(y,\omega) = \tilde{w}_p\left(\Phi^{-1}(y,\omega),\omega\right), \quad \nabla\tilde{w}_p \quad \textit{is stationary in the sense of (3)}, \\ \\ \mathbb{E}\left(\displaystyle\int_{\Phi(Q,\cdot)} \nabla w_p(y,\cdot)dy\right) = 0, \end{cases}$$

has a solution in $\left\{w \in L^2_{\rm loc}(\mathbb{R}^d, L^2(\Omega)), \quad \nabla w \in L^2_{\rm unif}(\mathbb{R}^d, L^2(\Omega))\right\}$. Moreover, this solution is unique up to the addition of a (random) constant.

Theorem 3. *Let $\mathcal{D}$ be a bounded smooth open subset of $\mathbb{R}^d$, and let $f \in H^{-1}(\mathcal{D})$. Let $A_{\rm per}$ and Φ satisfy the hypotheses of Theorem 2. Then the solution $u_\varepsilon(x,\omega)$ of (6) satisfies the following properties:*

(i) *$u_\varepsilon(x,\omega)$ converges to some $u_0(x)$ strongly in $L^2(\mathcal{D})$ and weakly in $H^1(\mathcal{D})$, almost surely;*

(ii) *the function u_0 is the solution to the homogenized problem:*

(11)
$$\begin{cases} -\mathrm{div}\left(A^*\nabla u\right) = f \quad \textit{in} \quad \mathcal{D}, \\ \\ u = 0 \quad \textit{on} \quad \partial\mathcal{D}. \end{cases}$$

In (11), the homogenized matrix A^* is defined by:

(12)
$$A^*_{ij} = \det\left(\mathbb{E}\left(\int_Q \nabla\Phi(z,\cdot)dz\right)\right)^{-1} \cdot \mathbb{E}\left(\int_{\Phi(Q,\cdot)} \left(e_i + \nabla w_{e_i}(y,\cdot)\right)^T A_{per}\left(\Phi^{-1}(y,\cdot)\right) e_j \, dy\right),$$

where for any $p \in \mathbb{R}^d$, w_p is the corrector defined by (10).

In the theorems above, we have used the notation $L^2_{\rm unif}$ for the *uniform* L^2 space, that is, $L^2_{\rm unif} = \left\{f \in L^2_{\rm loc}, \quad \sup_{x\in\mathbb{R}^d}, \|f\|_{L^2(\mathbb{R}^d)} < +\infty\right\}$.

It is worth noticing that, in general, the matrix $A_{\rm per} \circ \Phi^{-1}$ is not stationary, that is, it does not satisfy (3).

The above results have been extended to the nonlinear case in [1].

3. Deformation close to identity

In the case of a diffeomorphism Φ which is close to identity, that is, if

$$\Phi(x,\omega) = x + \eta\Psi(x,\omega),$$

where η is small, and if A_{per} is smooth, it is possible to expand the result A^* in powers of η, finding an expansion in which the first terms are defined by deterministic formulas:

$$A^* = A^0 + \eta A^1 + O(\eta^2), \tag{13}$$

where A^0 is the homogenized matrix associated to A_{per}, and A^1 is the expectation value of some linear functions of $\nabla\Psi$. Therefore, it may be computed directly as a deterministic function of $\mathbb{E}(\nabla\Psi)$. See [3] for the details.

This is particularly useful as far as numerical computations are considered. Indeed, if one assumes the above expansion for Φ, and if the first two terms in (13) are sufficient for the purpose at hand, the computational cost is greatly improved: instead of solving problem (10), which is set in the whole space $\mathbb{R}^d$, we only need to solve corrector-like problems on the periodic cell Q. See [4] for the details.

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Kinetic limit for a wave equation in a medium with weak random disorder

Maximilian Butz

Introduction

For a realistic description of wave propagation one has to account for possible inhomogeneities of the underlying medium. Physical examples include waves travelling in a shallow water of varying depth, elastic waves in composite materials or light propagating through air with temperature fluctuations.

When modeling the disorder of the medium as random fluctuations of the index of refraction, there are three space scales of the problem: the correlation length of the fluctuations (CL), the typical wavelength (WL), and the observation scale (OS) on which we want to understand the energy transport of the wave.

Cases that have been mathematically rigorously studied make use of a clear scale separation of wavelength and correlation length ($WL \ll CL \approx OS$ in [4], or $WL \ll Cl \ll OS$ in [1]) or model the random medium as time dependent ([2] for the case of a random Schrödinger equation).

A particularly interesting case, however, is when the waves can fully interact with the inhomogeneities, i.e. $WL \approx CL = \mathcal{O}(1)$. We consider the system in the kinetic limit, with weak $\mathcal{O}(\sqrt{\varepsilon})$ disorder and observe the propagation behavior on large $\mathcal{O}(1/\varepsilon)$ space and time scales.

In this scaling, Erdös and Yau [3] investigate a Schrödinger equation with weak random potential,

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi = (-\Delta + \sqrt{\varepsilon}V)\psi. \tag{1}$$

while [6] consider a discrete analog of the present problem, the propagation of elastic vibrations through a cubic crystal lattice,

$$m_y \frac{\mathrm{d}^2}{\mathrm{d}t^2} u_y = \left(\Delta_{\text{lattice}} u\right)_y, \tag{2}$$

where the presence of different isotopes leads to $\mathcal{O}(\sqrt{\varepsilon})$ fluctuations of the atom masses m_y. As the space variable $y \in \mathbb{Z}^3$ is discrete the Fourier space is compact. In both cases the main object of the analysis is the *Wigner function* to be introduced below, and the limit is governed by a linear Boltzmann equation.

In my talk I want to present a rigorous proof of the kinetic limit for the case of a *continuous* wave equation. As the main goal is to understand how to deal with the randomness of the medium and the scaling limit, the wave equation itself will be chosen as simple as possible, a scalar wave equation on $\mathbb{R}^d$,

$$\frac{\partial^2}{\partial t^2} u(x,t) = c(x)^2 \Delta u(x,t). \tag{3}$$

Wigner Functions

We start (3) with initial conditions

$$\begin{aligned} u(x,0) &= u_0(x) \\ \frac{\partial}{\partial t}u(x,0) &= v_0(x), \end{aligned} \tag{4}$$

where $u_0 \in H^1\left(\mathbb{R}^d;\mathbb{R}\right)$ and $\frac{v_0}{c} \in L^2\left(\mathbb{R}^d;\mathbb{R}\right)$. The speed of wave propagation is assumed to have average one, and to be perturbed in the neighborhood of the points (y_n) generated by a Poisson point process (with Lebesgue measure as intensity measure) on $\mathbb{R}^d$. So it reads

$$c(x) = 1 + \sqrt{\varepsilon}\xi(x) \tag{5}$$

with a small parameter $\varepsilon > 0$ and a random field

$$\xi(x) = \sum_{n\in\mathbb{N}} \phi(x - y_n) - \int_{\mathbb{R}^d} \phi(y)\mathrm{d}y \tag{6}$$

where ϕ is a positive function on $\mathbb{R}^d$ with certain smoothness and decay conditions.

With $\Omega = \sqrt{-\Delta}$ we define $\psi = \psi(x,t)$ as

$$\psi = \begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\Omega u + i\partial_t u/c\\ \Omega u - i\partial_t u/c\end{pmatrix} \tag{7}$$

and arrive at a Schrödinger-type equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi^\varepsilon = H_\varepsilon \psi^\varepsilon. \tag{8}$$

The selfadjoint operator H_ε is random and ε-dependent by

$$\begin{aligned} H_\varepsilon &= H_0 + \sqrt{\varepsilon}V \\ &= \begin{pmatrix}\Omega & 0\\ 0 & -\Omega\end{pmatrix} + \frac{\sqrt{\varepsilon}}{2}\begin{pmatrix}\Omega\xi + \xi\Omega & -\Omega\xi + \xi\Omega\\ \Omega\xi - \xi\Omega & -\Omega\xi - \xi\Omega\end{pmatrix}. \end{aligned} \tag{9}$$

The Wigner transform of ψ^ε is a 2×2 matrix-valued function defined on the macroscopic (x,k) phase space,

$$\begin{aligned} &W^\varepsilon_{\sigma'\sigma}[\psi^\varepsilon](x,k) \\ &= \varepsilon^{-d}\int_{\mathbb{R}^d} \mathrm{d}y\, e^{i2\pi k\cdot y}\overline{\psi^\varepsilon_{\sigma'}\left(\frac{x}{\varepsilon} + \frac{y}{2}\right)}\psi^\varepsilon_\sigma\left(\frac{x}{\varepsilon} - \frac{y}{2}\right). \end{aligned} \tag{10}$$

We now want to understand the limit behavior of the disorder-averaged Wigner function $W^\varepsilon_{++}[\psi^\varepsilon(t/\varepsilon)]$. Typically, one would test weak convergence with Schwartz functions J on $\mathbb{R}^{2d}$,

$$\left\langle J, W^\varepsilon_{++}\right\rangle = \int_{\mathbb{R}^{2d}} \mathrm{d}x\,\mathrm{d}k\,\overline{J(x,k)}W^\varepsilon_{++}(x,k). \tag{11}$$

However, the dispersion relation $\omega(k) = 2\pi|k|$ of the wave equation is not smooth at the origin, so we obtain a higher resolution at $k \approx 0$ in a similar manner to [5]:

$$\left\langle\!\left\langle a, W^{\varepsilon}_{++} \right\rangle\!\right\rangle = \int_{\mathbb{R}^{2d}} \mathrm{d}x\,\mathrm{d}k\, \overline{a\left(x, k, \frac{k}{\varepsilon}\right)} W^{\varepsilon}_{++}(x,k). \tag{12}$$

Roughly speaking $a(x,k,q)$ is uniformly Schwartz in x,k, smooth in q and converges to a radial limit $a(x,k,q) \to b(x,k,q/|q|)$ as $|q| \to \infty$.

For this class of test functions and initial conditions $\psi^{\varepsilon}(t=0)$ bounded in $L^2\left(\mathbb{R}^d;\mathbb{C}^2\right)$ and tight on momentum and macroscopic position space, we can prove our main result.

Main Result

Let all above assumptions hold and fix a space dimension $d \geq 2$. Then there exists a subsequence $\varepsilon \to 0$ and positive, bounded Borel measures μ_0 on $\mathbb{R}^d \times \left(\mathbb{R}^d \setminus \{0\}\right)$ and μ_0^H on $\mathbb{R}^d \times S^{d-1}$ as well as a vector $\varphi_0 \in L^2\left(\mathbb{R}^d;\mathbb{C}\right)$ such that for all a as described above and all $t \geq 0$

$$\begin{aligned} &\lim_{\varepsilon\to 0} \mathbb{E}\left[\left\langle\!\left\langle a, W^{\varepsilon}_{++}[\psi^{\varepsilon}(t/\varepsilon)] \right\rangle\!\right\rangle\right] = \\ &\quad = \int_{\mathbb{R}^d\times(\mathbb{R}^d\setminus\{0\})} \mu_t(\mathrm{d}x,\mathrm{d}k)\overline{b(x,k,k/|k|)} \\ &\qquad + \int_{\mathbb{R}^d\times S^{d-1}} \mu_t^H(\mathrm{d}x,\mathrm{d}q)\overline{b(x,0,q)} \\ &\qquad + \left\langle a_0, W^1[\varphi_t]\right\rangle \end{aligned} \tag{13}$$

with $a_0(x,q) = a(x,0,q)$, W^1 a non-scaled Wigner function. The time-evolution of the limit object $\left(\mu_t, \mu_t^H, \varphi_t\right)$ from the initial state $\left(\mu_0, \mu_0^H, \varphi_0\right)$ reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\mu_t(x,k) = -\frac{k}{|k|}\cdot\nabla_x\mu_t(x,k) + \int_{\mathbb{R}^d} \nu_k(\mathrm{d}k')(\mu_t(x,k') - \mu_t(x,k)) \tag{14}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mu_t^H(x,q) = -\frac{q}{|q|}\cdot\nabla_x\mu_t^H(x,q) \tag{15}$$

$$\widehat{\varphi_t}(q) = e^{-2\pi i|q|t}\widehat{\varphi_0}(q), \tag{16}$$

with measure ν_k given by

$$\nu_k(\mathrm{d}k') = |\hat{\phi}(k-k')|^2 2\pi\delta(2\pi|k| - 2\pi|k'|)|2\pi k|^2\mathrm{d}k'. \tag{17}$$

Thus, in the limit, wave motion disintegrates into three decoupled limit dynamics: Microscopic waves with wavelengths of the same order of magnitude as the correlation length of the medium, which scatter off the inhomogeneities; on macroscopic scales their energy transport is given by a linear Boltzmann equation (14), with a collision kernel encoding the microscopic properties of the medium. Mesoscopic waves have wavelengths much larger than the correlation length but much smaller than the observation scale, thus they do not scatter and they appear on macroscopic scale as solution of a mere transport equation (15). Finally, there are macroscopic waves with wavelengths that are still resolved in the scaling limit,

they do not scatter either and thus are solutions of an unperturbed wave equation (16).

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Towards an optimization of the slip length of viscous fluids near rough walls

Anne-Laure Dalibard-Roux

(joint work with D. Gérard-Varet, D. Bucur, M. Bonnivard)

In this talk, I will present some recent results about wall laws for viscous fluids in the vicinity of a rough boundary. When the roughness is random stationary and ergodic, one can prove that in general, the wall law is Dirichlet at first order, and Navier at second order with an effective slip length of the same order as the amplitude and the wave length of the roughness. The derivation of the Navier wall law involves a multi scale expansion with a boundary layer corrector, in the spirit of homogenization problems.

Once the wall law is derived, the issue is to design roughness profiles which maximize the slip length, so as to minimize energy losses. We will review different tools which enable us either to prove or to guess which profiles are optimal (domain derivation techniques, numerical simulations, periodic homogenization theory, direct computation).

Generalized multiscale finite element method with oversampling

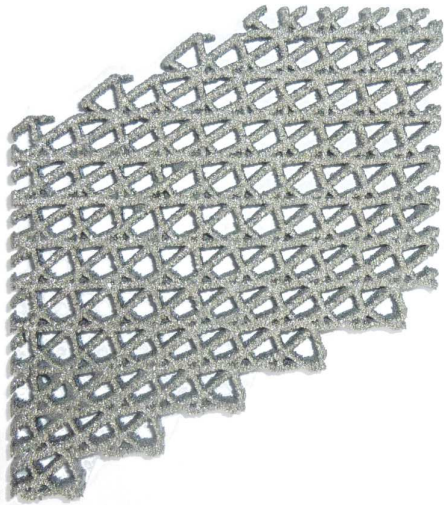
Yalchin Efendiev

In this talk, I describe generalized multiscale finite element method. In this method, as a construction of offline and online spaces, we propose an efficient local model reduction technique for multiscale problems. I discuss oversampling technique within GMsFEM and present convergence results. Numerical results are presented.

Optimization of structurally graded materials

Virginie Ehrlacher
(joint work with C. Le Bris, F. Legoll, G. Leugering, M. Stingl, F. Wein)

We consider microstructured materials whose composition evolves gradually at the macroscopic scale. An example of such material is shown in the picture below.



Our aim is to optimize the microstructure of such a material with respect to given loading scenarios and boundary conditions. More precisely, let $d \in \mathbb{N}^*$, $\Omega \subset \mathbb{R}^d$ and $S \subset \Omega$ an open subset of Ω. We assume that the domain Ω is occupied by a given linear elastic material in the domain S, characterized by a linear elasticity tensor $\left(E^0_{ijkl}\right)_{1\leq i,j,k,l\leq d}$, and by void in the domain $\Omega \setminus S$. More precisely, the linear elastic tensor of the microstructured material is given by

$$\forall 1 \leq i,j,k,l \leq d,\ \forall x \in \Omega, \quad E^S_{ijkl}(x) = \chi_S(x) E^0_{ijkl},$$

where

$$\forall x \in \Omega, \quad \chi_S(x) := \begin{cases} 1 \text{ if } x \in S, \\ \eta \text{ if } x \notin S, \end{cases}$$

where $\eta > 0$ is a small regularization parameter.

For the sake of simplicity, we will assume that the material is subject to external volumic forces $\mathbf{f} \in \left(L^2(\Omega)\right)^d$ and that Dirichlet boundary conditions are imposed on the displacement field. Thus, if the material occupying the domain Ω is characterized by a linear elasticity tensor field $(E_{ijkl}(x))_{1\leq i,j,k,l}$, the displacement field $\mathbf{u}^E$ of the material is the unique solution of (using Einstein's relations)

$$(1) \qquad \begin{cases} \text{find } \mathbf{u}^E \in \left(H^1_0(\Omega)\right)^d \text{ such that} \\ \forall \mathbf{v} \in \left(H^1_0(\Omega)\right)^d,\ \int_\Omega E_{ijkl}(x) e_{ij}\left(\mathbf{u}^E\right) e_{kl}\left(\mathbf{v}\right)\, dx = \int_\Omega \mathbf{f} \cdot \mathbf{v}, \end{cases}$$

where for all $1 \leq i, j \leq d$ and all $\mathbf{v} = (v_k)_{1 \leq k \leq d} \in \left(H^1_{\mathrm{loc}}(\mathbb{R}^d)\right)^d$,

$$e_{ij}(\mathbf{v}) := \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right).$$

For the sake of simplicity, using a slight abuse of notation, we shall denote by $E\mathbf{u}^E = \mathbf{f}$ to refer to the fact that $\mathbf{u}^E$ is the unique solution of problem (1).

Typical optimization problems we would like to consider are of the following form:

$$\text{(2)} \qquad \text{Find } S_{opt} \text{ such that } S_{opt} \in \underset{\substack{S \in \mathcal{S} \\ E^S \mathbf{u}^{E^S} = \mathbf{f} \\ C\left(\mathbf{u}^{E^S}\right) \leq c}}{\operatorname{argmin}} \mathcal{J}\left(\mathbf{u}^{E^S}, S\right),$$

where

- $\mathcal{S}$ is an admissible set of structures S, which encodes the structural constraints of the material to optimize;
- $\mathcal{J}$ is a cost functional to minimize;
- C denotes some constraints which must be satisfied on $\mathbf{u}^{E^S}$.

Unfortunately, it is well-known that a minimization problem of the form (2) is ill-posed in general [1].

We propose an alternative way of considering this problem: let $\mathbf{g} : \Omega \to \mathbb{R}^d$ be a macroscopic mapping, let $\varepsilon > 0$ be a small real number, $Y = (0,1)^d$ the unit cube of $\mathbb{R}^d$ and $\chi_{\mathrm{per}} \in L^\infty_{\mathrm{per}}(Y, \{\eta, 1\})$ a fixed Y-periodic function with values in $\{\eta, 1\}$. Instead of considering materials whose microstructure is characterized by a general subset S of the domain Ω, we are going to consider structures S such that their characteristic function χ_S is of the form

$$\forall x \in \Omega, \quad \chi_S(x) = \chi_{\mathrm{per}}\left(\frac{\mathbf{g}(x)}{\varepsilon}\right).$$

Our aim is then to keep χ_{per} and ε fixed and optimize the structure of the material by optimizing the choice of the macroscopic mapping $\mathbf{g}$.

We would like to consider two different strategies: the first one consists in using the homogenization formulae proved by Bensoussan, Lions and Papanicolaou in the limit when the size of a microcell of the material goes to 0 to model the properties of the macroscopic material; the second one consists in taking into account the fact that the size of the microcell is indeed small, but not 0, and to use an adapted finite element method such as a Multiscale Finite Element Method (MsFEM) to compute efficiently the properties of this material. In order to perform these computations in practice, it will be necessary to use advanced reduced-order modeling methods such as reduced basis or greedy algorithms. This is currently work in progress.

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Stochastic Homogenization for Small Isotropic Perturbations of the Heat Equation

Benjamin Fehrman

In this talk, we describe some analytic methods used to understand the limiting behavior of solutions u^ϵ to drift-diffusion equations

$$(1) \qquad \begin{cases} u_t^\epsilon - \operatorname{tr}(A(\frac{x}{\epsilon},\omega)D^2u^\epsilon) + \frac{1}{\epsilon}b(\frac{x}{\epsilon},\omega)Du^\epsilon = u_1(x) & \text{on } \mathbb{R}^d \times (0,\infty), \\ u^\epsilon = u_0 & \text{on } \mathbb{R}^d \times \{0\}, \end{cases}$$

which are small, isotropic perturbations of the heat equation.

Precisely, the coefficients are bounded, Lipschitz continuous, stationary ergodic and, additionally, satisfy a restricted isotropy condition introduced by Bricmont and Kupiainen [1] in the discrete setting and considered by Sznitman and Zeitouni [3] in the continuous setting. For every orthogonal transformation r preserving the coordinate axis, for every $x \in \mathbb{R}^d$,

$$(2) \qquad (b(rx,\cdot), A(rx,\cdot)) \text{ and } (rb(x,\cdot), rA(x,\cdot)r^t) \text{ have the same law.}$$

Furthermore, the coefficients satisfy a finite range dependence.

We will focus on the following result.

Proposition 1. [3] *($d \geq 3$) There exists $\eta > 0$ and $\overline{\alpha} > 0$ such that if*

$$|b(x,\omega| \leq \eta \text{ and } |A(x,\omega) - I| \leq \eta$$

then, almost surely, as $\epsilon \to 0$,

$$u^\epsilon \to \overline{u} \text{ locally uniformly on } \mathbb{R}^d \times [0,\infty),$$

for $\overline{u}$ satisfying

$$\begin{cases} \overline{u}_t - \overline{\alpha}\Delta\overline{u} = u_1 & \text{on } \mathbb{R}^d \times (0,\infty), \\ \overline{u} = u_0 & \text{on } \mathbb{R}^d \times \{0\}. \end{cases}$$

The essential difficulty toward obtaining homogenization is the lack of estimates, uniform in ϵ, for the solutions of (1). As a result, and in contrast to the case $b = 0$, see Papanicolaou and Varadhan [2], an invariant measure will not exist, in general, for the underlying process.

The proof therefore follows by an induction argument which propagates pde analogues of the localization, trapping and contraction controls appearing in [3] along a sequence of finer length scales. The finite range dependence and isotropy are used to ensure that these controls are satisfied, with high probability, on a large portion of space as the length scale approaches zero.

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Model reduction in homogeneous chaos spaces

Roger Ghanem

Optimal basis are sought through a rotation of Gaussian variables with respect to which polynomial chaos spans are constructed. Those bases are used in solving partial differential equations whose coefficients are random variables or processes. A number of arguments are also presented for the selection of these rotations. The resulting approximations reduce very high-dimensional problems into either a 1-dimensional problem or a sequence of 1-dimensional problems

A quantitative two-scale expansion in stochastic homogenization

Antoine Gloria

(joint work with Stefan Neukamm, Felix Otto)

Consider a discrete elliptic equation on the (discretized) unit torus, with iid conductivities. We then show that the L^2-norm is probability of the discrete H^1-norm in space of the first two terms of the two-scale expansion decays as "ε" (up to a logarithm in dimension 2). The proof relies on a covariance estimate, bounds on the moment of the corrector, an estimate of the error on the approximation of the homogenized coefficients by periodization, and annealed estimates on the random Green's function (first two derivatives).

Asymptotic behaviors for the Random Schrödinger Equation with Slowly Decaying Correlations

Christophe Gomez

The topic of the talk concerned wave propagation in random media with slowly decaying correlations. The motivation of this study comes from data collections in real environments, such as laser beams propagation through the atmosphere, geophysics, and medical imaging, showing the possibility to encounter such propagation media. Waves propagating in such environment undergo multiple scattering and it is necessary to understand this mechanism for application purposes. For random environments with rapidly decaying correlations wave scattering is described through the notion of *scattering mean free path* describing the expected propagation distance for which a signal becomes partially coherent. However, for

random media with slowly decaying correlations the *scattering mean free path* is not defined anymore. Nevertheless, as described below, it is possible to derived kinetic models for wave decoherence in such random media.

Monochromatic wave propagation can be described using the so-called paraxial wave equation given by the following random Schrödinger equation :

$$i\kappa\partial_z\phi + \frac{1}{2}\Delta_{\mathbf{x}}\phi + \kappa^2\sigma V(z,\mathbf{x})\phi = 0$$

where ϕ is the wave field amplitude, z is the main propagation axis coordinate, $\kappa = 2\pi/\lambda$ is the wavenumber (λ is the wavelength), and $\mathbf{x} \in \mathbb{R}^d$ the transverse section variable. The fluctuations of the propagation medium are given by V and σ represents the amplitude of the fluctuations. The problem was to understand the scattering effects for high frequency waves. A classical tool to do so is the following Wigner transform

$$W(z,\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^d}\int d\mathbf{y} e^{i\mathbf{k}\cdot\mathbf{y}}\phi\big(z,\mathbf{x}-l_c\frac{\mathbf{y}}{2}\big)\overline{\phi\big(z,\mathbf{x}+l_c\frac{\mathbf{y}}{2}\big)}$$

which is the spatial Fourier transform of the two points correlation function of the wave field. This tool describes the loss of coherence of the wave field ϕ on a spatial correlation scale l_c through diffusion phenomena on the wavevector $\mathbf{k}$. In this talk, we have characterized anomalous diffusion phenomena of the wavevector over several propagation scales. If the wave propagates over large distances, cumulative scattering effects may start to become significant. The first decoherence effects happen after a propagation distance L_1 on a correlation scale $l_{c,1}$ (related to the propagation distance) and can be described thanks to the following stochastic partial differential equation

$$\begin{aligned} dW(z,\mathbf{x},\mathbf{k}) = &-\sigma(\theta)(-\Delta_{\mathbf{k}})^{\theta/2}W(z,\mathbf{x},\mathbf{k}) \\ &+ i\int d\mathcal{B}_z(d\mathbf{p})e^{i\mathbf{x}\cdot\mathbf{p}}\Big(W\big(z,\mathbf{x},\mathbf{k}-\frac{\mathbf{p}}{2}\big) - W\big(z,\mathbf{x},\mathbf{k}+\frac{\mathbf{p}}{2}\big)\Big),\ \theta\in(0,1), \end{aligned}$$

where $(\mathcal{B}_z)_z$ is a Wiener process depending on the statical properties of the random medium (as well as θ and $\sigma(\theta)$), and whose solution is

$$W(z,\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^d}\int d\mathbf{q}\widehat{W}^{\mathbf{k}}(0,\mathbf{x},\mathbf{q})\exp\Big(i\mathbf{k}\cdot\mathbf{q} + i\int\mathcal{B}_z(d\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}(e^{-i\mathbf{q}\cdot\mathbf{p}/2} - e^{i\mathbf{q}\cdot\mathbf{p}/2})\Big).$$

The random part of the previous equation suggests an uncertainty on the wavevector diffusion behavior. However, when the wave propagates further ($L_2 \gg L_1$) the randomness averages out, the loss of coherence of the wave field happens on smaller spatial scales $l_{c,2} \ll l_{c,1}$, and can be described by the following fractional heat equation

$$\partial_z W(z,\mathbf{x},\mathbf{k}) = -\sigma(\theta)(-\Delta_{\mathbf{k}})^{\theta/2}W(z,\mathbf{x},\mathbf{k}).$$

The meaning of $l_{c,2} \ll l_{c,1}$ when $L_2 \gg L_1$ is that we lose first the coherence of the wave field on its large structures before losing it on its smaller structures. Finally, for larger propagation distances ($L_3 \gg L_2 \gg L_1$) the smallest scales of the wave

field $l_{c,3} \ll l_{c,2} \ll l_{c,1}$ are also affected and the loss of coherence can be described thanks to the following radiative transport equation

$$\partial_z W(z,\mathbf{x},\mathbf{k}) + \mathbf{k}\cdot\nabla_{\mathbf{x}} W(z,\mathbf{x},\mathbf{k}) = \int \sigma(\mathbf{p})\big(W(z,\mathbf{x},\mathbf{k}+\mathbf{p}) - W(z,\mathbf{x},\mathbf{k})\big),$$

where $\sigma(\mathbf{p})$ described how the wave field is scattered, and depends on the statical properties of the random medium. The three previous regimes show that all the spatial scales of the wave field are affected, some of them earlier than if the medium has rapidly decaying correlations, and it is not possible to defined a *scattering mean free path*, it would be 0. In the other hand, this means that the wave field is strongly affected throughout the propagation and produce a very nice smoothing effect in $\mathbf{k}$ and $\mathbf{x}$. These results have been published in the two following papers :

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Deterministic and stochastic homogenization problems with new applications in nanotechnology

Clemens Heitzinger

(joint work with Pierre Degond, Peter Markowich, and Christian Ringhofer)

Introduction

Non-standard deterministic and stochastic homogenization problems arise naturally from the modeling of recent devices in nanotechnology and nanostructured metamaterials. Non-standard situations are, e.g., homogenization at surfaces, and using systems of equations to describe the physics. Related problems arise from the modeling of confined structures such as nanopores and ion channels.

An overview of recent results is given. For the concrete applications discussed here, very good agreement with experimental data has been achieved in numerical simulations based on these homogenized model equations.

In nanotechnology, homogenization problems arise immediately due to the inherently different length scales of single features and whole devices. Examples of potentially great impact are nanowire biosensors [1, 2, 3, 4, 5] and nanowire gas sensors [6, 7], as nanowires have several advantages for sensing applications.

In these and related applications, stochastic homogenization problems also arise naturally in addition to deterministic ones. Inevitable noise and fluctuations result in fluctuations in the functional that corresponds to the sensor response, and quantifying these uncertainties makes it possible to determine the signal-to-noise ratio.

Homogenization results

One of the first problems solved was a homogenization problem for the Poisson equation with a periodic, highly oscillatory charge concentration at a material interface [8]. We found that the highly oscillatory charges are replaced by two interface conditions after homogenization. The two interface conditions are jumps in the solution and in essentially its normal derivative, and the sizes of the jumps depend on the surface-charge density and the dipole-moment density of the boundary layer. Based on this result and an existence and local-uniqueness result for a system of equations [9], it has became possible to study the current-voltage characteristics of realistic nanowire sensors in 2D and 3D simulations [10]. In order to simulate nanowires with very large aspect ratios, we additionally developed the first parallel algorithm for the drift-diffusion-Poisson system with jumps at an interface [11]. Comparison with measurements of different devices yielded excellent agreement. Therefore, this model enables the rational design and optimization of nanowire bio- and gas sensors despite the nonlinear interdependence between design parameters [10, 12, 5].

In the next step, an effective equation for the covariance of the solution of the Poisson equation was derived in [13] for the problem with a stochastic boundary layer. Given the stochastic process of the boundary layer, the variance of the solution can be calculated efficiently as the diagonal of the solution of the effective equation for the covariance. Numerical results were also discussed and compared to the Monte-Carlo method.

A problem with a stochastic boundary layer was considered numerically in [14], where the actual probability distribution of the molecules was calculated from their electrostatic free energy by solving the nonlinear Poisson-Boltzmann equation. This approach based in the physics of the problem goes beyond the popular assumption of normal distributions. The numerical results indicate how the fluctuations and the noise in nanowire devices can be reduced.

For the simulation of the functional devices mentioned above, transport equations are needed. Therefore we have been working on the homogenization of the most general system for many-particle systems, namely the Boltzmann-Poisson system

$$-\nabla \cdot (A_\epsilon \nabla u_\epsilon) = \rho_\epsilon + g_\epsilon, \tag{1a}$$

$$\partial_t f_\epsilon + \frac{1}{\epsilon}\{E_\epsilon, f_\epsilon\}_{xv} = \frac{1}{\epsilon^2} Q(f_\epsilon) \tag{1b}$$

in a diffusive scaling. This system is the most general approach towards the simulation of these devices. Again, highly oscillatory charge concentrations live at a surface or a manifold. A drift-diffusion equation with effective coefficients can be derived by homogenization of the system (1).

Nanopores and ion channels lead to related multiscale problems. When modeling confined structures, the essential problem is that bulk coefficients are not correct. Therefore, a multiscale problem involving transport through confined

structures was solved in [15]. The main model equation is the Boltzmann equation (1b), a (6 + 1)-dimensional equation. The result is a (2 + 1)-dimensional diffusion-type transport equation whose transport coefficients are given – even in closed form – by the (harmonic) confinement potential. For the first time, the physically correct coefficients in the transport equation can be calculated. Additionally, the computational effort is considerably decreased; currents and fluxes can be calculated directly in contrast to time consuming particle Monte-Carlo simulations. Very good agreement with measurements of various ion channels was found [16].

Conclusions

New homogenization problems arising from multiscale problems in applications in nanotechnology were solved. Numerical simulations based on the homogenized equations were developed and simulation results were compared with measurements of nanoscale devices. Very good agreement was found.

Current and future work involves more sophisticated model equations and systems of equations. There is also plenty of opportunity to use stochastic homogenization to quantify noise, fluctuations, and uncertainties.

Acknowledgments

This is joint work with Pierre Degond (Toulouse), Robert W. Dutton and Yang Liu (Stanford), Peter A. Markowich (Cambridge), Mark A. Reed and Aleksandar Vacic (Yale), and Christian Ringhofer (ASU).

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Corrector Analysis for Some Heterogeneous Multi-Scale Schemes

Wenjia Jing
(joint work with Guillaume Bal)

It is well known that homogenization theories provide natural benchmarks for multi-scale numerical methods designed to solve partial differential equations with highly oscillatory coefficient. In this talk, we introduce the so-termed corrector theory which concerns the distributions of the fluctuations in a heterogenous PDE compared with the homogenized one. We show that corrector theories provide natural benchmarks for multi-scale numerical methods to evaluate their ability in capturing the fluctuations of the heterogeneous PDEs, which is important in many applications and is often among the main objectives of multi-scale methods. Using benchmarks of this kind, and considering several methods in the general framework of heterogeneous multi-scale methods (HMM) of E and Engquist, we investigate the competition between savings in the computation and accuracy in capturing the fluctuations. Further, our corrector theory may provide remedies for the contradiction between the two.

More precisely, let u_ϵ and u_0 denote the solutions to the heterogeneous PDE and the homogenized one, where some coefficient $q_\epsilon(x,\omega) = q(\frac{x}{\epsilon},\omega)$ of the former is rescaled from a stationary ergodic random field $q(x,\omega)$ on some probability space $(\Omega,\mathcal{F},\mathbb{P})$. Let $\mathbb{E}$ denote the expectation. The fluctuation in the heterogeneous PDE is defined to be $u_\epsilon - \mathbb{E}u_\epsilon$. The corrector theory is therefore of the form

$$\frac{u_\epsilon(x,\omega) - \mathbb{E}u_\epsilon(x,\omega)}{\epsilon^\gamma} \xrightarrow[\epsilon\to 0]{\text{distribution}} \sigma \int G(x,y)u_0(y)\, dW^\gamma(y),$$

where ϵ^γ is the order of the fluctuation in the L^2 norm, $G(x,y)$ is the Green's function of the homogenized equation, σ is some constant depending on q and W^γ is some Gaussian process. Depending on the settings, the convergence makes sense as in distribution of continuous paths, L^2 paths, or merely weakly in x. The result depends on the de-correlation structure of $q(\cdot,\omega)$. In particular, when q is short range correlated, $\gamma = \frac{d}{2}$ and $W^{\frac{d}{2}}$ is the standard multi-parameter Wiener process; when q is a function of a stationary Gaussian field whose correlation function behaves like $c|x|^{-\alpha}, \alpha < d$ for large $|x|$, then $\gamma = \frac{\alpha}{2}$ and $W^{\frac{\alpha}{2}}$ is a Gaussian random field with correlation function $c|x-y|^{-\alpha}$. Such corrector theories are difficult to obtain for general PDEs but are available for the one dimensional steady diffusion operator $-\frac{d}{dx}\left(a_\epsilon(x)\frac{d}{dx}\right)$ and for the elliptic operator with random potential $(P(x,D)+q_0)+q_\epsilon(x)$. We refer to [9, 7, 1, 3, 4, 2] for more details.

Based on the corrector theory, we build a benchmark to test the performances of multi-scale numerical methods in capturing the fluctuations of the heterogeneous problem. Let u_ϵ^h be the solution to the heterogeneous equation given by the numerical methods with discretization size h, and let u_0^h be the solution to the homogenized equation given by the same method. Consider the following diagram:

$$\begin{array}{ccc} \frac{u_\epsilon^h - u_0^h}{\epsilon^{\frac{\alpha\wedge d}{2}}}(x,\omega) & \xrightarrow[(i)]{h\to 0} & \frac{u_\epsilon - u_0}{\epsilon^{\frac{\alpha\wedge d}{2}}}(x,\omega) \\ \epsilon\to 0 \big\downarrow (ii) & & (iii) \big\downarrow \epsilon\to 0 \\ \mathcal{U}^h_{\alpha\wedge d}(x;W^{\alpha\wedge d}) & \xrightarrow[(iv)]{h\to 0} & \mathcal{U}_{\alpha\wedge d}(x;W^{\alpha\wedge d}). \end{array}$$

The scaling $\alpha\wedge d$ depends on the de-correlation structure of q as remarked. Path (iv) is precisely the corrector theory before. We are interested in Paths (ii) and (iii). What is the intermediate distribution when $\epsilon \downarrow 0$ while h is fixed? More importantly, does this distribution converges to the one given by the corrector theory when $h \downarrow 0$?

We analyze this diagram using the aforementioned ODE/PDE and random field models for some numerical methods in the framework of HMM [8]. There, besides h, there is another parameter $\delta \le h$, the scale on which fine computations are made. Usually, δ is much larger than ϵ so as to capture the homogenization limit and smaller than h to reduce computations. We identify the intermediate limit $\mathcal{U}_d^{h,\delta}$ and further observe: For short range correlated medium, its limit is $(h/\delta)^{\frac{d}{2}}\mathcal{U}_d$. For long range correlated medium, however, the intermediate $\mathcal{U}_\alpha^{h,\delta}$ converges to the correct limit $\mathcal{U}_\alpha$ even for $\delta < h$. Therefore, savings in computation may come at a cost of amplifying the fluctuations (depending on the medium). Our theory should help to remedy this possible amplification effect.

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Asymptotics of solutions of the stochastic lattice wave equation

Tomasz Komorowski
(joint work with S. Olla, L. Ryzhik)

We consider the long time limit for the solutions of a discrete wave equation with weak stochastic forcing. The multiplicative noise conserves energy, and in the unpinned case also conserves momentum. We obtain a time-inhomogeneous Ornstein-Uhlenbeck equation for the limit wave function that holds for both square integrable and statistically homogeneous initial data. The limit is understood in the pointwise sense in the former case, and in the weak sense in the latter. On the other hand, the week limit for square integrable initial data is deterministic.

Monte Carlo simulations in media with interfaces

Antoine Lejay
(joint work with Sylvain Maire and Géraldine Pichot)

Diffusion problems in media with interfaces between sub-domains are ubiquitous. Discontinuities in the diffusivity, or thin layers, lead for example to such problems.

We are interested in developing Monte Carlo methods, where a quantity of interest (pressure, concentration, effective coefficient, ...) is computed by using the empirical distribution of a cloud of particles moving independently and randomly in such media. Applications may be found in geophysics, brain imaging, atmospheric study, population ecology, astrophysics, oceanography, chemistry, ...

More precisely, we consider a one-dimensional infinite medium with an interface at 0 separating two parts of constant diffusivity $D(x) = D^-$ for $x < 0$ and $D(x) = D^+$ for $x > 0$. The concentration of a fluid evolving in the media is governed by the Fick's second law

$$(\star) \qquad \partial_t C(t,x) = \nabla(D(x)\nabla C(t,x)),\ x \neq 0,\ t > 0 \text{ and } C(0,x) = C_0(x).$$

As such, $(\star)$ does not define properly the PDE unless one specifies some conditions at 0. There are two kind of interfaces conditions we consider here:

$$(\mathcal{I}1) \qquad \begin{cases} C(t,0-) = C(t,0+), \\ (1-q)D^-\nabla C(t,0-) = (1+q)D^+\nabla C(t,0+) \end{cases}$$

for some $q \in (-1,1)$ and

$$(\mathcal{I}2) \qquad \begin{cases} D^+ = D^-, \\ \nabla C(t,0-) = \nabla C(t,0+), \\ \lambda(C(t,0+) - C(t,0-)) = D^{\pm}\nabla C(t,0\pm). \end{cases}$$

With $q = 0$ in condition $(\mathcal{I}1)$, it is a rewriting of $(\star)$ on $\mathbb{R}$ with the divergence form operator $\nabla(D\nabla\cdot)$, where this equation is interpreted as a diffraction problem (See *e.g.* [3]). With $q = (D(0-) - D(0+))/(D(0+) + D(0-))$, then it corresponds indeed in solving $\partial_t C(t,x) = D(x)\nabla C(t,x)$ over the whole domain. In general, this interface condition can be reached as the limit by homogenization of a process with constant diffusivity and a drift periodic on each side of the interface [2].

Condition $(\mathcal{I}2)$ is obtained as the limit of a thin layer problem, that is when the diffusivity is equal to $\epsilon\lambda$ on the layer of width ϵ around 0 decreases to 0 (See *e.g.* [9]).

Monte Carlo simulations. We are looking at simulating particles starting from x whose positions at time t have for density the fundamental solution $p(t,x,\cdot)$ of the problem $(\star)$, with respect to the x variable, with the appropriate interface condition.

The successive positions of the particles $t \mapsto X_t$ form continuous but irregular paths. We then aim at simulating a discretized version $(X_0, X_{\delta t}, X_{2\delta t}, \ldots, X_T)$ of $(X_t)_{t\in[0,T]}$ for a small time step δt.

For both interfaces conditions, X is a (strong) Markov process so that the distribution of $X_{(k+1)\delta t}$ given $(X_0, \ldots, X_{k\delta t})$ depends only on $X_{k\delta t}$. However, X is not in general solution to a Stochastic Differential Equation (SDE).

Here, we are interested in the behavior of the particle at the interface. Our results are easily generalized when D varies smoothly away from 0, in presence of several interfaces or boundary conditions. This is why we take D piecewise constant for the sake of simplicity.

Until it reaches the interface, the particle moves like a Brownian motion of diffusivity $2D^{\pm}$. Thus, the successive positions of the particles are easily simulated by $X_{(k+1)\delta t} = X_{k\delta t} + \sqrt{2D(X_{k\delta t})\delta t} \times \xi$ where ξ is a centered, unit, Gaussian random variable independent from $X_{k\delta t}$. Yet this is only an approximation as there is always a positive probability that the particle crosses the interface between $k\delta t$

and $(k+1)\delta t$. However, as long as $|X_{k\delta t}| \gg \sqrt{\delta t}$, this probability is exponentially small and may be neglected.

We are then concerned by setting up algorithms when $X_{k\delta t}$ belongs to an interval of length proportional to $\sqrt{\delta t}$ around 0.

Condition ($\mathcal{I}1$)**.** With $\Phi(x) = \int_0^x \mathrm{d}y/\sqrt{2D(y)}$, the stochastic process $Y_t = \Phi(X_t)$ is solution to the SDE with local time

$$Y_t = Y_0 + W_t + \theta L_t^0(Y),$$

where W is a Brownian motion, $L_t^0(Y)$ is the local time of Y at 0 and $\theta \in (-1, 1)$ is a function of D^+, D^- and q. For example, with a divergence form operator $\nabla(D\nabla\cdot)$, $\theta = (\sqrt{D^+} - \sqrt{D^-})/(\sqrt{D^+} + \sqrt{D^-})$ while with a non-divergence form operator $D\triangle$, $\theta = (\sqrt{D^-} - \sqrt{D^+})/(\sqrt{D^+} + \sqrt{D^-})$.

The local time $L_t^0(Y)$ characterizes the time spend at 0 by the process: $L_t^0(Y) = \lim_{\epsilon\to 0}(2\epsilon)^{-1}\lambda(\{s \le t; Y_s \in [-\epsilon, \epsilon]\})$, where λ is the Lebesgue measure. The paths $t \mapsto L_t^0(Y)$ of this process are continuous and non-decreasing. They increase only on a set of measure 0 which is the closure of $\{t \ge 0; Y_t = 0\}$. These properties are a by-product of the irregularities of the paths of the Brownian motion.

The process Y is called a *Skew Brownian motion* [6]. Using its properties, several algorithms may be given. Also, its density has a simple form: $p(t, x, y) = \gamma(t, y - x) + \mathrm{sgn}(y)\theta\gamma(t, |x| + |y|)$, where $\gamma(t, x) = (2\pi t)^{1/2} \exp(-|y - x|^2/2t)$ is the Gaussian density.

In [8], we propose a simulation method in which $Y_{(k+1)\delta t}$ is exactly simulated when $Y_{k\delta t} = x$ is known using the expression of its density $p(\delta t, x, \cdot)$. Other algorithms, either based on probabilistic or analytic considerations, are also possible (See [8] for references).

These works justify the old heuristic that the interface acts like a permeable barrier. But due to the irregularities of the path, one has to look more closely to the properties of the process X or Y to give a sound meaning to this statement.

Although we present here some results specific to one-dimensional media, other algorithms have been proposed for multi-dimensional media with locally isotropic or orthotropic coefficients with a flat interface. In particular, in [7], we propose schemes with a better order of convergence than just moving the component of the process in the normal direction of the interface as in the one-dimensional case. For layered media, the scheme proposed in [5], which relies on some considerations of stochastic analysis, provides a simple and exact simulation technique.

Condition ($\mathcal{I}2$)**.** The interface condition ($\mathcal{I}2$) is seen as a semi-permeable barrier: the particle is reflected on the interface until it crosses it and starts afresh on the other side.

Using tools from stochastic analysis and the properties of the elastic Brownian motion which is linked to the Robin boundary conditions, we construct in [4] a diffusion process X associated to ($\star$) with the interface condition ($\mathcal{I}2$) by gluing together elastic Brownian motions. The time at which the particle passes for the first time to the other side of the interface is the smallest time at which the local time of the Brownian motion is greater than an independent exponential random

variable of parameter λ when $D = 1/2$. We also provide a simple simulation algorithm.

Open problems. Many problems remain open regarding interface conditions, among them:

- The presence of a drift/convection term (See however [1]).
- The multi-dimensional case when the diffusivity tensor is not diagonal on each side of the interface.
- High contrasts ($D^+ \gg D^-$), where some techniques related to rare events simulations shall be used.

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Variance reduction approaches in stochastic homogenization

Frédéric Legoll
(joint work with William Minvielle)

This work is concerned with the construction of variance reduction approaches in stochastic homogenization, that aim at better approximating the homogenized coefficients.

1. Introduction

Let $\mathcal{D}$ be a smooth bounded domain in $\mathbb{R}^d$ and let $f \in L^2(\mathcal{D})$. We consider the elliptic boundary value problem

$$-\operatorname{div}\left(A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right) = f \ \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \ \text{ on } \partial\mathcal{D}, \tag{1}$$

where ε is a small parameter. The matrix A is assumed to be bounded, uniformly elliptic, random and stationary in the sense that

$$\forall k \in \mathbb{Z}^d, \quad A(x+k,\omega) = A(x,\tau_k\omega) \quad \text{a.e. in } \mathbb{R}^d \text{ and a.s.}, \tag{2}$$

where $(\tau_k)_{k\in\mathbb{Z}^d}$ is a group action on the ambient probability space which is assumed to preserve the measure and be ergodic. We refer e.g. to [1] for all details on the probabilistic setting, which we skip here for the sake of brevity. We simply point out that we adopt here a *discrete* stationary setting, in contrast to many works in the literature, where a *continuous* stationary setting is used. The former is indeed more adapted to our work than the latter.

In that setting, it is well-known (see e.g. [5, 11]) that the solution $u^\varepsilon(\cdot,\omega)$ to (1) converges (weakly in $H^1_0(\mathcal{D})$ and strongly in $L^2(\mathcal{D})$, almost surely) to $u^\star$, solution to the homogenized problem

$$-\operatorname{div}(A^\star \nabla u^\star) = f \ \text{ in } \mathcal{D}, \quad u^\star = 0 \ \text{ on } \partial\mathcal{D}, \tag{3}$$

where the homogenized matrix $A^\star$ is *deterministic* and given by

$$A^\star_{ij} = \mathbb{E}\left[\int_Q e_i^T \ A(y,\cdot)\ (\nabla w_{e_j}(y,\cdot) + e_j)\, dy\right], \quad Q = (0,1)^d, \quad 1 \le i,j \le d, \tag{4}$$

where $\{e_i\}_{i=1}^d$ is the canonical basis of $\mathbb{R}^d$ and where, for any vector $p \in \mathbb{R}^d$, the *corrector* w_p is the solution (unique up to the addition of a random constant) to

$$\begin{cases} -\operatorname{div}[A(\nabla w_p + p)] = 0 \ \text{ on } \mathbb{R}^d, \\ \nabla w_p \text{ is stationary in the sense of (2)}, \quad \displaystyle\int_Q \mathbb{E}(\nabla w_p) = 0. \end{cases} \tag{5}$$

The corrector problem (5) is set on $\mathbb{R}^d$, and thus challenging to solve in practice. A standard approximation is to consider a truncated version of that problem on the so-called supercell $Q_N = (-N,N)^d$,

$$-\operatorname{div}\left[A(\cdot,\omega)\left(p + \nabla w_p^N(\cdot,\omega)\right)\right] = 0, \quad w_p^N(\cdot,\omega) \text{ is } Q_N\text{-periodic}, \tag{6}$$

and infer the apparent homogenized matrix $A^\star_N$ defined by

$$[A^\star_N(\omega)]_{ij} := \frac{1}{|Q_N|}\int_{Q_N} e_i^T A(y,\omega)\left(e_j + \nabla w^N_{e_j}(y,\omega)\right) dy. \tag{7}$$

We note that, although $A^\star$ itself is a deterministic object, its practical approximation $A^\star_N$ is random. It is only in the limit of infinitely large domains Q_N that the deterministic value is attained. Indeed, we know from [8] that $\lim\limits_{N\to\infty} A^\star_N(\omega) = A^\star$ a.s. Questions about rates of convergence in terms of the truncation size N have been addressed in [8], and in a recent series of works by A. Gloria and F. Otto [10].

Our aim is to design a technique that, for finite N, allows to compute $A^\star_N$ more effectively, i.e. with a smaller variance. More precisely, we decompose the error as

$$A^\star - A^\star_N(\omega) = \left(A^\star - \mathbb{E}\left[A^\star_N\right]\right) + \left(\mathbb{E}\left[A^\star_N\right] - A^\star_N(\omega)\right),$$

where the first term is a systematic error and the second term is a statistical error. In what follows, we focus on how to efficiently compute $\mathbb{E}\,[A_N^\star]$.

To that aim, a direct approach is the standard Monte Carlo approach, which consists in considering M independent realizations $A^m(y,\omega)$ of the random coefficient, and computing for each of them the approximate homogenized matrix $A^\star_{N,m}(\omega)$ using (6)–(7). In turn, the expectation $\mathbb{E}(A_N^\star)$ is approximated by

$$I_M := \frac{1}{M}\sum_{m=1}^{M} A^\star_{N,m}(\omega).$$

Using the Central Limit Theorem, it is commonly admitted that, for any $1 \le i,j \le d$, we have (with a probability equal to 95 %),

$$\left|\mathbb{E}([A_N^\star]_{ij}) - [I_M]_{ij}\right| \le 1.96\,\frac{\sqrt{\mathbb{V}\mathrm{ar}([A_N^\star]_{ij})}}{\sqrt{M}}. \tag{8}$$

Variance reduction techniques aim at improving on this estimate, by decreasing the prefactor in the above right-hand side. We have shown in [9, 6, 7, 13] that the technique of antithetic variables can be used to design more efficient approaches. In this work, we use another variance reduction technique, the so-called control variate approach, which builds on a surrogate model.

2. A weakly stochastic case: rare defects in a periodic structure

We describe here a model introduced in [2, 3, 4], that we will use in Section 3 to build our surrogate model. Consider the case when the random coefficient A writes

$$A(x,\omega) = A_{\rm per}(x) + b_\eta(x,\omega)\,C_{\rm per}(x),$$

where both $A_{\rm per}$ and $C_{\rm per}$ are $\mathbb{Z}^d$-periodic matrices, and

$$b_\eta(x,\omega) = \sum_{k\in\mathbb{Z}^d} 1_{Q+k}(x)\,B_\eta^k(\omega), \quad Q=(0,1)^d,$$

where $\left\{B_\eta^k\right\}_{k\in\mathbb{Z}^d}$ are i.i.d. Bernoulli random variables:

$$\mathbb{P}(B_\eta^k=1)=\eta, \quad \mathbb{P}(B_\eta^k=0)=1-\eta.$$

When η is a small parameter, $A = A_{\rm per}$ "most of the time". This model represents a periodic structure (described by $A = A_{\rm per}$) that may contains defects (modelled by $A_{\rm per} + C_{\rm per}$). When η is small, these defects are rare.

The above setting allows to model a large class of materials (including composite materials where some fibers have been deleted). The random checkerboard case also falls within that setting, by taking $A_{\rm per}(x) = \alpha$, $A_{\rm per}(x) + C_{\rm per}(x) = \beta$, and $\eta = 1/2$: on each cell $Q + k$, A is equal to α or β with equal probability.

We now return to the computation of the apparent homogenized matrix $A_N^\star(\omega)$ on the supercell Q_N, following (6)–(7). We first observe that a realization of the matrix A on Q_N is uniquely determined by the collection of the B_k^η (valued

in $\{0,1\}$) in each cell $k+Q$ of Q_N. By enumerating all possible realizations of $A(x,\omega)$ on Q_N, one obtains an expansion of $\mathbb{E}\left[A_N^\star\right]$ in powers of η (see [2, 3]):

$$\begin{aligned}\mathbb{E}\left[A_N^\star\right] &= \sum_{\omega \text{ s.t. } 0 \text{ defect}} A_N^\star(\omega)\mathbb{P}(\omega) + \sum_{\omega \text{ s.t. } 1 \text{ defect}} A_N^\star(\omega)\mathbb{P}(\omega) + \dots \\ &= A_{\rm per}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + O(\eta^3). \qquad (9)\end{aligned}$$

The leading order term is given by periodic homogenization: for any $p \in \mathbb{R}^d$,

$$A_{\rm per}^\star p = \int_Q A_{\rm per}(\nabla w_p^0 + p) \quad \text{with} \quad -\operatorname{div}\left[A_{\rm per}\left(p+\nabla w_p^0\right)\right] = 0, \quad w_p^0 \text{ is } Q\text{-periodic.}$$

The first-order correction writes

$$\overline{A}_1^{\star,N} = \frac{1}{|Q_N|}\sum_{k\in I_N} \mathcal{A}_k^{1\,\rm def}, \quad I_N = \left\{k\in\mathbb{Z}^d,\ k+Q\subset Q_N\right\},$$

where $\mathcal{A}_k^{1\,\rm def}$ is the contribution of a configuration with a unique defect located in the cell $k+Q$:

$$\forall p\in\mathbb{R}^d, \quad \mathcal{A}_k^{1\,\rm def} p = \int_{Q_N} A_1^k(\nabla w_p^{1,k}+p) - \int_{Q_N} A_{\rm per}(\nabla w_p^0 + p)$$

where $A_1^k = A_{\rm per} + \mathbf{1}_{Q+k} C_{\rm per}$ and

$$-\operatorname{div}\left[A_1^k\left(p+\nabla w_p^{1,k}\right)\right] = 0, \quad w_p^{1,k} \text{ is } Q_N\text{-periodic.} \qquad (10)$$

Remark 1. *The first order correction $\overline{A}_1^{\star,N}$ in* (9) *involves configurations with* one *defect. Likewise, the second order correction $\overline{A}_2^{\star,N}$ involves configurations with* two *defects. See* [2, 3, 4, 12] *for more details. On a different note, we observe that the contribution $\mathcal{A}_k^{1\,\rm def}$ is actually independent of k, due to the use of periodic boundary conditions in* (10).

3. A control variate approach

Using the above defect-type model, we now build an approximate model for $A_N^\star(\omega)$. We observe that, in the expansion (9), the first order correction satisfies

$$\eta\overline{A}_1^{\star,N} = \frac{\eta}{|Q_N|}\sum_{k\in I_N}\mathcal{A}_k^{1\,\rm def} = \mathbb{E}\left[A_1^{\star,N}\right], \qquad (11)$$

where we have introduced the random variable

$$A_1^{\star,N}(\omega) := \frac{1}{|Q_N|}\sum_{k\in I_N} B_\eta^k(\omega)\ \mathcal{A}_k^{1\,\rm def}.$$

We recall that $B_\eta^k = 1$ if there is a defect in the cell $Q+k$ (which happens with probability η) and $B_\eta^k = 0$ otherwise. We hence introduce

$$A_{\rm app}^\star(\omega) := A_{\rm per}^\star + A_1^{\star,N}(\omega) = A_{\rm per}^\star + \frac{1}{|Q_N|}\sum_{k\in I_N} B_\eta^k(\omega)\ \mathcal{A}_k^{1\,\rm def},$$

notice that, in view of (9) and (11),

$$\mathbb{E}\left[A_N^\star\right] = \mathbb{E}\left[A_{\rm app}^\star\right] + \eta^2 \overline{A}_2^{\star,N} + \cdots$$

and think of $A_{\rm app}^\star(\omega)$ as a good approximation of $A_N^\star(\omega)$. This is actually confirmed by the fact that, for any function φ,

$$\mathbb{E}\left[\varphi\left(A_N^\star\right)\right] = \mathbb{E}\left[\varphi\left(A_{\rm app}^\star\right)\right] + O\left(\eta^2\right).$$

The outline of our approach is as follows:

- draw $B_\eta^k(\omega)$ in each cell $Q + k \subset Q_N$. This determines the field $A(x,\omega)$ on Q_N.
- compute the associated approximate homogenized coefficient $A_N^\star(\omega)$ by solving (6)–(7).
- in parallel to this task, reconstruct from the specific realization of the set of $B_\eta^k(\omega)$ the field $A_{\rm app}^\star(\omega)$ and introduce the random variable

$$C_N^\star(\omega) := A_N^\star(\omega) - \rho\left(A_{\rm app}^\star(\omega) - \mathbb{E}\left[A_{\rm app}^\star\right]\right), \tag{12}$$

  where ρ is a deterministic parameter. Note that $\mathbb{E}\left[A_{\rm app}^\star\right]$ is analytically computable.

Observing that $\mathbb{E}\left[A_N^\star(\omega)\right] = \mathbb{E}\left[C_N^\star(\omega)\right]$, we next run the Monte Carlo approach on the random variable $C_N^\star(\omega)$. We hence introduce the estimator

$$J_M := \frac{1}{M}\sum_{m=1}^{M} C_{N,m}^\star(\omega),$$

which satisfies

$$\left|\mathbb{E}([A_N^\star]_{ij}) - [J_M]_{ij}\right| \le 1.96\ \frac{\sqrt{\mathbb{V}\mathrm{ar}([C_N^\star]_{ij})}}{\sqrt{M}}.$$

Comparing this confidence interval with (8), we see that the accuracy has been improved if $\mathbb{V}\mathrm{ar}([C_N^\star]_{ij}) < \mathbb{V}\mathrm{ar}([A_N^\star]_{ij})$. This condition is satisfied when choosing the deterministic parameter ρ in (12) as the one that minimizes the variance of $[C_N^\star(\omega)]_{ij}$.

We refer to [14] for a complete description of the approach, some elements of analysis, and comprehensive numerical results that demonstrate its efficiency in the regime $\eta \approx 1/2$: in that regime, defects are not rare, the asymptotic approximation described in Section 2 (namely, (9)) may be inaccurate, but it still can be used to define a surrogate model.

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Optimal Local Bases for Heterogeneous Media and Hierarchical Structures

Robert Lipton
(joint work with Ivo Babŭska)

Large multi-scale systems exhibit a cascade of substructure spread across several length scales. The importance of accurate numerical simulation for these systems is ever increasing due to the high cost of experimental testing of large structures made from heterogeneous materials. The computational modeling of such heterogeneous systems or structures is a very large problem that requires the use of parallel computers.

In order for a numerical method to be adequate it must be able to utilize many local computations performed independently on single processors or clusters of processors of reasonable size. Additionally because of their multi-scale nature these problems have many degrees of freedom and one seeks numerical approaches based upon dimension reduction. Unfortunately in many cases no clear scale separation is present and "the standard" methods of homogenization do not apply.

In this research effort we address both the problems of parallelization and dimension reduction and introduce a multi-scale finite element method composed of a global Galerkin scheme using optimal local basis functions. The local bases are supported on subdomains of prescribed diameter within the computational domain. There is great flexibility as there is no apriori restriction on the choice of subdomains. The notion of the Kolmogorov n-width is used to characterize a new optimal class of local bases. It is shown that these bases provide local approximations to the actual solution with exponentially decreasing error. For this choice the global Galerkin approximation converges exponentially with the coarse scale degrees of freedom.

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MsFEM à la Crouzeix-Raviart on perforated domains

Alexei Lozinski

(joint work with Claude Le Bris, Frédéric Legoll)

We are intereseted in the numerical solution of two following multicale problems

$$\begin{cases} -\nabla \cdot (a_\varepsilon \nabla u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{1}$$

$$\begin{cases} -\Delta u = f & \text{in } \Omega_\varepsilon := \Omega \setminus B_\varepsilon \\ u = 0 & \text{on } \partial\Omega_\varepsilon \end{cases} \tag{2}$$

In both cases, Ω represents a bounded domain in $\mathbb{R}^2$; a in Problem (1) is a highly oscillating coefficient ($0 < \alpha \leq a_\varepsilon(x) \leq \beta$ with some positive constants α and β) and B_ε in Problem (2) represents numerous holes in Ω. The first problem has been extensively studied both theoretically and numerically. One of the most popular numerical approaches for it is the multiscale finite element method (MsFEM), see the book [1] for a review. In this presentation, we discuss a new variant of this method [2], which is inspired by the classical Crouzeix-Raviart finite elements. The results that we obtain with this method for problems of type (1), although good, are less accurate than those by oversampling MsFEM. Nevertheless, the study of Crouzeix-Raviart MsFEM for this problem is useful at least as a starting point for developing an efficient MsFEM approach for problems of type (2), which have not yet been studied numerically in the context of MsFEM-type approaches to the best of our knowledge. We show in [3] that Crouzeix-Raviart MsFEM can be easily adapted to this context if we enrich the multiscale finite element space by carefully chosen bubble functions.

Let us describe in more detail our method for Problem (1). We introduce a regular mesh $\mathcal{T}_H$ (which may consist of triangles or quadrangles) on Ω and denote by $\mathcal{E}_H$ the ensemble of irs internal edges. The size H of the mesh cells in $\mathcal{T}_H$ is supposed to be larger than ε (the characteristic length of oscillations in a) so that usual finite elements cannot be efficiently used on this mesh. We are thus looking for a new approximating space V_H which is well adapted to Problem (1) and has a localized basis, i.e. a basis consisting of functions with supports covering a small number of cells of $\mathcal{T}_H$. We allow V_H to be non-conforming, i.e. to contain the functions that are discontinuous on the edges of the mesh $\mathcal{T}_H$ (note that it is also the case for the oversampling MsFEM). We enforce however a "weak" continuity of our numerical solution by requiring that the average of the jump vanishes on each edge. The natural functional space for our purposes is thus larger than $H_0^1(\Omega)$ and can be introduced as

$$W_H = \left\{ u \in L^2(\Omega) : u_H|_T \in H^1(T)\ \forall T \in \mathcal{T}_H \text{ and } \int_E [u] = 0\ \forall E \in \mathcal{E}_H \right\}$$

$[u]$ denoting the jump of u over an edge. Decompose now W_H into the sum of resolved and unresolved scales $W_H = V_H \oplus^{\perp_a} W_H^0$ where

$$W_H^0 = \{u \in W_H : \int_E u = 0,\ \forall E \in \mathcal{E}_H\},\ V_H = \{u \in W_H : a_H(u,v) = 0,\ \forall v \in W_H^0\}$$

with $a_H(u,v) = \sum_{T\in\mathcal{T}_H} \int_T a_\varepsilon \nabla u \cdot \nabla v$. It is easy to see that the space V_H is of finite dimension and it has a localized basis. Indeed, $V_H = \text{span}\,(\phi_e,\ e \in \mathcal{E}_H)$ where ϕ_e is constructed for any internal edge e of the mesh as follows: denoting by T_1 and T_2 the two mesh elements that share the edge e and by by Γ_i^k $(i = 1, \ldots, N_\Gamma)$ the edges composing the boundary of T_k ($k = 1$ or 2) numbered so that $\Gamma_1^1 = \Gamma_1^2 = e$, we define ϕ_e as the function with support in $T_1 \cup T_2$ that solves

$$-\nabla \cdot [a_\varepsilon(x)\nabla\phi_e] = 0 \text{ in } T_k,\ k = 1,2 \tag{3}$$

$$\int_{\Gamma_i^k} \phi_e = \delta_{i1} \text{ for } i = 1, \ldots, N_\Gamma,\ k = 1,2 \tag{4}$$

$$n \cdot a_\varepsilon \nabla\phi_e = \lambda_i^k \text{ on } \Gamma_i^k,\ i = 1, \ldots, N_\Gamma,\ k = 1,2 \tag{5}$$

with some constants λ_i^k. In practice, the basis functions ϕ_e should be precomputed numerically using a sufficiently fine mesh. Then, the approximated solution u_H to (1) is found as

$$u_H \in V_H : \quad a_H(u_H, v_H) = (f, v_H)_{L^2(\Omega)} \quad \forall v_H \in V_H. \tag{6}$$

We have proved the following error estimate in the periodic case:

Theorem 1. *Under the hypothesis $a_\varepsilon(x) = a_{1\text{-periodic}}(\frac{x}{\varepsilon})$, the MsFEM solution u_H satisfies*

$$|u - u_H|_{H^1} \le CH\|f\|_{L^2} + C\left(\sqrt{\varepsilon} + H + \sqrt{\frac{\varepsilon}{H}}\right)\|\nabla u^\star\|_{C^1},$$

where C is a constant independent of H and $u^\star$ is the homogenized solution to (1) in the limit $\varepsilon \to 0$.

We now turn to Problem (2). One could apply to this problem exactly the same method as before. The only difference would be that one replaces the bilinear form by $a_H(u,v) = \sum_{T\in\mathcal{T}_H} \int_{T\setminus B_\varepsilon} \nabla u \cdot \nabla v$ and the MsFEM basis functions are constructed as the solutions of local problems on perforated mesh cells, i.e. ϕ_e for any edge $e \in \mathcal{E}_H$ satisfies $-\Delta\phi_e = 0$ in $T_k \setminus B_\varepsilon$, $k = 1, 2$, $\phi_e|_{\partial B_\varepsilon} = 0$ accompanied with boundary conditions similar to (4)–(5). This method turns out to be unsatisfactory in practice since the basis functions computed in this way decay exponentially fast when one moves away from an edge, and thus a Galerkin approximation on such a basis can miss completely the exact solution in the regions well inside the mesh elements. We need therefore to enrich the approximation space. This enrichment can be still presented as a decomposition of W_H into the sum of resolved and unresolved scales $W_H = \tilde{V}_H \oplus^{\perp_a} \tilde{W}_H^0$ where the new space of unresolved scales $\tilde{W}_H^0$ is smaller than before

$$\tilde{W}_H^0 = \{u \in W_H \text{ such that } \int_E u = 0,\ \forall E \in \mathcal{E}_H \text{ and } \int_T u = 0,\ \forall T \in \mathcal{T}_H\}$$

and the new approximation space is still the orthogonal (with respect to the form a_H) complement of $\tilde{W}_H^0$. One can see that $\tilde{V}_H = \text{span}\,(\phi_e,\ e \in \mathcal{E}_H) \oplus \text{span}\,(\phi_T^b,\ T \in \mathcal{T}_H)$ where ϕ_e are constructed for any internal edge e as outlined above and the new basis functions ϕ_T^b are associated to each element T of the mesh and are constructed as solutions to

$$-\Delta\phi_T^b = 1 \text{ in } T \setminus B_\varepsilon, \quad \phi_T^b|_{\partial B_\varepsilon} = 0, \quad \phi_T^b|_{\partial T} = 0.$$

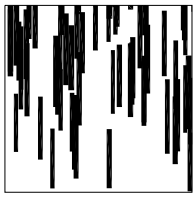
We call ϕ_T^b the MsFEM bubble functions as they share with classical finite element bubble function the property of vanishing on all the edges of the mesh. We have proved the following error estimate in the periodic case:

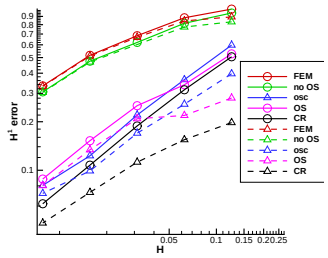
Theorem 2. *Under the hypothesis of a periodic micro-structure, i.e. B_ε being an ε- periodic array of identical holes, and under some technical assumption on the mesh $\mathcal{T}_H$, the MsFEM solutions $u_H \in \tilde{V}_H$ to (6) with V_H replaced by $\tilde{V}_H$ satisfies*

$$|u - u_H|_{H^1(\Omega)} \leq C\varepsilon \left(\sqrt{\varepsilon} + H + \sqrt{\frac{\varepsilon}{H}}\right) ||f||_{W^{2,\infty}(\Omega)}$$

where C is a constant independent of H.

The numerical experiments confirm a similar behavior of the method also in the non-periodic case. As an example, the following figure presents the results for Problem (2) with $\Omega = (0,1)^2$ and the holes B_ε as in the picture on the left. The picture on the right gives the convergence curves ($|u - u_H|_{H^1}$ versus H) on rectangular meshes of step H for a variety of methods, "FEM" for standard $\mathbb{Q}_1$ FEM, "noOS", "osc", "OS" for classical MsFEM variants with respectively linear, oscillating and oversapling boundary conditions, and "CR" for our Crouzeix-Raviart MsFEM. In all the cases, the dashed curves stand for the variants of the corresponding method enriched by the bubble functions.





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Kinetic theory and the discrete nonlinear Schrödinger equation

Jani Lukkarinen

It is common practice to approximate a weakly nonlinear wave equation through a kinetic transport equation of the Boltzmann type. The precise mathematical meaning and domain of applicability of such approximations is still an open question. In this talk, I present an overview of the present understanding of how such transport equations may arise from wave equations with weak interactions, and comment on how the problem is related to the larger research program of understanding the origin of diffusive transport of energy in these systems, i.e., to proving the validity of Fourier's law.

The following presents a physical scenario for the expected time-evolution of a dynamical system with *normal thermal conductivity*:

- $t = 0$**:** The system is started with a "typical", sufficiently well-behaved, *initial state*. This can be either deterministic or stochastic.
- $t = O(1)$**:** The state of the system should approach *local equilibrium*: time-averaged, local observables should be well approximated by the corresponding expectation in some thermal equilibrium state. The choice of state typically still depends on time and spatial position. For instance, in the "simplest" Hamiltonian examples, this would lead to approximation of the evolution of the full system via evolution of a temperature distribution $T(x, t)$, considered as parameters of canonical Gibbs states for the local statistics.
- $t = O(L^2)$**:** For macroscopic times, the system should relax towards equilibrium, unless some outside forcing is imposed (here $L \gg 1$ is a macroscopic

length, for instance, the diameter of the system). The relaxation should happen via local equilibrium states and involve diffusion of energy; for instance, Fourier's law should hold and the above parameters $T(x,t)$ satisfy a heat equation with some thermal conductivity function $\kappa(T)$.

Very little of the validity of the above scenario has been mathematically proven so far. Most of the progress has been in studies of systems with stochastic dynamics which allows for various new tools and simplifications compared to purely Hamiltonian dynamical systems.

One motivation for introduction of stochastic states, even when the dynamics is deterministic, is due to the following practical obstacles present in any real physical experiment or simulation.

(1) The initial data may be only *partially prepared or measured*.
(2) Measurements have only a *finite time-resolution* $t_0 > 0$.
(3) Most of the above systems involve a vast number of degrees of freedom, and even though one can prove that the problem is mathematically well-posed, the actual computation of the solution for a given initial state at a given time is often not possible, not even in any meaningful approximation. A simple oscillator serves to illustrate the point: suppose $\omega \in \mathbb{R}_+$ is irrational and consider $\psi_t := \mathrm{e}^{\mathrm{i}2\pi\omega t}$, $t \geq 0$. To compute the value of ψ_t, it is necessary to compute the fractional part of ωt. At the very least, this requires storing the *value* of ω in accuracy which is greater than $1/t$. Thus for large enough $t \gg 1$ this becomes impossible using any physical computing device with finite memory.

Hence, when studying large scale properties of macroscopic systems, it looks more reasonable to aim at descriptions using a stochastic state μ_t (a probability measure) for the dynamical degrees of freedom ψ_t. These could be defined (using the Riesz-Markov representation theorem) by

$$\int \mathrm{d}\mu_t(\psi)\, F(\psi) := \frac{1}{t_0} \int_t^{t+t_0} \mathrm{d}s \int \mathrm{d}\nu_0(\psi_0)\, F(\psi_s[\psi_0])\,, \tag{1}$$

where F is any *observable*, ν_0 *describes the uncertainty* in the initial data and $t_0 > 0$ *the time-resolution*. In the simple oscillator example in item 3, $\psi_s[\psi_0] = \mathrm{e}^{\mathrm{i}2\pi\omega s}$, and as soon as $\omega t_0 \gg 1$, the measure μ_t is very well approximated, uniformly in t, by the uniform measure on the unit circle. In other words, as long as one is not interested in time-scales shorter than the period of oscillation, the uniform measure serves as an accurate approximation for any t, even though the exact value of ψ_t could never be computed. In addition to (1), other definitions for μ_t are certainly possible, and depending on the problem a well-chosen averaging procedure might simplify the estimates considerably.

One instance in which a mathematical control of some parts of the physical scenario has begun to look feasible, is given by kinetic scaling limits of weakly perturbed wave-equations. There one considers a *small perturbation* (strength $\lambda > 0$) of a *transport dominated system* (a system where the motion is described by constant velocity, i.e., ballistic, motion). The goal is to see some remnants of

the above physical scenario by suitably rescaling time and taking $\lambda \to 0$. More precisely, for weakly perturbed wave-type equations we expect to find the following behaviour:

- $t = 0$**:** Assume a random initial state with *fast spatial decay of correlations*.
- $t = O(\lambda^{-1})$**:** Wave motion continues, but with a possibly modified dispersion relation. The state *approaches a Gaussian* distribution and *becomes homogenized*, with variation on the scale t.
- $t = O(\lambda^{-2})$**:** Wave motion gets interrupted by "collisions". Effect of collisions on the covariance is described by some *wave Boltzmann equation*.
- $t = o(\lambda^{-3})$**:** The Boltzmann equation should force the covariance locally towards an equilibrium covariance.

Should the above scheme work, one would expect the state of the system to remain close to a local equilibrium state also for later times, although exceptions to this rule are also possible (such as the exponentially slow "freezing" expected in two-dimensional Anderson models).

As an explicit test-case of the above scheme, I refer to a joint work with Herbert Spohn concerning a discrete Schrödinger equation with a weak nonlinear interaction [1]. We derive an explicit equation—indirectly related to the conjectured Boltzmann equation of the system—for the decay of field-field time-correlations in a regular thermal Gibbs state, compensated for fast oscillations and in the kinetic scaling limit. The proof is based on a regularized perturbation expansion and uses heavily the stationarity of the initial state which implies ℓ_1-summability of the cumulants of the field at any fixed time.

The result in [1] describes a compensated scaling limit of time-correlations. The chosen observable might appear somewhat artificial since it involves taking $\lambda \to 0$ with $t = O(\lambda^{-2})$. However, the result could become useful for development of *more efficient numerical algorithms* for small λ by resolving fast oscillations and lowest order effects. More precisely, the result proven in [1] implies that for $t = O(\lambda^{-2})$

$$\mathbb{E}[\widehat{\psi}_0(k')^* \widehat{\psi}_t(k)] \approx \delta_\Lambda(k' - k) W(k) \mathrm{e}^{-\mathrm{i}\omega^\lambda_{\mathrm{ren}}(k)t} \mathrm{e}^{-|\lambda^2 t|\Gamma_1(k)} ,$$

where the equilibrium covariance $W(k)$, the renormalized dispersion relation $\omega^\lambda_{\mathrm{ren}}(k)$ and the decay rate $\Gamma_1(k) \geq 0$ are explicitly computable functions of the wave-vector $k \in \mathbb{T}^d$. To see what happens at later times, it might help to cancel out the known oscillations and to study

$$\mathbb{E}[\widehat{\phi}_0(k')^* \widehat{\phi}_t(k)] - \delta_\Lambda(k' - k) W(k) \mathrm{e}^{-|\lambda^2 t|\Gamma_1(k)} ,$$

where $\widehat{\phi}_t(k) := \mathrm{e}^{\mathrm{i}\omega^\lambda_{\mathrm{ren}}(k)t} \widehat{\psi}_t(k)$.

If the full kinetic conjecture could be proven, this should be of even greater use since it would allow experimenting with algorithms which start by solving the limit Boltzmann equation for the given initial data and then employ the approximation which is obtained from the solution by scaling back powers of λ. However, as with most of the above discussion, at present such considerations should be at

best considered as conjectures, and much more work is needed before a full mathematical understanding, including domain of validity, of such schemes will have been developed.

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Multiscale methods for transport processes through membranes

Maria Neuss-Radu

In this paper we develop multiscale methods appropriate for the homogenization of processes in domains containing thin heterogeneous layers. Our model problem consists of a reaction-diffusion system in such a domain. Both, the size of the heterogeneities and the thickness of the layer are of order ε. Performing an asymptotic analysis with respect to the scale parameter ε, we derive an effective model which consists of reaction-diffusion equations on two domains separated by an interface, together with appropriate transmission conditions across this interface. These conditions are determined solving micro-problems on the standard periodicity cell in the layer. Thereby, the techniques developed in [1, 2] for the derivation of effective transmission conditions across flat interfaces are further extended to include curved membranes. This step requires new concepts like periodicity on thin curved layers, and two-scale convergence with respect to manifold charts, see [3].

Let $\varepsilon > 0$ be a sequence of strictly positive numbers which goes to zero. We consider a bounded domain $\Omega \subset \mathbb{R}^n,\ n \geq 2$, consisting of three subdomains: the bulk regions $\Omega_\varepsilon^+,\ \Omega_\varepsilon^-$, and the thin heterogeneous layer Ω_ε^M, separated by the interfaces S_ε^+ and S_ε^-, see Figure 1 (left). Thus we have

$$\Omega = \Omega_\varepsilon^+ \cup \Omega_\varepsilon^- \cup \Omega_\varepsilon^M \cup S_\varepsilon^+ \cup S_\varepsilon^-.$$

The outer unit normal at the boundaries of the domains Ω and Ω_ε^M is also denoted by ν. The restrictions of functions defined on Ω to the subdomains $\Omega_\varepsilon^+,\ \Omega_\varepsilon^-$, and Ω_ε^M are denoted by the superscripts $+,\ -$, and M respectively. In the domain Ω, we consider the following reaction-diffusion equation for the unknown function $u_\varepsilon : (0,T) \times \Omega \to \mathbb{R}$:

$$\begin{aligned} \partial_t u_\varepsilon^+ - D^+ \Delta u_\varepsilon^+ &= f(x, u_\varepsilon^+) && \text{in } (0,T) \times \Omega_\varepsilon^+ \\ \partial_t u_\varepsilon^- - D^- \Delta u_\varepsilon^- &= f(x, u_\varepsilon^-) && \text{in } (0,T) \times \Omega_\varepsilon^- \\ \tfrac{1}{\varepsilon} \partial_t u_\varepsilon^M - \nabla \cdot (\varepsilon D_\varepsilon^M(x) \nabla u_\varepsilon^M) &= \tfrac{1}{\varepsilon}\, g_\varepsilon\left(x, u_\varepsilon^M\right) && \text{in } (0,T) \times \Omega_\varepsilon^M \end{aligned} \tag{1}$$

subjected to the following boundary conditions:

$$u_\varepsilon = u_D \quad \text{on } \partial\Omega \tag{2}$$

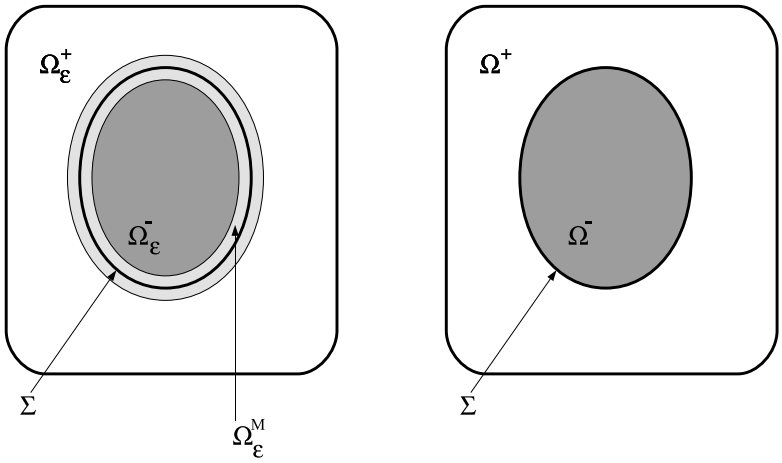

FIGURE 1. Left: The microscopic domain Ω composed of the two bulk domains Ω_ε^+, and Ω_ε^-, and the membrane domain Ω_ε^M. Right: The macroscopic domain consisting of the two bulk regions Ω^+, and Ω^- separated by the interface Σ.

and initial conditions:

$$u_\varepsilon(0,x) = \begin{cases} U_0(x), & x \in \Omega_\varepsilon^+ \\ U_0^M\left(\bar{x}, \frac{x_n}{\varepsilon}\right), & x \in \Omega_\varepsilon^M \\ U_0(x), & x \in \Omega_\varepsilon^- \end{cases} \tag{3}$$

On the interfaces S_ε^+ and S_ε^- we require the natural transmition conditions, i.e. the continuity of the solutions and of the normal fluxes:

$$\begin{aligned} u_\varepsilon^\pm &= u_\varepsilon^M && \text{on } S_\varepsilon^\pm \\ D^\pm \nabla u_\varepsilon^\pm \cdot \nu &= \varepsilon D_\varepsilon^M(x) \nabla u_\varepsilon^M \cdot \nu && \text{on } S_\varepsilon^\pm. \end{aligned} \tag{4}$$

The microscopic heterogeneous structure of the membrane Ω_ε^M is reflected in the diffusion coefficients D_ε^M and the reaction term g_ε, which we assume to be locally ε-periodic, see Definition 1 below.

Definition 1 (Locally periodic functions on thin curved layers)**.** *A sequence of functions $a_\varepsilon : \Omega_\varepsilon^M \to \mathbb{R}$ is called locally ε-periodic if there exists an atlas $\mathcal{A}_\Sigma = \{(U_i, \varphi_i)\}_{i=1,\dots,N}$ of Σ consisting of charts*

$$U_i \ni \mathbf{x}' \mapsto \sigma = \varphi_i(\mathbf{x}') \in V_i \subset \Sigma \tag{5}$$

mapping open sets $U_i \subset \mathbb{R}^{n-1}$ to open sets $V_i \subset \Sigma$ such that

$$a_\varepsilon(x) = a_\varepsilon(\mathcal{T}(\sigma,\rho)) = a_i\left(\varphi_i^{-1}(\sigma), \frac{\varphi_i^{-1}(\sigma)}{\varepsilon}, \frac{\rho}{\varepsilon}\right), \tag{6}$$

with smooth functions $a_i : U_i \times [0,1]^{n-1} \times [-1,1] \to \mathbb{R}$, $i = 1, \dots, N$, *which are* 1*-periodic in the second variable. We denote by*

$$Z = Y \times [-1,1] = [0,1]^{n-1} \times [-1,1],$$

the standard cell in the chart domain.

To model the behavior of the solutions u_ε for small values of the parameter ε, we investigate the asymptotic behavior of the sequence u_ε when $\varepsilon \to 0$. Then, the thin layer Ω_ε^M approaches the interface Σ. The domains Ω_ε^+ and Ω_ε^- tend to the domains Ω^+ and Ω^- respectively, see Figure 1, (right). We extend the notion of two-scale convergence introduced in [1] to curved thin layers. Furthermore, we are able to show strong two-scale convergence of the sequence u_ε in the membrane domain. Using these results, we prove that for $\varepsilon \to 0$ the sequence $(u_\varepsilon^+, u_\varepsilon^-, u_\varepsilon^M)$ converges to the limit $(u_0^+, u_0^-, (u_i^M)_{i=1,\dots,N})$ satisfying the following effective model:

Theorem 2. *The limit functions* u_0^+ *and* u_0^- *satisfy the following initial-boundary-value problem on* Ω^+ *respective* Ω^- :

$$\begin{aligned} \partial_t u_0^\pm(t,x) - D^\pm \Delta u_0^\pm(t,x) &= f(x, u_0^\pm(t,x)), \quad (t,x) \in (0,T) \times \Omega^\pm \\ u_0^+(t,x) &= u_D(t,x), \quad (t,x) \in (0,T) \times \partial\Omega \\ u_0^\pm(0,x) &= U_0(x), \quad x \in \Omega^\pm, \end{aligned}$$

together with the effective transmission conditions on the interface Σ*, formulated in the chart coordinates of the atlas* $\mathcal{A}_\Sigma$

$$D^\pm \nabla u_0^\pm(t, \mathcal{T}_i(\mathbf{x}', 0)) \cdot \nu(\mathcal{T}_i(\mathbf{x}', 0)) = \int_{S^\pm} D_i^M(\mathbf{x}', \mathbf{y}) \frac{\partial u_i^M}{\partial \mathbf{y}_n}(t, \mathbf{x}', \mathbf{y}) d\mathbf{y}',$$

for $\mathbf{x}' \in U_i$, $i = 1, \dots, N$, *and* $t \in (0,T)$.

The limit functions u_i^M, $i = 1, \dots, N$ *which enter the transmission conditions are solutions to the following local problems, also given with respect to the chart coordinates*

$$\begin{aligned} &\partial_t u_i^M(t, \mathbf{x}', \mathbf{y}) - \sum_{j=1}^{n-1} \frac{\partial}{\partial \mathbf{y}_j} \left\{ D_i^M(\mathbf{x}', \mathbf{y}) g_i^{jk}(\mathbf{x}') \frac{\partial u_i^M}{\partial \mathbf{y}_k}(t, \mathbf{x}', \mathbf{y}) \right\} \\ &- \frac{\partial}{\partial \mathbf{y}_n} \left\{ D_i^M(\mathbf{x}', \mathbf{y}) \frac{\partial u_i^M}{\partial \mathbf{y}_n}(t, \mathbf{x}', \mathbf{y}) \right\} = g_i^M(\mathbf{x}', \mathbf{y}, u_i^M(t, \mathbf{x}', \mathbf{y})), \\ &\qquad\qquad (t, \mathbf{y}) \in (0,T) \times Z, \text{ a.e. } \mathbf{x}' \in U_i \\ &u_i^M(t, \mathbf{x}', \mathbf{y}', \pm 1) = u_0^\pm(t, \mathcal{T}_i(\mathbf{x}', 0)), \quad (t, \mathbf{y}') \in (0,T) \times Y, \text{ a.e. } \mathbf{x}' \in U_i \\ &u_i^M \text{ periodic in } Y = [0,1]^{n-1} \\ &u_i^M(0, \mathbf{x}', \mathbf{y}) = U_0^M(\mathbf{x}', \mathbf{y}_n), \quad \mathbf{y} \in Z, \text{ a.e. } \mathbf{x}' \in U_i. \end{aligned}$$

where the tensor

$$G_i(\mathbf{x}') = \left(g_i^{jk}(\mathbf{x}') \right)_{j,k=1,\dots,n-1} \tag{7}$$

is the inverse of the metric tensor $G^i(\mathbf{x}')$ *of* Σ *in the chart* (U_i, φ_i) *defined by*

$$G^i(\mathbf{x}') = \left(g^i_{jk}(\mathbf{x}')\right)_{j,k=1,\ldots,n-1} = \left(\sum_{l=1}^{n} \frac{\partial \varphi_{il}}{\partial x_j}(\mathbf{x}') \frac{\partial \varphi_{il}}{\partial x_k}(\mathbf{x}')\right)_{j,k=1,\ldots,n-1}.$$

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Random fields representations for stochastic elliptic boundary value problem and statistical inverse problems

Anthony Nouy

(joint work with Christian Soize)

We present new results for the identification of random fields through statistical inverse problem involving a stochastic elliptic boundary value problem [2]. A general class of non-Gaussian positive-definite matrix-valued random fields adapted to the statistical inverse problems is introduced and its properties are analyzed. Using a parametrization of discretized random fields in this class, a complete identification procedure is proposed. New results of the mathematical and numerical analyzes of the parameterized stochastic elliptic boundary value problem are presented. The numerical solution of this parametric stochastic problem provides an explicit approximation of the application that maps the parameterized general class of random fields to the corresponding set of random solutions. This approximation can be used during the identification procedure in order to avoid the solution of multiple forward stochastic problems. Since the proposed general class of random fields possibly contain random fields which are not uniformly bounded, a particular mathematical analysis is developed [3] and dedicated approximation methods are introduced. In order to make affordable the construction of an approximation of a very high-dimensional map, complexity reduction methods are introduced and are based on the use of low-rank approximation methods [1] that exploit the tensor structure of the solution which results from the parametrization of the general class of random fields.

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From averaging to homogenization in cellular flows.

Alexei Novikov
(joint work with G.Iyer, T.Komorowski, L.Ryzhik)

Consider an advection diffusion equation of the form

$$\partial_t \varphi + Av(x) \cdot \nabla \varphi - \Delta \varphi = 0. \tag{1}$$

where A is the non-dimensional strength of a prescribed vector field $v(x)$. Under reasonable assumptions when $A \to \infty$, the solution φ becomes constant on the trajectories of v. Indeed, dividing (1) by A and passing to the limit $A \to \infty$ formally shows

$$v(x) \cdot \nabla \varphi = 0,$$

which, of course, forces φ to be constant along trajectories of v. Well known "averaging" results [2] study the slow evolution of $\varphi(t, x)$ across various trajectories.

On the other hand, if we fix $A = 1$, classical homogenization results (see e.g. [1]) determine the long time behavior of solutions of (1). For such results it is usually convenient to choose $\varepsilon \ll 1$ small, and rescale (1) to time scales of order $1/\epsilon^2$, and distance scales of order $1/\epsilon$. This gives

$$\partial_t \varphi_\varepsilon + \frac{1}{\varepsilon} v\left(\frac{x}{\varepsilon}\right) \cdot \nabla \varphi_\varepsilon - \Delta \varphi_\varepsilon = 0. \tag{2}$$

Assuming v is periodic and mean-zero, and that the initial condition varies slowly (i.e. $\varphi_\epsilon(x, 0)$ is independent of ϵ), standard homogenization results show that $\varphi_\epsilon \to \bar{\varphi}$, as $\epsilon \to 0$. Further, $\bar{\varphi}$ is the solution of the effective problem

$$\frac{\partial \bar{\varphi}}{\partial t} = \nabla \cdot (\bar{\sigma} \nabla \varphi), \tag{3}$$

and $\bar{\sigma}$ is the effective diffusion matrix, which can be computed as follows. Define the correctors $\chi_1, \ldots, \chi_n$ to be the mean-zero periodic solutions of

$$-\Delta \chi_j + v(x) \cdot \nabla \chi_j = -v_j(x), \quad j = 1, \ldots, n. \tag{4}$$

Then

$$\bar{\sigma}_{ij} = \delta_{ij} + \frac{1}{|Q|} \int_Q \nabla \chi_i \cdot \nabla \chi_j \, dx, \quad i, j = 1, \ldots, n. \tag{5}$$

Q is the period cell of the flow $v(x)$, and δ_{ij} is the Kronecker delta function.

The main focus of this work is to study a transition between the two well known regimes described above. To this end, rescale (1) by choosing time scales of the order $1/\epsilon^2$ and length scales of order $1/\epsilon$. This gives

$$\partial_t \varphi_{\varepsilon,A} + \frac{A}{\varepsilon} v\left(\frac{x}{\varepsilon}\right) \cdot \nabla \varphi_{\varepsilon,A} - \Delta \varphi_{\varepsilon,A} = 0, \tag{6}$$

where $A \gg 1$ and $\varepsilon \ll 1$ are two *independent* parameters. Of course, if we keep ϵ fixed, and send $A \to \infty$, the well known averaging results apply. Alternately, if we keep A fixed and send $\epsilon \to 0$, we are in the regime of standard homogenization results. The present paper considers (6) with *both* $\epsilon \to 0$ and $A \to \infty$. Our main result [3] shows that if v is a $2D$ cellular flow, then we see a sharp transition between the homogenization and averaging regimes at $A \approx 1/\epsilon^4$.

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A quantitative theory in stochastic homogenization

Felix Otto

We consider a scalar elliptic equation $\nabla^* a \nabla u = f$ on the d-dimensional lattice $\mathbb{Z}^d$ with a random coefficients field a, that is assumed to be uniformly elliptic in the sense of $\lambda \mathrm{id} \le a(x) \le \mathrm{id}$ for all sites $x \in \mathbb{Z}^d$ for some fixed $\lambda > 0$. Under the mere assumption of stationarity and ergodicity of the ensemble $\langle \cdot \rangle$, Kozlov and Papanicolaou & Varadhan have shown that for a right hand side f that varies on a length large scale L, the solution u converges to a deterministic solution of a homogenized problem.

In this talk, we optimally quantify this convergence: If the correlations are integrable, the fluctuations $u(x) - \langle u(x) \rangle$ satisfy a Central Limit Theorem scaling. The integrability of correlations is encoded by the assumption that the ensemble $\langle \cdot \rangle$ satisfies a Logarithmic Sobolev Inequality (LSI). This means that there exists a constant $\rho > 0$ such that for all functions $\zeta(a) > 0$ of the coefficient field a, one has

$$\langle \zeta \ln \frac{\zeta}{\langle \zeta \rangle} \rangle \le \frac{1}{2\rho} \Big\langle \sum_{x \in \mathbb{Z}^d} \big| \frac{\partial \zeta}{\partial a(x)} \big|^2 \Big\rangle,$$

where $\frac{\partial \zeta}{\partial a(x)}$ denotes the partial derivative of ζ with respect to the value $a(x)$ of the coefficient field at site x. In fact, we appeal to a slightly weakened version of LSI that is in particular satisfied for any independently and identically distributed $\{a(x)\}_{x \in \mathbb{Z}^d}$.

The main insight is that the assumption of LSI allows to upgrade the annealed estimates on first and (mixed) second derivatives of the Green's function $G(a; x, y)$ by Delmotte & Deuschel, namely

$$\begin{aligned} \langle |\nabla_x G(x,y)|^2 \rangle^{\frac{1}{2}} &\le C(d,\lambda)|x-y|^{1-d}, \\ \langle |\nabla_x \nabla_y G(x,y)| \rangle &\le C(d,\lambda)|x-y|^{-d} \end{aligned}$$

to stochastic moments of arbitrary order $p < \infty$:

$$\begin{aligned} \langle |\nabla_x G(x,y)|^p \rangle^{\frac{1}{p}} &\leq C(d,\lambda,\rho,p)|x-y|^{1-d}, \\ \langle |\nabla_x \nabla_y G(x,y)|^p \rangle^{\frac{1}{p}} &\leq C(d,\lambda,\rho,p)|x-y|^{-d}. \end{aligned}$$

The latter is of independent interest since is shows that with high probability, the variable-coefficient Green's function G decays like the constant coefficient one, despite the fact that there are — necessarily ungeneric coefficient fields a — for which the Green's function has a worse decay.

This is joint work with Daniel Marahrens, see MPI MIS Preprint 69/2012 "Annealed estimates on the Green's function".

Random homogenisation of a highly oscillatory singular potential

Etienne Pardoux

(joint work with M. Hairer and A. Piatnitski)

We consider the parabolic PDE with space-time random potential given by

$$\begin{aligned} \partial_t u^\varepsilon(x,t) &= \partial_x^2 u^\varepsilon(x,t) + \varepsilon^{-\beta} V\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^\alpha}\right) u^\varepsilon(x,t) \,, \\ u^\varepsilon(x,0) &= u_0(x) \,, \end{aligned} \tag{1}$$

where $x \in \mathbb{R}$, $t \geq 0$ and V is a stationary centred random field. The homogenisation theory of equations of this type has been studied by a number of authors. The case when V is time-independent was considered in [6] and [1]. The articles [3], [4] considered a situation where V is a stationary process as a function of time, but periodic in space. Purely periodic / quasiperiodic operators with large potential were also studied several authors. A problem similar to ours, but with a Gaussian potential, was considered in [2].

For $\alpha \geq 2$ and $\beta = \frac{\alpha}{2}$, (1) was studied in [7], where it was shown that its solutions converge as $\varepsilon \to 0$ to the solutions to

$$\partial_t u(x,t) = \partial_x^2 u(x,t) + \bar{V} u(x,t) \,, \quad u(x,0) = u_0(x) \,, \tag{2}$$

where the constant $\bar{V}$ is given by

$$\bar{V} = \int_0^\infty \Phi(0,t)\, dt \,,$$

in the case $\alpha > 2$ and

$$\bar{V} = \int_0^\infty \int_{-\infty}^\infty \frac{e^{-\frac{x^2}{4t}}}{2\sqrt{\pi t}} \Phi(x,t)\, dx\, dt \,,$$

in the case $\alpha = 2$. Here, $\Phi(x,t) = \mathbb{E}V(0,0)V(x,t)$ is the correlation function of V which is assumed to decay sufficiently fast.

In the case $0 < \alpha < 2$, it was conjectured in [7] that the correct scaling to use in order to obtain a non-trivial limit is $\beta = 1/2 + \alpha/4$, but the corresponding value of $\bar{V}$ was not obtained. Furthermore, the techniques used there seem to break down

in this case. The main result of the present article is that the conjecture does indeed hold true and that the solutions to (1) do again converge to those of (2) as $\varepsilon \to 0$. This time, the limiting constant $\bar{V}$ is given by

$$\bar{V} = \frac{1}{2\sqrt{\pi}} \int_0^\infty \frac{\overline{\Phi}(t)}{\sqrt{t}}\, dt\ ,$$

where we have set $\overline{\Phi}(s) := \int_{\mathbb{R}} \Phi(x,s)dx$.

The techniques employed in the present article are very different from [7]: instead of relying on probabilistic techniques, we adapt the analytical techniques from [5].

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Spectrum-preserving two-scale decompositions with applications to numerical homogenization and eigensolvers

Daniel Peterseim

(joint work with A. Målqvist)

This note summarizes some recent results on linear elliptic problems with rough multiscale coefficients in the absence of strong assumptions such as periodicity or scale separation. Given a polyhedral domain $\Omega \subset \mathbb{R}^d$ and functions $A \in L^\infty(\Omega, \mathbb{R}^{d\times d}_{\mathrm{sym}})$ with uniform spectral bounds $\sigma(A(\cdot)) \subset [\alpha,\beta] \subset]0,\infty[$ and $g \in L^2(\Omega)$, consider the second order linear elliptic problem

(LP) find $u \in V := H^1_0(\Omega)$ such that

$$a(u,v) := \int_\Omega (A\nabla u)\cdot\nabla v = \int_\Omega gv =: (g,v) \quad \text{for all } v \in V,$$

and the associated eigenproblem

(EP) find pairs $(\lambda^{(\ell)}, u^{(\ell)}) \in \mathbb{R}_{>0} \times V \setminus \{0\}$, $\ell \in \mathbb{N}$ such that

$$a(u^{(\ell)}, v) = \lambda^{(\ell)} \int_\Omega u^{(\ell)} v =: (\lambda^{(\ell)} u^{(\ell)}, v) \quad \text{for all } v \in V.$$

If the diffusion coefficient A is highly variable then the numerical approximation of either problem is challenging. The underlying mesh width has to be sufficiently

small to resolve the oscillations and heterogeneities of A. For problems in geophysics or material sciences with characteristic geometric features on microscopic length scales, this so-called resolution condition is often so restrictive that the initial mesh must be chosen very fine and further refinement exceeds computer capacity.

In this note, a new numerical homogenization method is presented. It is related to some low-dimensional macroscopic generalized finite element space. The assembling of the corresponding linear system of equations requires microscopic computations only in local vertex patches of diameter $H\log(1/H)$; H being the macroscopic mesh size. The energy error of the method converges linearly with respect to H without any pre-asymptotic effects. Moreover, small (leading) eigenvalues of the operator are preserved on the macroscopic level in a superconvergent way (at least quartic with respect to H).

The framework presented here was mainly developed in [4, 5] and further investigated in [2, 3, 1]. References to alternative methods for numerical homogenization or upscaling may be found therein and in several contributions to this Oberwolfach workshop, e.g., by A. Abdulle, L. Berlyand, Y. Efendiev, R. Lipton, A. Lozinski, or L. Zhang. The question of how the different approaches compare in certain scenarios remains open. As major advantages of our approach we consider its generality, rigorousness and spectral properties.

1. Two-scale Decompositions

Our method is based on novel multiscale decompositions of H^1 into some macroscopic/coarse part V_{cs} plus some microscopic/fine part V_{fs}. Let $V_H \subset V$ denote the classical $P1$ finite element space with respect to some coarse mesh of width H. It is spanned by nodal basis functions ϕ_z for interior vertices $z \in \mathcal{N}$. The key tool is the Clément-type (quasi-)interpolation operator $\mathcal{I}_H : V \to V_H$ with $\mathcal{I}_H v := \sum_{z\in\mathcal{N}} \frac{(v,\phi_z)}{(1,\phi_z)}\phi_z$. Throughout this note, its kernel $V_{\mathrm{fs}} := \operatorname{kernel}\mathcal{I}_H$ defines microscopic functions.

Lemma 1 (L^2-orthogonal two-scale decomposition)**.**

$$V = V_H \oplus V_{\mathrm{fs}} \quad \textit{and} \quad (V_{\mathrm{cs}}, V_{\mathrm{fs}}) = 0.$$

The decomposition is orthogonalized with respect to the scalar product a induced by the problems (LP) and (EP). Let $\mathfrak{F} : V \to V_{\mathrm{fs}}$ denote the a-orthogonal projection onto the finescale space V_{fs}, that is $a(\mathfrak{F}v, w) = a(v, w)$ for all $w \in V_{\mathrm{fs}}$. A modified (operator-dependent) coarse space is then given by

$$V_{\mathrm{cs}} := (1-\mathfrak{F})V_H = \operatorname{span}\{(1-\mathfrak{F})\phi_z \mid z \in \mathcal{N}\}.$$

Lemma 2 (a-orthogonal two-scale decomposition)**.**

$$V = V_{\mathrm{cs}} \oplus V_{\mathrm{fs}} \quad \textit{and} \quad a(V_{\mathrm{cs}}, V_{\mathrm{fs}}) = 0.$$

The lemma immediately yields the desired error estimates for the Galerkin method with respect to V_{cs} (see Section 2). A further main observation is that the a-orthogonal decomposition remains almost orthogonal in L^2.

Lemma 3 (L^2-quasi-orthogonality of the a-orthogonal decomposition)**.**

$$\forall v_{\mathrm{cs}} \in V_{\mathrm{cs}} \forall v_{\mathrm{fs}} \in V_{\mathrm{fs}} : \ (v_{\mathrm{cs}}, v_{\mathrm{fs}}) \lesssim \alpha^{-1} H^2 \left|\left|A^{1/2}\nabla v_{\mathrm{cs}}\right|\right| \left|\left|A^{1/2}\nabla v_{\mathrm{fs}}\right|\right|.$$

Here and throughout the paper, the constant hidden in the notation $\lesssim$ only depends on Ω and interior angles of the finite element mesh. Lemma 3 indicates that V_{cs} is suitable for the discretization of the eigenproblem (see Section 3).

2. Galerkin approximation and sparse representation of V_{cs}

Let $u_{\mathrm{cs}} \in V_{\mathrm{cs}}$ denote the Galerkin approximation of u with respect to V_{cs}, i.e.,

$$a(u_{\mathrm{cs}}, v) = (f, v) \quad \text{for all } v \in V_{\mathrm{cs}}.$$

The error of this discretization is small (of order H) because $g \in L^2(\Omega)$ and u_{cs} is exactly the coarse part of u in the decomposition of Lemma 2.

Lemma 4 (Discretization error)**.**

$$\left|\left|A^{1/2}\nabla(u - u_{\mathrm{cs}})\right|\right| \lesssim \alpha^{-1/2} \left|\left|Hg\right|\right|.$$

Observe that V may be replaced with any subspace $V_h \supset V_H$. In practical computations, V_h is some high resolution FE space that is sufficiently rich to capture the characteristic scales of the problem. In addition to this finescale discretization, we need to find approximations of the corrector function $\mathfrak{F}\phi_z$ with local support in order to turn (2) into a feasible method. We introduce a new parameter, the localization parameter $k \in \mathbb{N}$ and define nodal patches $\omega_{z,1} := \operatorname{supp} \phi_z$ and $\omega_{z,k} := \cup\{T \in \mathcal{T}_H \mid T \cap \omega_{z,k-1} \neq \emptyset\}$ for $k \geq 2$.

Lemma 5 (Decay of correctors)**.**

$$\forall z \in \mathcal{N} \forall k \in \mathbb{N} : \ \left|\left|A^{1/2}\nabla\mathfrak{F}\phi_z\right|\right|_{L^2(\Omega\setminus\omega_{z,k})} \lesssim e^{-\sqrt{\alpha/\beta}k} \left|\left|A^{1/2}\nabla\mathfrak{F}\phi_z\right|\right|.$$

The exponential decay motivates the approximation of $\psi_z = \mathfrak{F}\phi_z \in V_{\mathrm{fs}}$ by $\psi_{z,k} \in V_{\mathrm{fs}}(\omega_{z,k}) := \{v \in V_{\mathrm{fs}} \mid v|_{\Omega\setminus\omega_{x,k}} = 0\}$, where

$$a(\psi_{z,k}, v) = a(\phi_z, v) \quad \text{for all } v \in V_{\mathrm{fs}}(\omega_{z,k}).$$

Thus, the approximate modified coarse space V_{cs}^k has a local basis

$$V_{\mathrm{cs}}^k = \operatorname{span}\{\phi_z - \psi_{z,k} \mid z \in \mathcal{N}\}.$$

The corresponding Galerkin approximation of (LP) is denoted u_{cs}^k.

Theorem 6 (Discretization error after localization)**.**

$$\textit{If } k \gtrsim \sqrt{\beta/\alpha}|\log(H)| \textit{ then } \left|\left|A^{1/2}\nabla(u - u_{\mathrm{cs}}^k)\right|\right| \lesssim H \left|\left|g\right|\right|.$$

Estimates for fully discrete version and estimates in L^2-norm can be found in [4] (see [3] for improved results with regard to hidden constants).

3. Approximation of Eigenvalues and Eigenvectors

A third characterization of a macroscopic functions may be given via the eigenfunctions related to the ℓ smallest eigenvalues $E_\ell := \text{span}\{u^{(1)}, \dots, u^{(\ell)}\}$. By revisiting Lemma 3 we observe that those macroscopic functions are already represented very accurately by V_{cs} (or V_{cs}^k for k sufficiently large).

Corollary 7 (L^2-quasi-orthogonality of the a-orthogonal decomposition of macroscopic functions)**.** *Let $\ell \in \mathbb{N}$ and let $u = u_{\text{cs}} + u_{\text{fs}} \in E_\ell$ with $||u|| = 1$, where $u_{\text{cs}} \in V_{\text{cs}}$ (resp. $u_{\text{fs}} \in V_{\text{fs}}$) denotes the coarse scale part (resp. fine scale part) of u according to the a-orthogonal decomposition in Lemma 2. Then it holds*

$$(u_{\text{cs}}, u_{\text{fs}}) \lesssim \sqrt{\ell}\alpha^{-2}(\lambda^{(\ell)})^2 H^4.$$

We approximate eigenpairs by solutions of the discrete eigenvalue problem: find $\lambda_H^{(\ell)} \in \mathbb{R}$ and non-trivial $u_{\text{cs}}^{(\ell)} \in V_{\text{cs}}$ such that

$$a(u_{\text{cs}}^{(\ell)}, v) = \lambda_H^{(\ell)}(u_{\text{cs}}^{(\ell)}, v) \quad \text{for all } v \in V_{\text{cs}}.$$

Theorem 8 (Bound for the eigenvalue error)**.** *Let H be sufficiently small so that $H \lesssim \ell^{-1/4}\sqrt{\alpha/\lambda^{(l)}}$. Then it holds*

$$\lambda_H^{(\ell)} - \lambda^{(\ell)} \lesssim \sqrt{\ell}(\lambda^{(\ell)})^3\alpha^{-2}H^4 \quad \textit{for all } \ell = 1, 2, \dots, N_H.$$

See [5] for estimates of the error in the corresponding eigenfunctions. Again, discretization ($V \to V_h$) and localization ($V_{\text{cs}} \to V_{\text{cs}}^k$) as in Section 2 are applicable.

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Anomalous diffusion approximation for kinetic equations

Marjolaine Puel

(joint work with N. B. Abdallah, A. Mellet)

We consider diffusion approximation for kinetic equations like linear Boltzmann or Fokker-Planck in the case where the equilibria are heavy tail functions, In the case, the classical diffusion scaling leads to an infinite diffusion coefficient. Then, we have to adapt the scaling and reorganize the different terms to obtain at the limit that the solution may be approximated by a equilibrium as a velocity profile multiplied by a density satisfying a fractional diffusion equation.

Homogenization of Fluid Flow and Transport in Porous Media including an Evolving Microstructure

Nadja Ray
(joint work with Tycho van Noorden, Peter Knabner)

1. Introduction

In recent years, there has been an increased interest in porous media applications that contain multiple evolving phases. Examples are unsaturated flow and two/multi-phase flow. Likewise, the evolution of the solid phase is an important aspect. Because of such structural changes, the pore space that is accessible for the phases and consequently the transport properties of the porous medium change. In order to capture effects of non-periodic media or of the underlying geometry's evolution in a macroscopic model, numerous extensions of classical upscaling methods have been applied.

In this work, we discuss the upscaling of a coupled fluid flow and transport problem using a level set formulation following [2]. In our model the evolving geometry is controlled by attachment/detachment processes or due to chemical surface reactions. Moreover, interaction potentials between particles and the porous matrix (e.g. electric forces) have to be taken into account additionally.

2. Pore Scale Model

2.1. Notation.

c_ε, u_0	concentration, transformed conc.	L_ε, L_0	level set function
v_ε, $\bar{v}_0$	fluid velocity, averaged fluid velocity	p_ε, p_0	pressure
Φ_ε, Φ_0	prescribed total interaction potential	f	surface reaction rate
η	kinematic viscosity	D	diffusivity
kT	Boltzmann constant times temperature	m	molecular mass
$\rho_{(\mathrm{l})}$	density of the liquid (l)/solid phase	ε	scale parameter
x, y, t	global/local space, time variable	$\boldsymbol{\nu}_\varepsilon$	normal vector

Similar as in standard homogenization theory, in the non-rigid framework, the unit cell $Y = \left[-\frac{1}{2}, +\frac{1}{2}\right]^2$ is made up of two open sets which vary in time: the liquid part $Y_l = Y_l(t, \boldsymbol{x})$ and the solid part $Y_s = Y_s(t, \boldsymbol{x})$. Moreover, the internal boundary is defined by $\Gamma(t, \boldsymbol{x}) = \overline{Y}_l(t, \boldsymbol{x}) \cap \overline{Y}_s(t, \boldsymbol{x})$. This implies that, the fluid part/pore space, the solid part, and the interior boundary of the porous medium are defined by $\Omega_\varepsilon = \Omega_\varepsilon(t, \boldsymbol{x}) := \bigcup_{ij} Y^{ij}_{\varepsilon,l}$, $\Omega \backslash \overline{\Omega}_\varepsilon = \Omega \backslash \overline{\Omega}_\varepsilon(t, \boldsymbol{x}) := \bigcup_{ij} Y^{ij}_{\varepsilon,s}$, and $\Gamma_\varepsilon = \Gamma_\varepsilon(t, \boldsymbol{x}) := \bigcup_{ij} \Gamma^{ij}_\varepsilon$, letting $\cdot^{ij}_\varepsilon$ denote the ε-scaled and shifted versions of Y_s, Y_l, and Γ respectively. At initial time $t = 0$, we assume that the solid parts do not touch or intersect the boundary of the unit cell Y, i.e. the fluid part $\Omega_\varepsilon(0, \boldsymbol{x})$ is connected.

2.2. **Outline of the Model Equations.** The following ε-scaled and coupled system of partial differential equations describes flow flow and transport at the pore scale: Incompressible Stokes equations (1a), (1b) determine the fluid velocity $\boldsymbol{v}_\varepsilon$

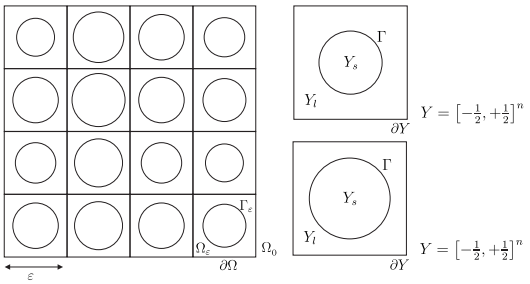

FIGURE 1. Geometrical setting and scale parameter ε: Domain Ω_0 and representation of a porous medium with porous matrix $\Omega_0 \backslash \Omega_\varepsilon$ and unit cells Y .

and the pressure p_ε while the transport equation (1d) for the concentration c_ε takes the processes of convection, diffusion into account. Moreover, a drift term with given interaction potential Φ_ε and a surface reaction rate f accounts for interaction with the porous matrix. Finally, the physically meaningful boundary conditions (1c), (1e) are carried out by conservation laws on the evolving solid-liquid interface $\Gamma_\varepsilon := \{x : L_\varepsilon(t,x) = 0\}$, which is characterized by means of the level set function L_ε via (1f). Moreover, the liquid phase is given by $\Omega_\varepsilon(t) = \{x : L_\varepsilon(t,x) > 0\}$.

$$-\varepsilon^2 \eta \Delta \boldsymbol{v}_\varepsilon + \tfrac{1}{\rho_1} \nabla p_\varepsilon = -\varepsilon \tfrac{1}{\rho_1 m} c_\varepsilon \nabla \Phi_\varepsilon \qquad x \in \Omega_\varepsilon(t),\ t \in (0, t^{\text{end}}) \tag{1a}$$

$$\nabla \cdot \boldsymbol{v}_\varepsilon = 0 \qquad x \in \Omega_\varepsilon(t),\ t \in (0, t^{\text{end}}), \tag{1b}$$

$$\boldsymbol{v}_\varepsilon = -\varepsilon \tfrac{\rho_1 - \rho}{\rho_1 \rho} f(c_\varepsilon, \rho) \boldsymbol{\nu}_\varepsilon \qquad x \in \Gamma_\varepsilon(t),\ t \in (0, t^{\text{end}}), \tag{1c}$$

$$\partial_t c_\varepsilon - \nabla \cdot (-v_\varepsilon c_\varepsilon + D \nabla c_\varepsilon + \tfrac{D}{kT} c_\varepsilon \nabla \Phi_\varepsilon) = 0 \qquad x \in \Omega_\varepsilon(t),\ t \in (0, t^{\text{end}}), \tag{1d}$$

$$(-v_\varepsilon c_\varepsilon + D \nabla c_\varepsilon + \tfrac{D}{kT} c_\varepsilon \nabla \Phi_\varepsilon) \cdot \boldsymbol{\nu}_\varepsilon$$

$$= \varepsilon \tfrac{1}{\rho} f(c_\varepsilon, \rho)(c_\varepsilon - \rho) \qquad x \in \Gamma_\varepsilon(t),\ t \in (0, t^{\text{end}}), \tag{1e}$$

$$\partial_t L_\varepsilon - \varepsilon \tfrac{1}{\rho} f(c_\varepsilon, \rho) |\nabla L_\varepsilon| = 0 \qquad x \in \Omega_0,\ t \in (0, t^{\text{end}}). \tag{1f}$$

3. Effective Model

3.1. **Two-scale Asymptotic Expansion.** In an attempt to identify the limit of system (1) for $\varepsilon \to 0$, we assume that a two-scale asymptotic expansion exists for all variables $\varphi_\varepsilon \in \{\boldsymbol{v}_\varepsilon, p_\varepsilon, c_\varepsilon, \Phi_\varepsilon\}$. In addition to these series in the scale parameter ε, we employ the following expansion for the spatial derivative:

$$\varphi_\varepsilon(t, \boldsymbol{x}) = \varphi_0(t, \boldsymbol{x}, \boldsymbol{y}) + \varepsilon \varphi_1(t, \boldsymbol{x}, \boldsymbol{y}) + \ldots, \quad \nabla \ = \nabla_{\boldsymbol{x}} + \tfrac{1}{\varepsilon} \nabla_{\boldsymbol{y}}, \quad \boldsymbol{y} = \boldsymbol{x}/\varepsilon. \tag{2a}$$

In the framework of a level set description, also the level set function L_ε itself and the normal vector $\boldsymbol{\nu}_\varepsilon$ have to be expanded according to the evolving microstructure. The expansion of the outer normal vector $\boldsymbol{\nu}_\varepsilon$ is expressed in terms of the level set function L_ε and for the two-dimensional setting the following relations

hold [2]:

$$L_\varepsilon(t,\boldsymbol{x}) = L_0(t,\boldsymbol{x},\boldsymbol{y}) + \varepsilon L_1(t,\boldsymbol{x},\boldsymbol{y}) + \varepsilon^2 L_2(t,\boldsymbol{x},\boldsymbol{y}) + \ldots, \quad \boldsymbol{y} = \boldsymbol{x}/\varepsilon, \tag{2b}$$

$$\boldsymbol{\nu}_\varepsilon = \boldsymbol{\nu}_0 + \varepsilon\boldsymbol{\nu}_1 + \ldots, \quad \boldsymbol{\nu}_0 = \tfrac{\nabla_{\boldsymbol{y}} L_0}{|\nabla_{\boldsymbol{y}} L_0|}, \quad \boldsymbol{\nu}_1 = \boldsymbol{\tau}_0 \tfrac{\boldsymbol{\tau}_0\cdot(\nabla_{\boldsymbol{x}} L_0 + \nabla_{\boldsymbol{y}} L_1)}{|\nabla_{\boldsymbol{y}} L_0|} \tag{2c}$$

with $\boldsymbol{\tau}_0 := \boldsymbol{\nu}_0^\perp$ denoting the unit tangent on Γ_0. We restrict ourselves to the two-dimensional setting here, since the representations (2b) together with the Lemmas 3.1 and 3.2 in [2] make it possible to simplify the following technical calculations considerably and to obtain reasonable upscaling results.

3.2. **Upscaling Results.** After inserting and evaluating the expansions (2) into system (1), the fully coupled Darcy-Convection-Diffusion system (3) is obtained by the upscaling procedure [1] which determines the averaged velocity $\bar{v}_0$, the pressure field p_0, the transformed concentration $c_0 = e^{-\frac{1}{kT}\Phi_0(t,x,y)}u_0$, and the level set L_0 on an averaged scale.

$$\bar{v}_0 = -\tfrac{1}{\eta\rho_1} K(t,x)\nabla_x p_0 \qquad t \in (0,t^{\mathrm{end}}),\ x \in \Omega_0, \tag{3a}$$

$$\nabla_x \cdot \bar{v}_0 = \tfrac{\rho_1-\rho}{\rho_1} F(t,x) \qquad t \in (0,t^{\mathrm{end}}),\ x \in \Omega_0, \tag{3b}$$

$$\partial_t(A(t,x)u_0) + \nabla_x \cdot (V(t,x)u_0)$$

$$-\nabla_x \cdot (\bar{D}(t,x)\nabla_x u_0) + F(t,x) = 0 \qquad t \in (0,t^{\mathrm{end}}),\ x \in \Omega_0, \tag{3c}$$

$$\partial_t L_0 - f(c_0(t,x),\rho)|\nabla_y L_0| = 0 \qquad t \in (0,t^{\mathrm{end}}),\ x \in \Omega_0,\ y \in Y. \tag{3d}$$

The time and space dependent, effective coefficients $K, A, V, \bar{D}, F$ are calculated by integrating solutions of time and space dependent cell problems [1].

Moreover, in [1] upscaling results are interpreted in the situation of clogging and numerical simulations are presented.

4. Concluing remarks

Our attempt can be seen as a first step toward capturing directly structural changes in a porous medium in a macroscopic model description. Moreover, the particular strength of our model lies in the fact that it is applicable for general interaction forces between the porous matrix and the concentration. However, the most important limitation lies in the fact that processes in a realistic 3D setting can not be considered. Consequently, further research is required to extend our model approaches from 2D to 3D. Another important issue for future research is the integration of intra particle interaction.

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Homogenization of plasticity equations with hardening using Finite-Element approaches

Ben Schweizer
(joint work with Marco Veneroni)

Plasticity equations describe the deformations e.g. of metal [1, 3]. As in elasticity, one describes the body at rest with a domain $\Omega \subset \mathbb{R}^n$, the deformation of the material point $x \in \Omega$ by $u(x) \in \mathbb{R}^n$, uses the symmetric gradient $\nabla^s u(x) = (\nabla u(x) + \nabla u(x)^T)/2$ to describe local deformations, and the stress tensor $\sigma(x)$ to describe inner forces. The balance of linear momentum is as in elasticity, (1a) with density ϱ and load f.

In contrast to elasticity, the stress tensor is *not* in a linear relation with $\nabla^s u(x)$. Instead, the deformation is decomposed (here: additively) into two parts, an elastic strain and a plastic strain, $\nabla^s u(x) = e(x) + p(x)$, such that with $e(x)$ Hooke's law is satisfied, $\sigma(x) = De(x)$ for some elasticity tensor D. The plastic strain can be considered as a component of a possibly larger vector of interior variables $\xi \in \mathbb{R}^N$; with a linear operator $B : \mathbb{R}^N \to \mathbb{R}^{n\times n}_s$ that maps into the space of symmetric matrices, we write $p = B\xi$ and obtain (1b) as stress-strain relation. Finally, in order to close the system, we have to introduce a *flow-rule* in (1c). It provides an ordinary differential equation for the internal variables $\xi(x,t) \in \mathbb{R}^N$. The nonlinear function $g : \mathbb{R}^N \to \mathbb{R}^N$ is assumed to be monotone and can be multi-valued. The flow rule expresses changes of the internal variables ξ under the influence of the forces σ. Hardening models include $L\xi$ in the argument of g, strictly monotone operators $L : \mathbb{R}^N \to \mathbb{R}^N$ contribute to regularity properties of solutions. In particular, p need not be regarded as a measure, but can be expected to be an element of $L^2(\Omega)$ for every time instance.

In the homogenization analysis, one is interested in oscillatory dependence of the material parameters on $x \in \Omega$, we therefore provide the material variables with a subscript η where $\eta > 0$ stands for the typical length scale in the heterogeneous model. Since the solution depends on the coefficients, we mark also the solution variables u^η, σ^η, and ξ^η with a superscript η. The system under consideration reads

$$\varrho_\eta \partial_t^2 u^\eta = \nabla \cdot \sigma^\eta + f \tag{1a}$$

$$\sigma^\eta = D_\eta(\nabla^s u^\eta - B_\eta \xi^\eta) \tag{1b}$$

$$\partial_t \xi^\eta \in g_\eta(B_\eta^T \sigma^\eta - L_\eta \xi^\eta) \tag{1c}$$

For a time horizon $T > 0$, the equations are posed on $\Omega_T = \Omega \times (0,T)$.

The homogenization of the plasticity system (1) was analyzed recently by several authors. The method of two-scale convergence was used in [9, 10, 11], quasi-stationary evolutions were the underlying concept in [4, 5], and a phase-shift construction was used in [2, 6]. Another method to derive similar results was introduced in [8]: Based on Tartar's original method of oscillating test functions in homogenization, we constructed oscillating test-functions from the two-scale limit

problem in order to prove the homogenization result. We note that all the approaches mentioned above have their own strengths. A strength of the approach in [8] is the simplicity and flexibility. In particular, the treatment of the wave equation (inclusion of $\varrho\partial_t^2 u$ in (1a)) is possible without any additional difficulties.

Why is the homogenization of the plasticity problem difficult? It is astonishing that the homogenization of this problem was only recently performed. Difficulties lie in the non-linear character of the equations and, in particular, in the differential inclusion (1c), which is typically formulated by imposing an energy-dissipation inequality. From our view-point, the main problem lies in the fact that solutions (of the two-scale problem) do not have sufficient regularity properties (in (x, y)). We circumvent this problem as follows: we *do not use* the solution of the two-scale problem to construct an oscillatory test-function, but we *do use* a Finite-Element approximation of the two-scale problem. This approximation has all the regularity properties that we need.

Results. We consider periodic homogenization. With the periodicity cell $Y = [0, 1)^n$ we assume that the material parameters are given as

$$D_\eta(x) = D\left(x, \frac{x}{\eta}\right), \quad L_\eta(x) = L\left(x, \frac{x}{\eta}\right), \quad B_\eta(x) = B\left(x, \frac{x}{\eta}\right),$$
$$\varrho_\eta(x) = \varrho\left(x, \frac{x}{\eta}\right), \quad g_\eta(\,\cdot\,; x) = g\left(\,\cdot\,; \frac{x}{\eta}\right).$$

The limit system for plasticity consists in a two-scale problem. In general, this problem cannot be decoupled — we do *not* obtain a single macroscopic plasticity system as an effective equation (except for the one-dimensional case, [7]). The unknowns in the two-scale problem are the macroscopic deformation $u : \Omega_T \to \mathbb{R}^n$, a corrector for the deformation $v : \Omega_T \times Y \to \mathbb{R}^n$, the two-scale internal variables $w : \Omega_T \times Y \to \mathbb{R}^N$, and the two-scale stress $z : \Omega_T \times Y \to \mathbb{R}^{n\times n}_s$. The two-scale system reads, for the averaged density $\bar\varrho(x) > 0$,

$$\bar\varrho\partial_t^2 u = \nabla \cdot \left(\int_Y z\, dy\right) + f \tag{2a}$$
$$z = D(\nabla_x^s u + \nabla_y^s v - Bw) \tag{2b}$$
$$\nabla_y \cdot z = 0 \tag{2c}$$
$$\partial_t w \in g(B^T z - Lw\,; y) \tag{2d}$$

The homogenization result takes the following form. We are currently working on optimal assumptions on the coefficients, the following formulation is meant to indicate work in progress (but we note that precise assumptions for a less general model with an indicatrix map g are given in [8]).

Theorem 1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded polygonal domain, $T > 0$. Let the maps $D(x)$ and $L(x)$ be monotone, uniformly bounded with uniformly bounded inverse operators. Let $g : \mathbb{R}^N \times Y \to \mathbb{R}^N$ be a multi-valued monotone operator. Let the density ϱ be strictly positive, we use $\bar\varrho(x) = \int_Y \varrho(x, y)\, dy$. Let initial data and boundary conditions be such that solutions to the oscillatory system and to the*

two-scale system exist. Let $(u^\eta, \sigma^\eta, \xi^\eta)$ *and* (u, v, w, z) *be solutions of problems* (1) *and* (2)*. Then, as* $\eta \to 0$*,*

$$\partial_t u^\eta \to \partial_t u \quad \textit{strongly in } L^2(\Omega_T),$$
$$\sigma^\eta \rightharpoonup \int_Y z\,dy, \quad \xi^\eta \rightharpoonup \int_Y w\,dy \quad \textit{weakly in } L^2(\Omega_T).$$

As indicated, the proof of the theorem is based on solutions of a semi-discrete version of the two-scale problem. More precisely, we define a space of piecewise affine finite elements $U_h \subset H^1(\Omega)$ and search for $u_h(.,t) \in U_h$. The other variables, $v_h(x,y,t)$, $z_h(x,y,t)$, and $w_h(x,y,t)$ are searched for in spaces of piecewise constant function in x. We solve

$$\int_\Omega \left(\int_Y z_h\,dy \right) : \nabla\psi = \int_\Omega (f - \bar{\varrho}\partial_t^2 u_h)\cdot\psi \qquad \forall\,\psi \in U_h \tag{3a}$$
$$z_h = D_h(\nabla^s u_h + \nabla_y^s v_h - B w_h) \tag{3b}$$
$$\nabla_y \cdot z_h = 0 \tag{3c}$$
$$\partial_t w_h \in g(B^T z_h - L w_h;\, y) \tag{3d}$$

For any function $\phi : \Omega \times Y \times (0,T) \to \mathbb{R}^m$, we construct an oscillatory test-function by setting $\phi_\eta(x,t) := \phi(x, x/\eta, t)$. Using the solution (u_h, v_h, z_h, w_h) of (3), constructing the oscillatory functions $(u_{h,\eta}, v_{h,\eta}, z_{h,\eta}, w_{h,\eta})$, and using them as test-functions in the original system and in (3), we can derive Theorem 1 with energy methods, using taylored div-curl-lemmas to show smallness of error terms.

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Performance of the Metropolis algorithm on a disordered tree: The Einstein relation

Ofer Zeitouni
(joint work with Pascal Maillart)

Consider a d-ary rooted tree ($d \geq 3$) where each edge e is assigned an i.i.d. (bounded) random variable $X(e)$ of negative mean. Assign to each vertex v the sum $S(v)$ of $X(e)$ over all edges connecting v to the root, and assume that the maximum S_n^* of $S(v)$ over all vertices v at distance n from the root tends to infinity (necessarily, linearly) as n tends to infinity. We analyze the Metropolis algorithm on the tree and show that under these assumptions there always exists a temperature $1/\beta$ of the algorithm so that it achieves a linear (positive) growth rate in linear time. This confirms a conjecture of Aldous [1]. The proof is obtained by establishing an Einstein relation for the Metropolis algorithm on the tree. The full paper is available at [2].

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Localized bases for numerical homogenization with arbitrary coefficients

Lei Zhang
(joint work with Houman Owhadi, Leonid Berlyand)

We introduce a new variational method for the numerical homogenization of divergence form elliptic, parabolic and hyperbolic equations with arbitrary rough (L^∞) coefficients. Our method does not rely on concepts of ergodicity or scale-separation but on compactness properties of the solution space and a new variational approach to homogenization. The approximation space is generated by an interpolation basis (over scattered points forming a mesh of resolution H) minimizing the L^2 norm of the source terms; its (pre-)computation involves minimizing $\mathcal{O}(H^{-d})$ quadratic (cell) problems on (super-)localized sub-domains of size $\mathcal{O}(H \ln(1/H))$. The resulting localized linear systems remain sparse and banded. The resulting interpolation basis functions are biharmonic (for $d \leq 3$ and polyharmonic for $d \geq 4$) for the operator $-\mathrm{div}(a\nabla\cdot)$ and can be seen as a generalization of polyharmonic splines to differential operators with arbitrary rough coefficients. The accuracy of the method ($\mathcal{O}(H)$ in energy norm and independent from aspect ratios of the mesh formed by the scattered points) is established via the introduction of a new class of higher-order Poincaré inequalities. The method bypasses (pre-)computations on the full domain and naturally generalizes to time dependent problems, it also

provides a natural solution to the inverse problem of recovering the solution of a divergence form elliptic equation from a finite number of point measurements.

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