AFRL-AFOSR-UK-TR-2013-0020

Multiscale problems in materials science: a mathematical approach to the role of uncertainty

Claude Lebris, F. Legoll, F. Thomines

Ecole Nationale des Ponts et Chaussées
6-8, Avenue Blaise Pascal
Marne la Vallée 77455, France

EOARD SPC 10-4002

Report Date: October 2012

Final Report from 29 October 2009 to 28 October 2012

Air Force Research Laboratory
Air Force Office of Scientific Research
European Office of Aerospace Research and Development
Unit 4515 Box 14, APO AE 09421

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From – To)*
29 October 2012	Final Report	29 October 2009 – 28 October 2012

4. TITLE AND SUBTITLE

Multiscale problems in materials science: a mathematical approach to the role of uncertainty

5a. CONTRACT NUMBER

FA8655-10-C-4002

5b. GRANT NUMBER

SPC 10-4002

5c. PROGRAM ELEMENT NUMBER

61102F

6. AUTHOR(S)

Claude Lebris, F. Legoll, F. Thomines

5d. PROJECT NUMBER

5d. TASK NUMBER

5e. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Ecole Nationale des Ponts et Chaussées
6-8, Avenue Blaise Pascal
Marne la Vallée 77455, France

8. PERFORMING ORGANIZATION REPORT NUMBER

N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

EOARD
Unit 4515
APO AE 09421

10. SPONSOR/MONITOR'S ACRONYM(S)

AFRL/AFOSR/IOE (EOARD)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

AFRL-AFOSR-UK-TR-2013-0020

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

One approach to uncertainty quantification in materials science problems is to use dedicated numerical approaches in a multiscale framework, such as the Multiscale Finite Element Method (MsFEM). In this report, we first consider a variant of stochastic homogenization, well suited to model materials that are periodic up to a random deformation. This variant admits a homogenized limit. However, the homogenized matrix is expensive to compute, as is often the case in stochastic homogenization. We propose here an efficient MsFEM-type approach dedicated to that setting. We next turn to studying the robustness of the MsFEM approach to perturbations of the equation coefficients that are non-oscillatory. Our idea is that MsFEM approaches are devoted to capturing the highly oscillatory modes of the solution, which are poorly captured by a standard FEM approach using a limited number of degrees of freedom. When the coefficient in the equation is modified by a non-oscillatory component, the high frequencies are not modified, and the MsFEM approach can be expected to be robust with respect to these perturbations. This is exactly the question we considered in the final portion of this three-year study.

15. SUBJECT TERMS

EOARD, computational materials science, multiscale modeling, finite element modeling, uncertainty quantification

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18, NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Randall Pollak, Lt Colonel, USAF
UNCLAS	UNCLAS	UNCLAS	SAR	79	19b. TELEPHONE NUMBER *(Include area code)* +44 1895616115, DSN 314-235-6115

Contract FA 8655-10-C-4002

Multiscale problems in materials science: a mathematical approach to the role of uncertainty

Report 2012 to the European Office of Aerospace Research and Development (EOARD)

C. Le Bris, F. Legoll, F. Thomines

October 2012

Contents

Summary

We report here on the work performed during the third year (october 2011 - october 2012) of the contract FA 8655-10-C-4002 on *Multiscale problems in materials science: a mathematical approach to the role of uncertainty.*

We recall that the bottom line of our work is to develop *affordable numerical methods* in the context of *heterogeneous*, possibly *stochastic* materials. Many partial differential equations of materials science indeed involve highly oscillatory coefficients and thus small length-scales. When the microstructure of the materials is periodic, or random and statistically homogeneous, homogenization theory can be used, and allows to appropriately define averaged equations from the original oscillatory equations. The theoretical aspects of

these problems are now well-understood, in general. On the other hand, the numerical aspects have received less attention from the mathematics community, in particular in the case of stationary ergodic random problems, which are one instance often used for modelling uncertainty of continuous media. In that latter case, standard methods available in the literature often lead to very, and sometimes prohibitively, costly computations.

The situation is even more challenging when no structural assumption (periodicity, statistical homogeneity, ...) on the materials microstructure can be made. In the absence of such an assumption, homogenization theory still holds, but does not provide any explicit formulae amenable (even possibly after some approximation) to numerical computation. One possibility is then to directly address the original problem (rather than passing to the limit of infinite scale separation), and to use dedicated numerical approaches for such multiscale problems, such as, for instance, the Multiscale Finite Element Method (MsFEM).

In this report, we first consider a variant of stochastic homogenization, well suited to model materials that are periodic up to a random deformation. We have already considered this variant in our previous report [3], but with a perspective different from the one here. This variant admits a homogenized limit. However, the homogenized matrix is expensive to compute, as is often the case in stochastic homogenization. We propose here an efficient MsFEM type approach dedicated to that setting.

We next turn to studying the robustness of the MsFEM approach to perturbations of the equation coefficients that are non oscillatory. Our idea is that MsFEM approaches are devoted to capturing the highly oscillatory modes of the solution, which are poorly captured by a standard FEM approach using a limited number of degrees of freedom. When the coefficient in the equation is modified by a non-oscillatory component, the high frequencies are not modified, and the MsFEM approach can be expected to be robust with respect to these perturbations. This is exactly the question we consider in the second part of this report.

The works described below have been performed by Claude Le Bris (PI), Frédéric Legoll (Co-PI) and Florian Thomines (third year Ph.D. student).

1 Introduction

During this third year of contract, we have pursued our effort on developing *affordable* numerical methods in the context of *stochastic homogenization*.

Many partial differential equations of materials science indeed involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems are one of the most famous instances of mathematical uncertainty of continuous media.

The purpose of this report is to present the recent progress we have made on this topic, with the aim *to make numerical random homogenization more practical*. As already mentioned in our two previous reports, because we cannot embrace all difficulties at once, the case under consideration here is a *simple, linear, scalar second order elliptic partial differential equation in divergence form*, for which a sound theoretical groundwork exists. We focus here on the different manners the problem can be handled from the *computational viewpoint*.

In this report, we are concerned with various questions related to the MsFEM approach. We recall that this is one approach (among others, see e.g. [13] for an alternative) to address highly oscillatory problems when the assumptions needed by the homogenization theory on the materials microstructure (such as periodicity, statistical homogeneity, ...) are not met. We have already contributions extending the range of applicability of that approach, see our publication [4] and the previous reports [2, Section 4] and [3, Section 3].

We begin, in Section 2, with a brief description of periodic homogenization and the MsFEM approach in a deterministic setting. The only purpose of that section is the consistency of this report.

In Section 3, we consider a variant of stochastic homogenization, introduced by the PI and co-workers in [9, 10] some years ago. This model is adequate to represent materials that are random deformations of a perfect periodic material. A typical example is a composite material with fibers. Fibers are all identical, they would be located on a periodic lattice in the ideal situation. However (for instance as a consequence of the manufacturing process), their actual positions are now random. In our previous report [3, Section 5], we have presented and analyzed a procedure to practically ap-

proximate the homogenized matrix. In this report, we propose a MsFEM type approach to compute an approximation of the solution to the original highly oscillatory problem. Although the setting is stochastic, it turns out that the approach we propose does not require the recomputation of the MsFEM basis functions for each new realization of the material. This is why the proposed approach is much less expensive than the natural adaptation of the MsFEM approach to the stochastic problem at hand. The performance of the approach is illustrated by some numerical tests, which demonstrate the accuracy of the computed approximation.

In Section 4, we next turn to a question which is originally motivated by inverse problems in multiscale science. Assume that we model our heterogeneous materials with the oscillatory coefficient $b(x)A^\varepsilon(x)$, and that we do not have a good knowledge of b. This situation corresponds to the case when we accurately know the properties of our materials, up to a slowly varying, macroscopic envelop. Otherwise stated, the high frequency modes are well identified, but the way they change over macroscopic distances is not well characterized. One possibility to define a relevant b is to search for b so that the homogenized properties of the materials are as close as possible to the ones that are observed in practice. We thus want to optimize on b, and are thus going to iterate on this function, until we find the best one. For each iterate, we need to very efficiently compute the corresponding homogenized properties or the homogenized solution (because such a computation is needed at each iteration of the optimization loop). In the specific setting considered here, the high frequency modes are independent of b, since b is only *slowly* varying. We thus expect that the MsFEM approach, which aims at properly taking into account the high frequencies present in the problem, should be insensitive to the choice of b. Otherwise formulated, we expect the MsFEM basis functions to be robust with respect to modifications on b. In Section 4.1, we consider the above case where the coefficient reads $b(x)A^\varepsilon(x)$, and indeed show that the MsFEM basis functions can be computed independently of b. As shown in Section 4.2, the situation is different, and more challenging, when the coefficient reads $b(x) + A^\varepsilon(x)$. For that latter case, we propose an approximation strategy based on Proper Generalized Decomposition ideas, and numerically demonstrate its efficiency. For the sake of simplicity, and because again we cannot embrace all difficulties at once, we only consider deterministic models in that Section 4.

We eventually collect in Section 5 some possible future directions of research that we may consider if EOARD decides to renew our funding.

2 Periodic homogenization and MsFEM approaches

[Detailed presentation can be read in [1, 2].]

For the consistency of this report, we recall in this section some groundwork on periodic homogenization and on related approaches for deterministic, non necessarily periodic, heterogeneous materials. More details can be read in our first report [2] and references therein, and also in the review article [1] that we published.

The problem under consideration writes

$$-\mathrm{div}\left[A^\varepsilon(x)\nabla u^\varepsilon\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\varepsilon(x) = 0 \ \text{ on } \partial\mathcal{D}, \tag{1}$$

where $\mathcal{D}$ is a regular, bounded domain in $\mathbb{R}^d$, and where, for any ε, the matrix A^ε is symmetric, bounded and definite positive. The parameter ε encodes the typical size of the heterogeneities. We manipulate for simplicity *symmetric* matrices, but the discussion carries over to non symmetric matrices up to slight modifications.

2.1 Periodic homogenization

Assume that, in (1), the matrix A^ε reads

$$A^\varepsilon(x) = A_{\mathrm{per}}\left(\frac{x}{\varepsilon}\right) \tag{2}$$

where the matrix A_{per} is symmetric definite positive and $\mathbb{Z}^d$-periodic. In this framework, it is well known that, as $\varepsilon \to 0$, the solution u^ε to (1)–(2) converges to $u^\star$ solution to the homogenized problem

$$-\mathrm{div}\left[A^\star_{\mathrm{per}}\nabla u^\star\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\star(x) = 0 \ \text{ on } \partial\mathcal{D}, \tag{3}$$

where the homogenized matrix $A^\star_{\mathrm{per}}$ reads

$$\forall 1 \le i,j \le d, \quad \left[A^\star_{\mathrm{per}}\right]_{ij} = \int_Q \left(e_i + \nabla w_{e_i}\right)^T A_{\mathrm{per}}\left(e_j + \nabla w_{e_j}\right), \tag{4}$$

where $Q = (0,1)^d$ and where, for any $p \in \mathbb{R}^d$, the so-called corrector w_p is the (unique up to the addition of a constant) solution to

$$\begin{cases} -\mathrm{div}\left[A_{\mathrm{per}}\left(p + \nabla w_p\right)\right] = 0 \quad \text{on } \mathbb{R}^d, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases} \tag{5}$$

The practical interest of the approach is evident. No small scale ε is present in the homogenized problem (3). At the price of only computing d periodic problems (5) (as many problems as dimensions in the ambient space), the solution to (1)–(2) can be efficiently approached for ε small. In contrast, a direct attack of (1)–(2) would require taking a meshsize smaller than ε, to appropriately capture the variation of the materials properties at the microstructure scale. The difficulty has been circumvented.

2.2 MsFEM approach

The homogenization result recalled in Section 2.1 heavily relies on the periodicity assumption (2). Although it is possible to somewhat relax this assumption and still obtain explicit formulae for the homogenized matrix, there are many cases of practical interest for which the existence of a homogenized matrix is known, but no explicit formulae are available. For practical purposes, alternative approaches are needed.

The Multiscale Finite Element Method (MsFEM approach) is one such approach (note that other approaches have also been proposed within the same paradigm, we refer e.g. to [13]). The MsFEM is designed to directly address the original problem (1) by performing a variational approximation using pre-computed basis functions χ_i^ε that are *adapted* to the problem. The method is not restricted to the periodic setting, in contrast to the homogenization theory recalled above. We do not assume that (2) holds. In the sequel, we briefly describe the approach, and refer to our publication [4] (see also [5]) for more details and comprehensive numerical tests.

In the sequel, we argue on the variational formulation of (1):

$$\text{Find } u^\varepsilon \in H_0^1(\mathcal{D}) \text{ such that}, \quad \forall v \in H_0^1(\mathcal{D}), \quad \mathcal{A}_\varepsilon(u^\varepsilon, v) = b(v), \tag{6}$$

where

$$\mathcal{A}_\varepsilon(u,v) = \int_{\mathcal{D}} (\nabla v(x))^T A^\varepsilon(x) \nabla u(x)\, dx \quad \text{and} \quad b(v) = \int_{\mathcal{D}} f(x) v(x)\, dx.$$

We introduce a classical P1 discretization of the domain $\mathcal{D}$, with L nodes, and denote χ_i^0, $i = 1, \ldots, L$, the basis functions.

Definition of the MsFEM basis functions Several definitions of the MsFEM basis functions have been proposed in the literature (see e.g. [16, 14, 11]). They give rise to different variants of the method. In the following, we present one of these variants. For any finite element (e.g. triangle) $\mathbf{K}$, we consider the problem

$$\left\{ \begin{array}{rl} -\mathrm{div}\left(A^\varepsilon(x)\nabla\chi_i^{\varepsilon,\mathbf{K}}\right) & = 0 \quad \text{in } \mathbf{K}, \\ \chi_i^{\varepsilon,\mathbf{K}} & = \chi_i^0|_{\mathbf{K}} \quad \text{on } \partial\mathbf{K}. \end{array} \right. \tag{7}$$

By construction, these functions $\chi_i^{\varepsilon,\mathbf{K}}$, that are *numerically* precomputed, *encode the fast oscillations* present in (1).

Note the similarity between (7) and the corrector problem (5). Note also that the problems (7), indexed by $\mathbf{K}$, are all independent from one another. They can hence be solved in parallel, using a discretization adapted to the small scale ε.

Macro scale problem We now introduce the finite dimensional space

$$\mathcal{W}_h := \mathrm{span}\left\{\chi_i^\varepsilon,\ i = 1, \ldots, L\right\},$$

where χ_i^ε is such that $\chi_i^\varepsilon|_{\mathbf{K}} = \chi_i^{\varepsilon,\mathbf{K}}$ for all $\mathbf{K}$, and proceed with a standard Galerkin approximation of (6) using $\mathcal{W}_h$:

$$\text{Find } u_h^\varepsilon \in \mathcal{W}_h \text{ such that}, \quad \forall v \in \mathcal{W}_h, \quad \mathcal{A}_\varepsilon(u_h^\varepsilon, v) = b(v). \tag{8}$$

The function u_h^ε is the MsFEM approximation of the exact solution u^ε. Note that the dimension of $\mathcal{W}_h$ is equal to L: the formulation (8) hence requires solving a linear system with only a limited number of degrees of freedom.

Numerical illustration In order to illustrate the MsFEM approach, we solve (1) in a one dimensional setting with

$$A^\varepsilon(x) = 5 + 50\sin^2\left(\frac{\pi x}{\varepsilon}\right),$$

on the domain $\mathcal{D} = (0, 1)$, with $\varepsilon = 0.025$ and $f = 1000$. We subdivide the interval $(0, 1)$ in $L = 10$ elements. On Figure 1, we plot the MsFEM basis functions in a reference element and the MsFEM solution u_h^ε.

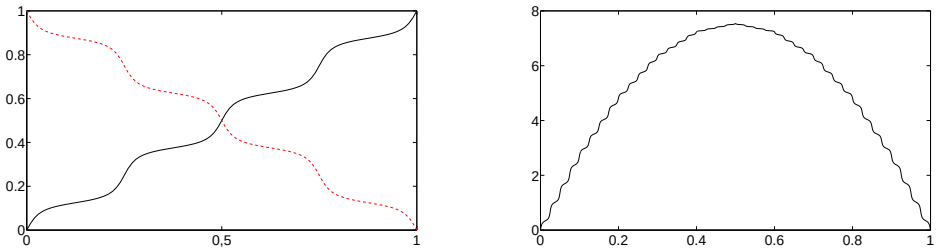

Figure 1: Left: Multiscale basis functions $\chi^{\varepsilon,\mathbf{K}}$ in the reference element. Right: MsFEM solution u_h^ε in the domain $(0,1)$.

3 A MsFEM type approach for a variant of stochastic homogenization

[Work expanded in [5].]

As announced in the conclusion of our previous report [3], we consider here a variant of the classical setting of stochastic homogenization, originally introduced a few years ago in [9, 10], and propose for that variant a MsFEM type approach. We briefly review the problem under consideration, before recalling the corresponding homogenization results and eventually describing our contribution.

3.1 A variant of stochastic homogenization and its homogenized limit

The equation under consideration is

$$-\mathrm{div}\left[A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\varepsilon(x,\omega) = 0 \ \text{ on } \partial\mathcal{D}, \tag{9}$$

where the matrix A is the composition of a $\mathbb{Z}^d$ periodic matrix A_{per} with a stochastic diffeomorphism Φ:

$$A\left(\frac{x}{\varepsilon},\omega\right) := A_{\mathrm{per}}\left[\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right]. \tag{10}$$

We assume that, almost surely, the map $\Phi(\cdot,\omega)$ is a well-behaved diffeomorphism from $\mathbb{R}^d$ to $\mathbb{R}^d$ (in the sense that $\mathrm{EssInf}_{\omega\in\Omega,x\in\mathbb{R}^d}\left(\det(\nabla\Phi(x,\omega))\right) = \nu >$

0 and $\mathrm{EssSup}_{\omega\in\Omega,x\in\mathbb{R}^d}|\nabla\Phi(x,\omega)| = M < +\infty$), and that it satisfies

$$\nabla\Phi \text{ is stationary.} \tag{11}$$

Formally, such a setting is well suited to model materials that are periodic, in a given reference configuration. The latter is only known up to a certain randomness. Materials we have in mind are ideally periodic materials, where some random deformation (modelled by Φ) has been introduced, for instance during the manufacturing process. Assumption (11) means that $\nabla\Phi$ is statistically homogeneous, i.e. the randomness is the same anywhere in the material. We refer e.g. to [2, Section 2.2] for a brief discussion of the notion of stationarity in the context of random homogenization.

The problem (9)-(10) admits a homogenized limit when ε vanishes. It is indeed shown in [9] that, under the above assumptions, the solution $u^\varepsilon(\cdot,\omega)$ to (9)-(10) converges as ε goes to 0 to $u^\star$, solution to the deterministic homogenized problem

$$-\mathrm{div}\left[A^\star\nabla u^\star\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\star(x) = 0 \ \text{ on } \partial\mathcal{D}.$$

The homogenized matrix $A^\star$ is given by, for any $1 \le i,j \le d$,

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

where $Q = (0,1)^d$ and where, for any $p \in \mathbb{R}^d$, w_p solves the corrector problem

$$\begin{cases} -\mathrm{div}\left[A_{\mathrm{per}}\left(\Phi^{-1}(y,\omega)\right)\left(p + \nabla w_p(y,\omega)\right)\right] = 0 \text{ in } \mathbb{R}^d, \\ w_p(y,\omega) = \widetilde{w}_p\left(\Phi^{-1}(y,\omega),\omega\right), \quad \nabla\widetilde{w}_p \text{ is stationary}, \\ \mathbb{E}\left(\displaystyle\int_{\Phi(Q,\cdot)} \nabla w_p(y,\cdot)dy\right) = 0. \end{cases} \tag{12}$$

3.2 A MsFEM-type approach

Our aim here is to propose a MsFEM-type approach for (9)-(10). One motivation is that, as is standard in stochastic homogenization, the corrector

problem (12) is set on the complete space $\mathbb{R}^d$, and is thus challenging to solve in practice.

Note that efficient MsFEM approaches are not easy to derive in stochastic settings, when the equation of interest writes in the general form

$$-\mathrm{div}\left[A^\varepsilon(x,\omega)\nabla u^\varepsilon(x,\omega)\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\varepsilon(x,\omega) = 0 \ \text{ on } \partial\mathcal{D}. \tag{13}$$

As pointed out in our first report (see [2, Section 4.1]), a natural adaptation of the deterministic MsFEM approach presented in Section 2.2 to the problem (13) would involve computing, for each new random realization of the matrix $A^\varepsilon(x,\omega)$, new highly oscillatory basis functions (see indeed (7)). This is prohibitively expensive. However, in particular settings, dedicated MsFEM-type approaches can be proposed. We have considered in our previous reports (see [2, Section 4.2] and [3, Section 3]) a weakly-stochastic setting, where the random matrix $A^\varepsilon(x,\omega)$ in (13) is a *small perturbation* of a deterministic matrix, and proposed for that particular setting an appropriate and efficient MsFEM approach (see our publication [4]). In what follows, we consider the particular setting (9)-(10), and use in an essential manner the fact that it is built upon a *periodic* matrix, randomly deformed.

We know from (12) that the expectation of $\widetilde{w}_p$ is a $\mathbb{Z}^d$ periodic function. Our approach is based on approximating the corrector $\widetilde{w}_p$ in (12) by a *periodic* function $\widetilde{w}_p^{\mathrm{per}}$.

To proceed, it is useful to write the corrector problem (12) in a variational form. As shown in [9], we have that

$$\mathbb{E}\left[\int_{\Phi(Q,\cdot)} (\nabla\psi(y,\omega))^T A_{\mathrm{per}}\left(\Phi^{-1}(y,\omega)\right)\left(p+\nabla w_p(y,\omega)\right)dy\right] = 0$$

for all $\widetilde{\psi}$ stationary, and where $\psi = \widetilde{\psi}\circ\Phi^{-1}$. The above expression can be rewritten, after a change of variables, as

$$\mathbb{E}\left[\int_Q \det(\nabla\Phi)\left(\nabla\widetilde{\psi}\right)^T(\nabla\Phi)^{-1}A_{\mathrm{per}}\left(p+(\nabla\Phi)^{-T}\nabla\widetilde{w}_p\right)\right] = 0.$$

We introduce the notation $\overline{\Phi} = \mathbb{E}(\Phi)$. Our idea is to approximate the random function $\widetilde{w}_p$ by a $\mathbb{Z}^d$ periodic function $\widetilde{w}_p^{\mathrm{per}}$, solution to

$$\int_Q \det\left(\nabla\overline{\Phi}\right)\left(\nabla\widetilde{\psi}\right)^T\left(\nabla\overline{\Phi}\right)^{-1}A_{\mathrm{per}}\left(p+\left(\nabla\overline{\Phi}\right)^{-T}\nabla\widetilde{w}_p^{\mathrm{per}}\right) = 0 \tag{14}$$

for all functions $\widetilde{\psi}$ that are $\mathbb{Z}^d$-periodic. Note that $\widetilde{w}_p^{\rm per}$ is uniquely defined (up to the addition of a constant) by the above problem.

Remark 1 *In general, the function $\widetilde{w}_p$ is* not *periodic. An explicit counter-example is given in [9]. In the numerical tests below, we will consider that particular example, and show that our approach yields accurate results even in that difficult case. See also Remark 4 below.*

Definition of the basis functions As in Section 2.2, we introduce a classical P1 discretization of the domain $\mathcal{D}$, with L nodes, and denote χ_i^0, $i = 1, \ldots, L$, the basis functions. We denote

$$\mathcal{V}_h := \mathrm{Span}(\chi_i^0)$$

the associated finite dimensional space.

Let $\widetilde{w}_p^{\rm per}$ be a solution to (14). We set

$$w_p^{\rm app}(x,\omega) := \widetilde{w}_p^{\rm per}\left(\Phi^{-1}(x,\omega)\right) \tag{15}$$

and introduce the vector $W(x,\omega) \in \mathbb{R}^d$, whose components are given by

$$W_j(x,\omega) = e_j^T W(x,\omega) := w_{e_j}^{\rm app}(x,\omega), \quad 1 \le j \le d.$$

The highly oscillatory basis functions are defined by

$$\chi_i^\varepsilon(x,\omega) := \chi_i^0\left(x + \varepsilon W\left(\frac{x}{\varepsilon},\omega\right)\right), \quad 1 \le i \le L.$$

Remark 2 *In the case when $\Phi(x,\omega) = x$, the problem* (9)-(10) *under consideration is exactly the highly oscillatory problem* (1)-(2)*, with a* periodic *matrix coefficient. In that case, the approach proposed above is identical to the MsFEM-type approach proposed in [11] to address* (1)-(2)*.*

Macro scale problem We introduce the finite dimensional space

$$\mathcal{W}_h := \mathrm{Span}(\chi_i^\varepsilon)$$

and proceed with a Petrov-Galerkin approximation of (9)-(10). The numerical approximation $u_h^\varepsilon \in \mathcal{W}_h$ is defined as the unique solution to the weak formulation

$$\forall v \in \mathcal{V}_h, \quad \int_{\mathcal{D}} (\nabla v(x))^T A_{\rm per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right) \nabla u_h^\varepsilon(x,\omega)\, dx = \int_{\mathcal{D}} f(x) v(x)\, dx. \tag{16}$$

The main feature of the proposed approach is that, although the highly oscillatory basis functions χ_i^ε are stochastic (and thus depend on the realization of the random material), we actually do not have to *solve* a new problem for each new realization of the material (i.e., for each new realization of the diffeomorphism Φ) to compute these basis functions. The basis functions are indeed given by (15), where the deterministic function $\widetilde{w}_p^{\rm per}$ has been precomputed. For each new realization, we thus only have to *evaluate* the new basis functions. This is the main advantage in terms of cost in comparison with a natural application of the MsFEM approach on the problem (9)-(10).

Note that, for each new realization of the material, we have to recompute the stiffness matrix of the problem, which is given by

$$K_{ij}(\omega) = \int_{\mathcal{D}} (\nabla \chi_i^0(x))^T A_{\rm per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right) \nabla \chi_j^\varepsilon(x,\omega)\, dx, \quad 1 \leq i,j \leq L.$$

A natural adaptation of the MsFEM approach on the problem (9)-(10) would also involve recomputing the stiffness matrix for each new realization.

Remark 3 *We have chosen in* (16) *to perform a Petrov-Galerkin approximation of the problem, where the space $\mathcal{V}_h$ of the test functions v is different from the space $\mathcal{W}_h$ of the numerical solution u_h^ε. It is also possible to use a Galerkin approximation, which yields results the accuracy of which is similar, although not as good, as the results presented below.*

Some elements of analysis in a one-dimensional setting In the one-dimensional setting, the corrector problem (12) reads

$$\left\{ \begin{array}{l} -\dfrac{d}{dy}\left[A_{\rm per}\left(\Phi^{-1}(y,\omega)\right)\left(1+\dfrac{dw}{dy}(y,\omega)\right)\right] = 0 \text{ in } \mathbb{R}, \\ w(y,\omega) = \widetilde{w}\left(\Phi^{-1}(y,\omega),\omega\right), \quad \dfrac{d\widetilde{w}}{dy} \text{ is stationary}, \\ \mathbb{E}\left(\displaystyle\int_{\Phi(Q,\cdot)} \frac{dw}{dy}(y,\cdot)dy\right) = 0. \end{array} \right. \tag{17}$$

This problem can be analytically solved, and we obtain that

$$\frac{dw}{dy}(y,\omega) = \frac{C}{A_{\rm per}(\Phi^{-1}(y,\omega))} - 1,$$

where C is a deterministic constant given by

$$\frac{1}{C} = \frac{1}{\mathbb{E}\left(\int_0^1 \Phi'(y,\cdot)dy\right)} \mathbb{E}\left(\int_0^1 \frac{1}{A_{\rm per}(y)} \Phi'(y,\cdot)dy\right). \tag{18}$$

Since $\widetilde{w}(y,\omega) = w(\Phi(y,\omega),\omega)$, we compute by the chain rule that

$$\frac{d\widetilde{w}}{dy}(y,\omega) = \frac{d\Phi}{dy}(y,\omega)\frac{dw}{dy}(\Phi(y,\omega),\omega) = \frac{d\Phi}{dy}(y,\omega)\left(\frac{C}{A_{\rm per}(y)} - 1\right). \tag{19}$$

We have now completely characterized the solution to the corrector problem (17). We next turn to the problem (14) that we introduced in our MsFEM-type approach. In the one-dimensional setting, this problem reads

$$\int_0^1 \frac{d\widetilde{\psi}}{dy} A_{\rm per}\left(1 + \left(\frac{d\overline{\Phi}}{dy}\right)^{-1} \frac{d\widetilde{w}^{\rm per}}{dy}\right) = 0$$

for all functions $\widetilde{\psi}$ that are $\mathbb{Z}$-periodic. Again using the specificities of the one-dimensional setting, we can analytically solve this problem, and obtain that

$$\frac{d\widetilde{w}^{\rm per}}{dy} = \frac{d\overline{\Phi}}{dy}\left(\frac{C}{A_{\rm per}} - 1\right) \tag{20}$$

where the constant C is again given by (18). Comparing (19) and (20), we see that the exact corrector $\widetilde{w}$ and our approximate solution $\widetilde{w}^{\rm per}$ are related by

$$\frac{d\widetilde{w}^{\rm per}}{dy} = \mathbb{E}\left(\frac{d\widetilde{w}}{dy}\right).$$

This somehow shows the consistency (at least in the one-dimensional setting) of our approximate problem (14). Note however that the one-dimensional case may be misleading in that respect, as it is the only case where the gradient of the corrector w_p solution to (12) is of the form of " a periodic function composed with the diffeomorphism Φ^{-1}". In general, this is not the case, as explicitly pointed out in [9]. Numerical tests are therefore of paramount importance to validate the approach.

Numerical tests We have considered the problem (9)-(10) on the domain $\mathcal{D} = (0,1)^2$, for two test cases represented on Figure 2. In both cases, the

periodic matrix A_{per} represents hard inclusions in a soft material. In the first test case (top row of Figure 2), inclusions have a circular shape, and the diffeomorphism Φ^{-1} corresponds to a translation of these inclusions by a random vector. More precisely, on each cell $k + Q$ (with $Q = (0, 1)^d$), the function Φ^{-1} is a translation by a random vector $X_k(\omega) \in \mathbb{R}^2$. The random variables X_k are independent and identically distributed. In the second case (bottom row of Figure 2), inclusions have a T shape, and the diffeomorphism Φ^{-1} corresponds to a rotation of these inclusions by a random angle θ, which can take four values, with equal probability: $\theta = 0$, $\pi/2$, π or $3\pi/2$.

Remark 4 *The second test case is inspired by (and the resulting function* Φ *is very close to) the counter-example discussed in [9]. It is shown there that, for this counter-example case, the gradient of the corrector* w_p *solution to* (12) *is not of the form of " a periodic function composed with the diffeomorphism* Φ^{-1}*". Despite this fact, we show below that the ansatz* (15) *(and the resulting MsFEM-type approach described above) actually yields accurate results (see the second line of Table 1).*

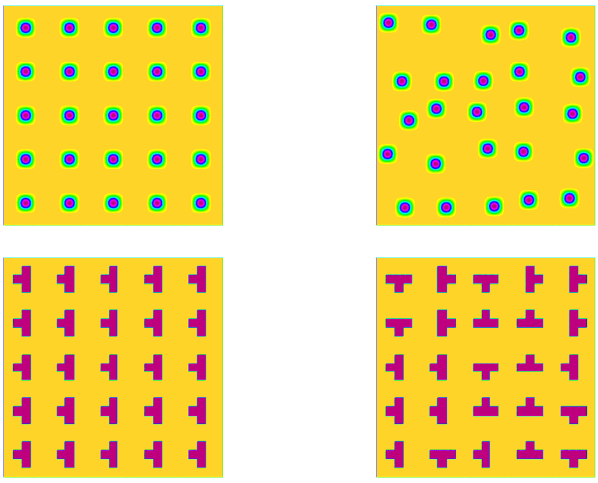

Figure 2: Left: the periodic material modelled by A_{per}. Right: a realization of $A_{\text{per}}(\Phi^{-1})$. Top row: Φ is a translation of circular inclusions. Bottom row: Φ is a rotation of T-shaped inclusions.

We work with the parameters $\varepsilon = 0.025$ and $H = 1/30$. The error between two random functions u_1 and u_2 is defined by

$$e(u_1, u_2) = \mathbb{E}\left(\frac{\|\nabla u_1 - \nabla u_2\|_{L^2(\mathcal{D})}}{\|\nabla u_2\|_{L^2(\mathcal{D})}}\right). \tag{21}$$

We have considered 30 realizations of Φ and approximated the above expectation as an empirical mean over these 30 realizations.

In Table 1, we compare the exact solution $u^\varepsilon(\cdot, \omega)$ of (9)-(10) (computed using a finite element method with a fine mesh of size $h = \varepsilon/40$ adapted to the small scales present in the problem) with the approximation $u_{\mathrm{BLL}}(\cdot, \omega)$ obtained using the approach described above and with the approximation $u_{\mathrm{MsFEM}}(\cdot, \omega)$ obtained using the standard MsFEM approach (as described in Section 2.2), with the recomputation of the basis functions for each new realization of Φ.

Of course, the computational cost to obtain many realizations of u_{BLL} is much smaller than that to obtain the same number of realizations of u_{MsFEM}. In the former case, and in contrast to the latter case, we do not have to recompute the highly oscillatory basis functions. On the other hand, our approach being a MsFEM type approach, the error $u^\varepsilon - u_{\mathrm{MsFEM}}$ seems to be the best error we can achieve. It is thus natural to compare the error we obtain, that is $u^\varepsilon - u_{\mathrm{BLL}}$, with that "reference" error.

Example	$e(u^\varepsilon, u_{\mathrm{MsFEM}})$	$e(u^\varepsilon, u_{\mathrm{BLL}})$	$e(u_{\mathrm{MsFEM}}, u_{\mathrm{BLL}})$
Translation	7.26%	10.38%	9.33%
Rotation	9.34%	10.58%	8.63%

Table 1: Errors (21) for the two test cases considered.

We observe that, for both test cases, the error $e(u^\varepsilon, u_{\mathrm{BLL}})$ is of the same order as the reference error $e(u^\varepsilon, u_{\mathrm{MsFEM}})$. Our approach thus yields an approximation u_{BLL} which is as accurate as the approximation u_{MsFEM} provided by a standard MsFEM approach, for a much smaller computational cost. Note also that the order of the error observed here (of 7 to 10 % in the H^1 norm) is the standard order obtained with MsFEM approaches (see e.g. [2, Section 4.2, Table 2]).

These first numerical results are encouraging. Note however that they both correspond to the specific case where $\nabla\Phi$ is piecewise constant. Definite conclusions on the interest of the approach yet need to be obtained, e.g. using test cases with more complex diffeomorphisms Φ.

4 Robustness of the MsFEM approach to a macroscopic perturbation of the diffusion coefficient

[Work expanded in [5].]

This section is devoted to a preliminary study of the following question. Assume that we know the corrector w_p associated to a periodic coefficient $A_{\rm per}$ by the corrector problem (5). Is it possible, using w_p, to approximate the corrector $\widetilde{w}_p$ associated to a macroscopic perturbation of $A_{\rm per}$? Otherwise formulated, once we know how to homogenize (1) with the coefficient $A^\varepsilon(x) = A_{\rm per}\left(\frac{x}{\varepsilon}\right)$, is it possible to efficiently homogenize (1) for the highly oscillatory matrix $\widetilde{A}^\varepsilon(x) = b(x)A_{\rm per}\left(\frac{x}{\varepsilon}\right)$, or $\widetilde{A}^\varepsilon(x) = b(x) + A_{\rm per}\left(\frac{x}{\varepsilon}\right)$? Note that, in both cases, the difference between $\widetilde{A}^\varepsilon(x)$ and $A^\varepsilon(x)$ only comes from a function b that has no small scale oscillation (thus the terminology "macroscopic perturbation"). In particular, the high frequencies present in $\widetilde{A}^\varepsilon(x)$ are identical to the high frequencies present in $A^\varepsilon(x)$. This is the reason why we expect that, once we have resolved these highly oscillatory modes for $A^\varepsilon(x)$, we may deduce the highly oscillatory modes of $\widetilde{A}^\varepsilon(x)$.

Remark 5 *The same question may be asked for the MsFEM highly oscillatory basis functions, rather than the periodic corrector. See Section 4.2 below.*

A motivation for this question is the following optimization problem. Assume that we model our material with some coefficient matrix $A^\varepsilon(x) = A_{\rm per}\left(\frac{x}{\varepsilon}\right) + b(x)$, that we know that the highly oscillatory component is accurate, and that we want to optimize on the macroscopic component b in order to reproduce with this model some known results (such as experimental data) on the homogenized behavior. In the optimization loop, we need to compute, for each new trial value of the function b, the homogenized coefficient. For the sake of efficiency, we thus need to perform this homogenization procedure with a computational cost as small as possible.

4.1 Multiplicative pertubation

As a first step, we consider a multiplicative perturbation. The coefficient $\widetilde{A}^\varepsilon(x)$ reads

$$\widetilde{A}^\varepsilon(x) = b(x) A_{\rm per}\left(\frac{x}{\varepsilon}\right), \tag{22}$$

where b is a scalar-valued function. The problem under consideration then reads

$$-\mathrm{div}\left[b(x) A_{\rm per}\left(\frac{x}{\varepsilon}\right)\nabla u^\varepsilon(x)\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\varepsilon = 0 \ \text{ on } \partial\mathcal{D}. \tag{23}$$

When $\varepsilon \to 0$, the function u^ε converges to $u^\star$, solution to the homogenized problem

$$-\mathrm{div}\left[A^\star(x)\nabla u^\star\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\star(x) = 0 \ \text{ on } \partial\mathcal{D},$$

where the homogenized matrix is given by $A^\star(x) = b(x) A^\star_{\rm per}$, where $A^\star_{\rm per}$ is defined by (4)-(5). In this case, the corrector associated to $\widetilde{A}^\varepsilon(x) = b(x) A_{\rm per}(x/\varepsilon)$ is identical to the corrector associated to $A^\varepsilon(x) = A_{\rm per}(x/\varepsilon)$.

In a MsFEM context, we have the same type of result. As in Section 2.2, introduce the P1 finite element space $\mathcal{V}_h = \mathrm{Span}(\chi_i^0,\ 1 \le i \le L)$. Compute the highly oscillatory basis function χ_i^ε by solving (7). These functions are therefore independent of the macroscopic function b. We next introduce the MsFEM space $\mathcal{W}_h = \mathrm{Span}(\chi_i^\varepsilon, 1 \le i \le L)$, and perform a Galerkin approximation of (23) using the space $\mathcal{W}_h$. Because of the specific structure (22), such an approach provides an approximation of u^ε solution to (23) whose accuracy is essentially independent of b. For each new trial function b, we do not have to recompute the MsFEM basis functions.

4.2 Additive pertubation

We now consider an additive perturbation, in the sense that the coefficient $\widetilde{A}^\varepsilon(x)$ reads

$$\widetilde{A}^\varepsilon(x) = b(x) + A_{\rm per}\left(\frac{x}{\varepsilon}\right). \tag{24}$$

We do not assume that b is much larger, or much smaller, than $A_{\rm per}$. The ratio $\dfrac{\|b\|_{L^\infty}}{\|A_{\rm per}\|_{L^\infty}}$ is of the order of one.

For the sake of simplicity, consider first the case when b is a constant function. The corrector equation associated to the coefficient (24) then reads

$$\begin{cases} -\mathrm{div}[(A_{\mathrm{per}}(y)+b)\,(p+\nabla\widetilde{w}_p(y))] = 0 \quad \text{on } \mathbb{R}^d, \\ \widetilde{w}_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases}$$

As can be seen on the one-dimensional case, there is no relation between $\widetilde{w}_p$ and the corrector w_p associated to the coefficient $A^\varepsilon(x) = A_{\mathrm{per}}(x/\varepsilon)$, which solves (5). This case is such much more challenging than the case considered in Section 4.1. In what follows, we propose a numerical approach, based on a tensor-product decomposition, to address this setting.

Principle In the sequel, we consider coefficients of the form

$$A^\varepsilon(x,\mu) = A_0^\varepsilon(x) + \mu b(x), \quad x \in \mathcal{D}, \quad \mu \in \Lambda, \tag{25}$$

where $\Lambda \subset \mathbb{R}^p$ is a bounded open set. The coefficient $A^\varepsilon(x,\mu)$ is thus equal to the highly oscillatory coefficient $A_0^\varepsilon(x)$, up to the addition of a macroscopic, non oscillatory function $\mu b(x)$. We do not assume that $A_0^\varepsilon(x)$ is periodic, and therefore put ourselves in the MsFEM context. Our aim is to efficiently compute the highly oscillatory basis functions $\chi_i^\varepsilon(x,\mu)$, solution, in each element $\mathbf{K}$, to

$$-\mathrm{div}\,[A^\varepsilon(x,\mu)\nabla\chi_i^\varepsilon(x,\mu)] = 0 \ \text{ in } \mathbf{K}, \quad \chi_i^\varepsilon(x,\mu) = \chi_i^0(x) \ \text{ on } \partial\mathbf{K}, \tag{26}$$

where χ_i^0 are the standard P1 finite element basis functions. In turn, the functions $\chi_i^\varepsilon(x,\mu)$ will be used to perform a Galerkin approximation of the problem

$$-\mathrm{div}\,[A^\varepsilon(x,\mu)\nabla u^\varepsilon(x,\mu)] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\varepsilon(\cdot,\mu) = 0 \ \text{ on } \partial\mathcal{D}, \tag{27}$$

for many values of the parameter $\mu \in \Lambda$.

This question has been addressed in [15], where an approach based on the expansion of $\chi_i^\varepsilon(x,\mu)$ in terms of a Neumann series is proposed. Our approach is different, and consists in adapting the Proper Generalized Decomposition (PGD) technique [17, 12, 19, 18] to the current context. More precisely, we are going to approximate χ_i^ε, function of the two variables x and μ, as a sum of products of a function depending only on x by a function depending only on μ.

We now proceed in details. We first change of unknown function and define

$$v_i^{\varepsilon,\mathbf{K}} = \chi_i^\varepsilon|_{\mathbf{K}} - \chi_i^0|_{\mathbf{K}}\,. \tag{28}$$

We infer from (26) that

$$-\mathrm{div}\left[A^\varepsilon(x,\mu)\left(\nabla\chi_i^0(x) + \nabla v_i^{\varepsilon,\mathbf{K}}(x,\mu)\right)\right] = 0 \ \text{ in } \mathbf{K}, \quad v_i^{\varepsilon,\mathbf{K}}(x,\mu) = 0 \ \text{ on } \partial\mathbf{K}. \tag{29}$$

The advantage of considering $v_i^{\varepsilon,\mathbf{K}}$ is that this function satisfies *homogeneous* boundary conditions on $\partial\mathbf{K}$, in contrast to χ_i^ε. Our approach is based on the assumption that $v_i^{\varepsilon,\mathbf{K}}(x,\mu)$ writes as follows:

$$v_i^{\varepsilon,\mathbf{K}}(x,\mu) \approx \sum_{j=1}^{N} g_{i,j}(\mu)\, f_{i,j}^{\varepsilon,\mathbf{K}}(x) \tag{30}$$

for a *small* number of terms N, where the functions $\mu \mapsto g_{i,j}(\mu)$ are independent of x and the functions $x \mapsto f_{i,j}^{\varepsilon,\mathbf{K}}(x)$ are independent of μ. Once these functions have been identified, computing the basis functions $\chi_i^\varepsilon(\cdot,\mu)$ for any value of μ just amounts to *evaluating* N functions of μ using (28) and (30), rather than *solving* the partial differential equations (26).

Algorithm The functions $g_{i,j}(\mu)$ and $f_{i,j}^{\varepsilon,\mathbf{K}}(x)$ are iteratively defined. Assume that they have been built for any $j \le k-1$. To build $g_{i,k}$ and $f_{i,k}^{\varepsilon,\mathbf{K}}$, we introduce two variational formulations. The first one consists in finding $f_{i,k}^{\varepsilon,\mathbf{K}} \in H_0^1(\mathbf{K})$ solution to

$$\forall w \in H_0^1(\mathbf{K}), \quad \mathcal{A}_k(f_{i,k}^{\varepsilon,\mathbf{K}}, w) = -\mathcal{F}_k(w), \tag{31}$$

with

$$\mathcal{A}_k(f_{i,k}^{\varepsilon,\mathbf{K}}, w) = \int_{\mathbf{K}}\int_\Lambda \left(A^\varepsilon(x,\mu)\nabla f_{i,k}^{\varepsilon,\mathbf{K}}(x)\cdot\nabla w(x)\right)\, g_{i,k}^2(\mu)\,dx\,d\mu$$

and

$$\mathcal{F}_k(w) = \int_{\mathbf{K}}\int_\Lambda \left(A^\varepsilon(x,\mu)\left(\nabla\chi_i^0(x) + \sum_{j=1}^{k-1} g_{i,j}(\mu)\nabla f_{i,j}^{\varepsilon,\mathbf{K}}(x)\right)\cdot\nabla w(x)\right) g_{i,k}(\mu)\,dx\,d\mu.$$

Note that it is natural to look for $f_{i,k}^{\varepsilon,\mathbf{K}}$ in the space $H_0^1(\mathbf{K})$, since $v_i^{\varepsilon,\mathbf{K}}$ satisfies homogeneous Dirichlet conditions on $\partial\mathbf{K}$.

The second variational formulation consists in finding $g_{i,k} \in L^2(\Lambda)$ such that

$$\forall h \in L^2(\Lambda), \quad \mathcal{B}_k(g_{i,k}, h) = -\mathcal{R}_k(h), \tag{32}$$

where

$$\mathcal{B}_k(g_{i,k}, h) = \int_{\mathbf{K}} \int_{\Lambda} \left(A^{\varepsilon}(x,\mu) \nabla f_{i,k}^{\varepsilon,\mathbf{K}}(x) \cdot \nabla f_{i,k}^{\varepsilon,\mathbf{K}}(x) \right) g_{i,k}(\mu) h(\mu)\, dx\, d\mu$$

and

$$\mathcal{R}_k(h) = \int_{\mathbf{K}} \int_{\Lambda} \left(A^{\varepsilon}(x,\mu) \left(\nabla \chi_i^0(x) + \sum_{j=1}^{k-1} g_{i,j}(\mu) \nabla f_{i,j}^{\varepsilon,\mathbf{K}}(x) \right) \cdot \nabla f_{i,k}^{\varepsilon,\mathbf{K}}(x) \right) h(\mu)\, dx\, d\mu.$$

Note that the two variational formulations (31) and (32) are coupled, as they both involve the unknown functions $f_{i,k}^{\varepsilon,\mathbf{K}}$ and $g_{i,k}$. However, each unknown function only depends on one variable (x or μ). Solving these two coupled problems is expected (and this is indeed the case) to be easier than solving a single problem on a function depending on both variables x and μ. One possibility to solve (31) and (32) is to use the following iterative algorithm. Let η be the accuracy we wish to reach and let e denote the error. We proceed as follows:

1. Initialization: set $e = 1$ and $g_{i,k}(\mu) = 1/\sqrt{|\Lambda|}$, so that $\|g_{i,k}\|_{L^2(\Lambda)} = 1$.
2. Iterate:
   (a) set $T = g_{i,k}(\mu)$;
   (b) find $f_{i,k}^{\varepsilon,\mathbf{K}}$ solution to (31);
   (c) find $g_{i,k}$ solution to (32);
   (d) multiply the function $g_{i,k}$ by a constant such that its L^2 norm is equal to 1: $g_{i,k} \leftarrow g_{i,k}/\sqrt{\int_{\Lambda} g_{i,k}^2}$;
   (e) compute the difference $e = \int_{\Lambda} (g_{i,k} - T)^2$ between the new and the old iterate;

(f) if $e > \eta$, go back to Step 2a.

In practice, at Steps 2b and 2c, both problems (31) and (32) can be solved by classical methods. For instance, we can discretize the bounded domain $\Lambda \subset \mathbb{R}^p$ and use a finite element method to solve (32), and likewise for (31).

Assume now that the functions $g_{i,k}$ and $f_{i,k}^{\varepsilon,\mathbf{K}}$ have been computed on each element $\mathbf{K}$ and for each $k \leq N$. We now want to solve (27), for some value of the parameter $\mu \in \Lambda$. We introduce the MsFEM space

$$\mathcal{W}_h^\mu := \mathrm{Span}\{\chi_i^\varepsilon(x,\mu)\}.$$

The Galerlin approximation $u_h^\varepsilon(x,\mu) \in \mathcal{W}_h^\mu$ of the solution $u^\varepsilon(x,\mu)$ to (27) is defined as the solution to

$$\forall v \in \mathcal{W}_h^\mu, \quad \int_{\mathcal{D}} (\nabla v)^T A^\varepsilon(\cdot,\mu) \nabla u_h^\varepsilon(\cdot,\mu) = \int_{\mathcal{D}} f v.$$

Numerical illustration We work in dimension two, with $A^\varepsilon(x_1,x_2,\mu) = a^\varepsilon(x_1,x_2,\mu)\,\mathrm{Id}$, where

$$a^\varepsilon(x_1,x_2,\mu) = 1 + 100\sin^2\left(\frac{\pi x_1}{\varepsilon}\right)\sin^2\left(\frac{\pi x_2}{\varepsilon}\right) + 100\,\mu, \quad (x_1,x_2) \in \mathbb{R}^2,$$

which is indeed of the form (25). The computational domain is $\mathcal{D} = (0,1)^2$ and the parameter domain is $\Lambda = (0,1)$. We set $\varepsilon = 0.05$. We compute the functions $g_{i,k}$ and $f_{i,k}^{\varepsilon,\mathbf{K}}$ as explained above, and evaluate the error

$$e_N^{\mathbf{K}}(\mu) = \frac{\left\| \nabla\chi_i^\varepsilon(\cdot,\mu) - \left[\nabla\chi_i^0 + \sum_{j=1}^N g_{i,j}(\mu)\nabla f_{i,j}^{\varepsilon,\mathbf{K}}\right]\right\|_{L^2(\mathbf{K})}}{\|\nabla\chi_i^\varepsilon(\cdot,\mu)\|_{L^2(\mathbf{K})}}, \tag{33}$$

where $\chi_i^\varepsilon(x,\mu)$ is the exact basis function for the parameter μ, which solves (26).

We have worked with the following numerical parameters. The open set Λ is discretized with a mesh of size $h_\Lambda = 0.1$. To solve (26), (31) or (32) in practice, each finite element $\mathbf{K}$ is discretized with a mesh of size $h = H/30$, where $H = \mathrm{diam}(\mathbf{K})$. We take $H = 1/7$.

In Table 2, we show the error (33) as a function of N, that is the number of terms used in (30) to approximate $v_i^{\varepsilon,\mathbf{K}}$. We observe a fast convergence of the error with respect to N. Two terms in (30) are actually enough to

N	$e_N^{\mathbf{K}}(\mu = 0.5)$	$e_N^{\mathbf{K}}(\mu = 0.67)$
1	18.15%	18.56%
2	3.78%	4.18%
3	3.11%	3.30%
4	2.82%	3.13%

Table 2: Error (33) for two values of the parameter μ (all these errors correspond to the same choice of finite element $\mathbf{K}$; similar results are obtained for a different choice).

obtain an approximation of $v_i^{\varepsilon,\mathbf{K}}$ (and therefore of χ_i^ε) with an error smaller than 5 %.

Obviously, these encouraging results are only preliminary. More tests are needed to get a better understanding of this approach, its limitations and the regime where it is indeed advantageous.

5 Proposed directions of research for an expected renewed funding

If EOARD decides to renew our funding, there are a number of directions of research on which we might consider proceeding (subject to EOARD approval of course). We summarize here some of them.

In Section 4, we have performed a preliminary study on the robustness of the MsFEM approach to perturbations that are non-oscillatory. This question is actually part of a much broader question, which is related to inverse problems in multiscale science.

A first remark is that all models that involve a random parameter require some knowledge on the distribution of this random parameter (actually, they most often require a *complete* knowledge of that distribution). In practice, access to this distribution is difficult. One is therefore bound to *assume* a given form (Gaussian, ...) for the distribution and proceed with the computation. A question of major practical interest is to *a posteriori* prove, or disprove the validity of this assumption. Otherwise stated, tests of hypotheses in the context of engineering problems is an important issue. A preliminary step, before trying to identify the *distribution* of the random parameters, is to assume a specific form of this distribution, depending on a few quantities (e.g.

assume a Gaussian distribution with an unknown variance) and identify these *quantities*. To solve this identification problem, it is important to be able to solve efficiently the forward problem (given the microscopic field A, compute the macroscopic, homogenized behavior). Efficient methods such as the ones proposed within this contract are then of paramount importance.

Another remark is that the question of inverse problems in materials science is of course not new. However, our context is very specific, owing to the fact that homogenization acts as a filter. Many features of the coefficient A^ε in the problem (1) (or its stochastic version (13)) are filtered out by the homogenization procedure. Several fields A^ε can lead to the same homogenized matrix $A^\star$. It is hence hopeless to try to recover the field A^ε from the sole knowledge of $A^\star$, or of properties of the homogenized material. From $A^\star$, one can only expect to recover *the class* of microscopic fields that correspond to this homogenized behavior. This class probably contains many materials, different at the fine scale, but equivalent from the macroscopic standpoint. All of these are thus admissible, if the only information we have is a macroscopic information.

References

References authored by the investigators in the context of the contract and cited in this report

[1] A. Anantharaman, R. Costaouec, C. Le Bris, F. Legoll and F. Thomines, *Introduction to numerical stochastic homogenization and the related computational challenges: some recent developments*, W. Bao and Q. Du eds., Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, Volume 22, pp. 197–272, 2011.

[2] C. Le Bris, F. Legoll and F. Thomines, *Multiscale problems in materials science: a mathematical approach to the role of uncertainty*, Report 2010 to the European Office of Aerospace Research and Development (EOARD), 2010.

[3] C. Le Bris, F. Legoll and F. Thomines, *Multiscale problems in materials science: a mathematical approach to the role of uncertainty*, Report

2011 to the European Office of Aerospace Research and Development (EOARD), 2011.

[4] C. Le Bris, F. Legoll and F. Thomines, *Multiscale finite element approach for "weakly" random problems and related issues*, submitted, `arXiv` preprint 1111.1524.

[5] F. Thomines, Ph.D. thesis of the Université Paris Est, Ecole des Ponts ParisTech, submitted (defense scheduled in November 2012).

References authored by the investigators in the context of the contract and not cited in this report

[6] X. Blanc, F. Legoll and A. Anantharaman, *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, `arXiv` preprint 1110.4767, accepted for publication in Applied Mathematics Research Express, available at http://amrx.oxfordjournals.org/content/early/2012/07/25/amrx.abs013.short?rss=1

[7] C. Le Bris, F. Legoll and F. Thomines, *Rate of convergence of a two-scale expansion for some weakly stochastic homogenization problems*, `arXiv` preprint 1110.5206, accepted for publication in Asymptotic Analysis.

[8] C. Le Bris and F. Thomines, *A Reduced Basis approach for some weakly stochastic multiscale problems*, Chinese Annals of Mathematics Series B, 33(5):657–672, 2012.

References authored by the investigators and not related to the contract

[9] X. Blanc, C. Le Bris and P.-L. Lions, *Une variante de la théorie de l'homogénéisation stochastique des opérateurs elliptiques [A variant of stochastic homogenization theory for elliptic operators]*, C. R. Acad. Sci. Série I, 343:717–724, 2006.

[10] X. Blanc, C. Le Bris and P.-L. Lions, *Stochastic homogenization and random lattices*, Journal de Mathématiques Pures et Appliquées, 88:34–63, 2007.

General references by other authors

[11] G. Allaire and R. Brizzi, *A multiscale finite element method for numerical homogenization*, SIAM Multiscale Modeling & Simulation, 4(3):790–812, 2005.

[12] A. Ammar, B. Mokdad, F. Chinesta and R. Keunings, *A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modelling of complex fluids*, Journal of Non-Newtonian Fluid Mechanics, 139(3):153–176, 2006.

[13] W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden, *Heterogeneous multiscale methods: a review*, Comm. Comput. Phys., 2(3):367–450, 2007.

[14] Y.R. Efendiev, T.Y. Hou and X.-H. Wu, *Convergence of a nonconforming multiscale finite element method*, SIAM Journal on Numerical Analysis, 37(3):888–910, 2000.

[15] V. Ginting, A. Malqvist and M. Presho, *A novel method for solving multiscale elliptic problems with randomly perturbed data*, SIAM Multiscale Modeling & Simulation, 8(3):977–996, 2010.

[16] T.Y. Hou and X.-H. Wu, *A multiscale finite element method for elliptic problems in composite materials and porous media*, Journal of Computational Physics, 134(1):169–189, 1997.

[17] P. Ladevèze, *Nonlinear Computational Structural Mechanics - New Approaches and Non-Incremental Methods of Calculation*, Springer Verlag, 1999.

[18] C. Le Bris, T. Lelièvre and Y. Maday, *Results and questions on a nonlinear approximation approach for solving high-dimensional partial differential equations*, Constructive Approximation, 30(3):621–651, 2009.

[19] A. Nouy, *Proper Generalized Decompositions and separated representations for the numerical solution of high dimensional stochastic problems*, Archives of Computational Methods in Engineering, 17:403–434, 2010.

Contract FA 8655-10-C-4002

Multiscale problems in materials science: a mathematical approach to the role of uncertainty

Report 2011 to the European Office of Aerospace Research and Development (EOARD)

C. Le Bris, F. Legoll, F. Thomines

October 2011

Contents

Summary

We report here on the work performed during the second year (october 2010 - october 2011) of the contract FA 8655-10-C-4002 on *Multiscale problems in materials science: a mathematical approach to the role of uncertainty.*

We recall that the bottom line of our work is to develop *affordable numerical methods* in the context of *stochastic homogenization.* Many partial differential equations of materials science indeed involve highly oscillatory coefficients and thus small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic

random problems (and the associated stochastic homogenization theory) are one instance for modelling uncertainty of continuous media. The theoretical aspects of these problems are now well-understood, in general. On the other hand, the numerical aspects have received less attention from the mathematics community. Standard methods available in the literature often lead to very, and sometimes prohibitively, costly computations.

In this report, we first focus on a class of materials of moderate difficulty but of significant relevance, that of random materials where the amount of randomness is *small*. They can be considered as *stochastic perturbations of deterministic materials*. We have presented in the previous report (see [3]) a possible extension of the well-known Multiscale Finite Element Method (MsFEM) to such a weakly stochastic setting, along with detailed numerical results. We are now in position to provide a complete analysis of the approach, extending that available for the deterministic setting.

We next consider a different weakly stochastic setting. Rather than perturbing the deterministic material by frequent but small random amounts, we consider a setting in which the deterministic material is rarely perturbed. However, when it occurs, the perturbation is large. Because this setting is a weakly stochastic setting, the workload to compute the homogenized matrix is already smaller than in generic stochastic homogenization. We show here how to further reduce the workload by using a Reduced Basis approach.

We finally turn to a variant of stochastic homogenization, where the randomness is not small, and describe in that context a truncation procedure to compute, in practice, an approximation of the homogenized coefficient.

The works described below have been performed by Claude Le Bris (PI), Frédéric Legoll (Co-PI) and Florian Thomines (second year Ph.D. student).

1 Introduction

During this second year of contract, we have pursued our effort on developing *affordable* numerical methods in the context of *stochastic homogenization*.

Many partial differential equations of materials science indeed involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems are one of the most famous instances of mathematical uncertainty of continuous media.

The purpose of this report is to present the recent progress we have made on this topic, with the aim *to make numerical random homogenization more practical*. As already mentioned in the previous report, because we cannot embrace all difficulties at once, the case under consideration here is a *simple, linear, scalar second order elliptic partial differential equation in divergence form*, for which a sound theoretical groundwork exists. We focus here on the different manners the problem can be handled from the *computational viewpoint*.

We begin, in Section 2, with a brief description of stochastic homogenization, the only purpose of which is the consistency of this report.

As pointed out above, random homogenization for general stochastic materials is very costly. Yet, it turns out that it is possible to identify classes of materials of moderate difficulty but of significant relevance, where stochastic homogenization theory and practice can be reduced to more affordable, less computationally demanding problems. These materials are neither periodic (because such an oversimplifying assumption is rarely met in practice), nor fully stochastic. They can be considered as an intermediate case, that of *stochastic perturbations of deterministic (possibly periodic) materials*. Note that many practical situations, involving actual materials or media, can be considered, at a good level of approximation, as perturbations of a deterministic (often periodic) setting (see e.g. [15]). In this report, we discuss two different weakly stochastic settings, and for each of them, we present an efficient numerical approach to handle it. First, in Section 3, we provide an analysis of a variant of the Multiscale Finite Element Method (MsFEM), well adapted to the case when the matrix describing the properties of the material is the sum of a deterministic term and a small random term. This variant has been introduced in the previous report (see [3]), and extensive numerical tests have been reported there. As explained below, we now have a complete understanding of the approach, from the analysis viewpoint. We wish to emphasize the fact that considering a stochastic perturbation of a deterministic problem and handling it with a multiscale technique developed in the deterministic setting is not restricted to the case of the MsFEM. Similar entreprises can probably be undertaken in other settings, such as those proposed in [19].

In Section 4, we turn to a different weakly stochastic setting, introduced by the PI and a collaborator of his in [8, 9, 10]. This model is well suited for representing materials with rare, but non small, perturbations with re-

spect to a deterministic situation. A typical example is a composite material embedding fibers, located, say, on a perfect, periodic lattice. The random perturbation then consists in *deleting* some fibers (see Figure 1 below). This setting is a weakly stochastic setting, as we assume that such an accident occurs very rarely. However, it is clear that the local properties (at the microscopic level) of the material are significantly changed if the fiber is indeed deleted. In the sequel, we show that the Reduced Basis approach can be used in that context to speed-up the computation of the homogenized coefficient.

In Section 5, we next turn to a non-weakly stochastic setting, and consider a variant of stochastic homogenization, introduced by the PI and co-workers in [11, 12] some years ago. This model is well suited to represent materials that are random deformations of a perfect periodic material. A typical example is, again, a composite material with fibers. Fibers are all identical, they would be located on a periodic lattice in the ideal situation. However (for instance as a consequence of the manufacturing process), their actual positions are now random. In the sequel, we present and analyze a procedure to practically approximate the homogenized matrix.

We collect in Section 6 some conclusions about the work performed so far, and future directions.

2 Basics of stochastic homogenization

[Detailed presentation can be read in [2, 3].]

For the consistency of this report and the convenience of the reader not familiar with the theory, we recall here some groundwork in stochastic homogenization, underlining why stochastic homogenization often leads to extremely expensive computations. More details can be read in [3] and references therein, and also in the review article [2] that we published.

The typical random homogenization problem writes

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

where A is a bounded, definite positive, stationary (i.e. statistically homogeneous) random matrix (see [3]). In this framework, it is well known that, as $\varepsilon \to 0$, the solution u^ε to (1) converges to $u^\star$ solution to

$$-\mathrm{div}\left[A^\star \nabla u^\star\right] = f(x) \ \text{ in } \mathcal{D}, \qquad u^\star(x) = 0 \ \text{ on } \partial\mathcal{D}, \tag{2}$$

where the homogenized matrix $A^\star$ reads

$$[A^\star]_{ij} = \mathbb{E}\left[\int_Q \left(e_i + \nabla w_{e_i}(y,\cdot)\right)^T A(y,\cdot)\left(e_j + \nabla w_{e_j}(y,\cdot)\right)\, dy\right],$$

where $Q = (0,1)^d$ and where, for any $p \in \mathbb{R}^d$, the so-called corrector w_p is the (unique up to the addition of a constant) solution to

$$\left\{\begin{array}{l} -\mathrm{div}\left[A\left(y,\omega\right)\left(p + \nabla w_p(y,\omega)\right)\right] = 0 \quad \text{on} \quad \mathbb{R}^d, \\ \nabla w_p \text{ is stationary}, \quad \mathbb{E}\left(\displaystyle\int_Q \nabla w_p(y,\cdot)\, dy\right) = 0. \end{array}\right. \tag{3}$$

From the computational viewpoint, solving (3) is challenging, because it is posed on the *entire space* $\mathbb{R}^d$. The traditional approach is to truncate (3) on a bounded domain, say the cube $Q_N = (-N,N)^d$, and complement it with e.g. periodic boundary conditions. We are thus left with solving the truncated corrector problem

$$\left\{\begin{array}{l} -\mathrm{div}\,\left(A(\cdot,\omega)\left(p + \nabla w_p^N(\cdot,\omega)\right)\right) = 0 \quad \text{on} \quad \mathbb{R}^d, \\ w_p^N(\cdot,\omega) \text{ is } Q_N\text{-periodic}. \end{array}\right. \tag{4}$$

In turn, the homogenized matrix $A^\star$ is approximated by the matrix

$$[A_N^\star]_{ij}\left(\omega\right) = \frac{1}{|Q_N|}\int_{Q_N}\left(e_i + \nabla w_{e_i}^N(y,\omega)\right)^T A(y,\omega)\left(e_j + \nabla w_{e_j}^N(y,\omega)\right)\, dy.$$

Although $A^\star$ itself is a deterministic object, its practical approximation $A_N^\star(\omega)$ is random. It is only in the limit of infinitely large domains Q_N that the deterministic value is attained. Indeed, as shown in [17, Theorem 1], we have

$$\lim_{N\to\infty} A_N^\star(\omega) = A^\star. \tag{5}$$

Errors between $A_N^\star(\omega)$ and $A^\star$ are due to (i) the truncation, and (ii) the fact that the truncated problem is random in nature. Because of the truncation, $\mathbb{E}\left[A_N^\star\right] \neq A^\star$. At fixed N, there is a systematic bias, which can only be reduced by taking sufficiently large domains Q_N. In addition, computing $\mathbb{E}\left[A_N^\star\right]$ is also expensive. Indeed, a large number M of independent realizations of $A_N^\star(\omega)$ should be considered to compute an empirical mean, in the spirit of Monte Carlo methods. It is only in the limit $M \to \infty$ that the exact mean $\mathbb{E}\left[A_N^\star\right]$ is recovered.

The overall computation described above, that involves solving several independent realizations of (4) on presumably large a domain Q_N, is thus very expensive.

3 A weakly-stochastic MsFEM approach

[Work expanded in [1, 4, 5].]

Following the encouraging numerical results reported in [3] on the variant of the MsFEM for weakly stochastic settings, we have pursued our efforts and obtained a complete analysis of the proposed approach, that we describe in the sequel. For clarity, we begin this section by briefly recalling our approach.

3.1 The proposed approach

We consider the problem

$$-\mathrm{div}(A_\eta^\varepsilon(\cdot,\omega)\nabla u_\eta^\varepsilon(\cdot,\omega)) = f \ \text{ in } \mathcal{D}, \quad u_\eta^\varepsilon(\cdot,\omega) = 0 \ \text{ on } \partial\mathcal{D}, \tag{6}$$

where $A_\eta^\varepsilon(\cdot,\omega) \in (L^\infty(\mathcal{D}))^{d\times d}$ is a random matrix satisfying the standard coercivity and boundedness conditions. In contrast to (1), we do not assume that $A_\eta^\varepsilon(x,\omega) = A_\eta\left(\frac{x}{\epsilon},\omega\right)$ for a fixed stationary matrix A_η. The MsFEM approach is applicable in more general situations.

We suppose that $A_\eta^\varepsilon(x,\omega)$ is highly oscillatory in both its deterministic and stochastic components, and that it is a *perturbation* of a deterministic matrix, in the sense that

$$A_\eta^\varepsilon(x,\omega) = A_0^\varepsilon(x) + \eta A_1^\varepsilon(x,\omega), \tag{7}$$

where A_0^ε is a deterministic matrix and η is a small deterministic parameter. This model may be well suited for heterogeneous materials (or, more generally, media) that, although not periodic, are *not fully* stochastic, in the sense that they may be considered as a *perturbation* of a deterministic material.

We recall that the MsFEM approach aims at approximating the solution of (6) by performing a variational approximation of the problem using precomputed basis functions ϕ_i^ε that are *adapted* to the problem. The main idea of our proposed approach is to compute a set of *deterministic* MsFEM basis functions ϕ_i^ε using A_0^ε, the deterministic part of A_η^ε in the expansion (7), and then to perform Monte Carlo realizations at the macroscale level using a set of $\mathcal{M}$ realizations of the random matrix $\left\{A_\eta^{\varepsilon,m}(x,\omega)\right\}_{1\le m\le\mathcal{M}}$ (see [3] for a detailed presentation). Note that, for each of these realizations, we solve the *original* problem, with the *complete* matrix A_η^ε, and not only its deterministic part. Only the basis set is taken deterministic.

The deterministic basis functions ϕ_i^ε are computed only once, hence the computational saving in comparison to a natural adaptation of the MsFEM to the stochastic setting, where, for each realization of the random matrix A_η^ε, new basis functions are computed before solving the macroscopic problem.

As illustrated by the numerical tests reported in [3, 4], our proposed approach is extremely efficient when A_η^ε is a perturbation of A_0^ε. In addition, the small parameter η does not need to be extremely small for our approach to be highly competitive.

3.2 Analysis

We now turn to the analysis of our approach. We recall that, in the deterministic setting, a classical context for proving convergence of the MsFEM approach (see [21]) is the case when, in the reference highly oscillatory problem

$$-\mathrm{div}(A^\varepsilon \nabla u^\varepsilon) = f \ \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \ \text{ on } \partial\mathcal{D}, \tag{8}$$

the matrix reads $A^\varepsilon(x) = A_{per}\left(\dfrac{x}{\varepsilon}\right)$ for a fixed periodic matrix A_{per}. Likewise, to be able to perform our theoretical analysis in the stochastic setting, we assume that $A_\eta^\varepsilon(x,\omega) = A_\eta\left(\dfrac{x}{\varepsilon},\omega\right)$ for a fixed stationary random matrix A_η, although, we repeat it, the approach can be used in practice for more general cases. The problem (6) then admits a homogenized limit when ε vanishes.

Our proof follows the same lines as that in the deterministic setting, which we now briefly review. The MsFEM is a Galerkin approximation, the error of which is then estimated using the Céa lemma:

$$\|u^\varepsilon - u_M\|_{H^1(\mathcal{D})} \leq C \inf_{v_h \in \mathcal{W}_h} \|u^\varepsilon - v_h\|_{H^1(\mathcal{D})}, \tag{9}$$

where u^ε is the solution to the reference deterministic highly oscillatory problem (8), u_M is the MsFEM solution, $\mathcal{W}_h = \mathrm{Span}(\phi_i^\varepsilon)$ is the MsFEM basis set, and C is a constant independent of the small length-scale ε present in A^ε and of the macroscopic mesh-size h. Taking advantage of the homogenization setting, we introduce the two-scale expansion

$$v^\varepsilon = u^\star + \varepsilon \sum_{i=1}^{d} w_{e_i}^0\left(\frac{\cdot}{\varepsilon}\right) \frac{\partial u^\star}{\partial x_i}$$

of u^ε, where $u^\star$ is the homogenized solution and $w^0_{e_i}$ is the periodic corrector associated to $e_i \in \mathbb{R}^d$. We deduce from (9) that

$$\|u^\varepsilon - u_M\|_{H^1(\mathcal{D})} \leq C \left(\|u^\varepsilon - v^\varepsilon\|_{H^1(\mathcal{D})} + \inf_{v_h \in \mathcal{W}_h} \|v^\varepsilon - v_h\|_{H^1(\mathcal{D})} \right).$$

The first term in the above right-hand side is estimated using standard homogenization results on the *rate* of convergence of $v^\varepsilon - u^\varepsilon$. To estimate the second term, one considers a suitably chosen element $v_h \in \mathcal{W}_h$, for which $\|v^\varepsilon - v_h\|_{H^1}$ can be estimated directly. The main idea is that the highly oscillating part of v^ε can be well approached by an element in $\mathcal{W}_h$, since, by construction, the highly oscillatory basis functions ϕ^ε_i are defined by a problem similar to the corrector problem, and thus encode the same highly oscillatory behavior as that present in the correctors $w^0_{e_i}$. We are thus left with approximating the slowly varying components of v^ε, for which standard FEM estimates are used.

Following the same strategy in our stochastic setting, we estimate the distance between the solution u^ε_η to the reference stochastic problem (6)-(7) and the weakly stochastic MsFEM solution u_S as

$$\|u^\varepsilon_\eta(\cdot,\omega) - u_S(\cdot,\omega)\|_{H^1(\mathcal{D})} \leq C \Big(\|u^\varepsilon_\eta(\cdot,\omega) - v^\varepsilon_\eta(\cdot,\omega)\|_{H^1(\mathcal{D})} + \inf_{v_h \in \mathcal{W}_h} \|v^\varepsilon_\eta(\cdot,\omega) - v_h\|_{H^1(\mathcal{D})} \Big). \quad (10)$$

We observe that a key ingredient for the proof is the rate of convergence of the difference between the reference solution u^ε_η and its two-scale expansion v^ε_η. Such a result is classical in periodic homogenization, but, to the best of our knowledge, open in the *general* stationary case (in dimensions higher than one). One only knows that $u^\varepsilon_\eta - v^\varepsilon_\eta$ vanishes (in some appropriate norm) when $\varepsilon \to 0$. However, in the particular case when A^ε_η is only *weakly* stochastic, we have shown in [5, Theorem 2] such a result, useful to control the first term in (10):

$$\sqrt{\mathbb{E}\left(\|u^\varepsilon_\eta - v^\varepsilon_\eta\|^2_{H^1(\mathcal{D})} \right)} \leq C \left(\sqrt{\varepsilon} + \eta \sqrt{\varepsilon \ln(1/\varepsilon)} + \eta^2 \right),$$

where C is a constant independent of ε and η. This result relies on asymptotic properties of the Green function of the operator $L = -\text{div } [A_{per} \nabla \cdot]$, a topic of independent interest which has been investigated in [1].

Hence, exploiting the specificity of our weakly stochastic setting, we have estimated the error given by our approach as (see our main result, Theorem 10 in [4]):

$$\sqrt{\mathbb{E}\left[\|u_\eta^\varepsilon - u_S\|_{H_h^1}^2\right]} \leq C\left(\sqrt{\varepsilon} + h + \frac{\varepsilon}{h} + \eta\left(\frac{\varepsilon}{h}\right)^{d/2}\ln(N(h)) + \eta + \eta^2\mathcal{C}(\eta)\right),$$

where C is a constant independent of ε, h and η, $\mathcal{C}$ is a bounded function as η goes to 0, $N(h)$ is the number of elements in the mesh (roughly of order h^{-d} in dimension d), and $\|\cdot\|_{H_h^1}$ is a broken H^1 norm, defined by

$$\|u\|_{H_h^1} := \left(\sum_{\mathbf{K}\in\mathcal{T}_h}\|u\|_{H^1(\mathbf{K})}^2\right)^{1/2}$$

where, in the above sum, $\mathbf{K}$ is any element of the coarse mesh $\mathcal{T}_h$.

Remark 1 *As is often the case in the deterministic MsFEM, we use in [4] the oversampling technique, which is known to improve the accuracy of the numerical results. Consequently, the basis functions ϕ_i^ε do not belong to $H_0^1(\mathcal{D})$, hence the use of a broken H^1 norm in the above estimate. We refer to [4] for more details.*

It is worth noticing that, when $\eta = 0$ in (7), our approach reduces to the standard deterministic MsFEM (with oversampling), and the above estimate then agrees with those proved in [21].

4 Reduced Basis approach in a weakly stochastic homogenization setting

[Work expanded in [6].]

4.1 Summary of previous works

In the previous works [8, 9, 10], not funded by EOARD, the PI and a collaborator of his introduced the following weakly stochastic case.

Consider the highly oscillatory problem (1), where the matrix A reads

$$A(x,\omega) = A_{\text{per}}(x) + b_\eta(x,\omega)C_{\text{per}}(x) \tag{11}$$

where $A_{\rm per}$ and $C_{\rm per}$ are two periodic matrices, and

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

where $\left\{B^k_\eta\right\}_{k\in\mathbb{Z}^d}$ are i.i.d. scalar random variables, sharing the following law: $B^k_\eta = 1$ with probability η, and $B^k_\eta = 0$ with probability $1-\eta$. In the sequel, η is a small parameter, so that $A = A_{\rm per}$ "most of the time". We hence see that the perturbation introduced by $b_\eta(x,\omega)C_{\rm per}(x)$ in (11) is rare. On the other hand, since $A_{\rm per} + C_{\rm per}$ is very different from $A_{\rm per}$, the perturbation, when it occurs, is large. See Figure 1 for some illustration.

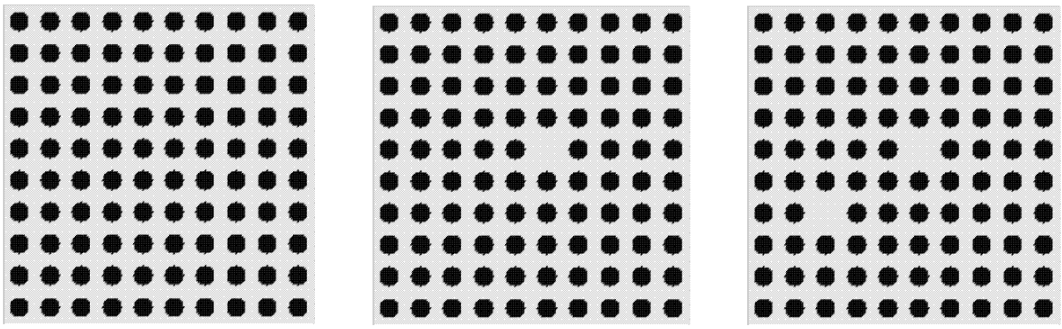

Figure 1: From left to right: perfect material (modelled with $A_{\rm per}$), material with one defect and two defects.

As explained in Section 2, we approximate $A^\star$ using the standard truncation method for the corrector problem (see (4)). By enumerating all possible realizations of $A(x,\omega)$ on Q_N, we obtain an expansion of $\mathbb{E}\left[A^\star_N\right]$ in powers of η (see [9, 10, 2]):

$$\mathbb{E}\left[A^\star_N\right] = A^\star_{\rm per} + \eta A_1^{\star,N} + \eta^2 A_2^{\star,N} + \cdots, \tag{12}$$

where

$$\begin{aligned}
A_1^{\star,N} e_i &= \int_{Q_N} A_1(\nabla w^{1,N}_{e_i} + e_i) - \int_{Q_N} A_{\rm per}(\nabla w^0_{e_i} + e_i), \\
A_2^{\star,N} e_i &= \frac{1}{2}\sum_{s=1}^{N^d-1} \left(\int_{Q_N} A_2^{1,s}(\nabla w^{2,s,N}_{e_i} + e_i) - 2\int_{Q_N} A_1(\nabla w^{1,N}_{e_i} + e_i) \right. \\
&\qquad \left. + \int_{Q_N} A_{\rm per}(\nabla w^0_{e_i} + e_i) \right),
\end{aligned} \tag{13}$$

where w_p^0 is the corrector associated to $A_{\rm per}$ (perfect material), solution to

$$-\mathrm{div}\left[A_{\rm per}\left(p+\nabla w_p^0\right)\right]=0, \quad w_p^0 \text{ is } Q\text{-periodic}, \tag{14}$$

and $w_p^{1,N}$ is the corrector associated to $A_1 = A_{\rm per} + \mathbf{1}_Q C_{\rm per}$ (material with one defect):

$$-\mathrm{div}\left[A_1\left(p+\nabla w_p^{1,N}\right)\right]=0, \quad w_p^{1,N} \text{ is } Q_N\text{-periodic}. \tag{15}$$

In turn, $w_p^{2,s,N}$ is the corrector associated to $A_2^{1,s} = A_{\rm per} + \mathbf{1}_Q C_{\rm per} + \mathbf{1}_{Q+s} C_{\rm per}$ (material with two defects, located in Q and $Q+s$):

$$-\mathrm{div}\left[A_2^{1,s}\left(p+\nabla w_p^{2,s,N}\right)\right]=0, \quad w_p^{2,s,N} \text{ is } Q_N\text{-periodic}. \tag{16}$$

Note that the periodic boundary conditions in (15)-(16) allow us to assume, without loss of generality, that the first defect is located in the cell Q.

It has been shown numerically in [9, 10] that the expansion (12) is not only valid in the asymptotic regime $\eta \ll 1$, but also for practical small values of η. In some cases, the expansion is even valid for values of η as large as 0.5, in which case the random variables B_η^k take value 0 and 1 with equal probability.

Note that the computation of $A_2^{\star,N}$, when necessary, requires to solve the corrector problems (16) for any value of s (the position of the second defect). In the sequel, we propose to use a Reduced Basis approach to solve these $N^d - 1$ problems, that are parameterized by s.

All the results of this section are illustrated with the same two-dimensional numerical example, that we now introduce. We take

$$A_{\rm per}(x,y) = 20\,\mathrm{Id}_2 + 100 \sum_{k\in\mathbb{Z}^2} \mathbf{1}_{Q+k}(x,y)\sin^2(\pi x)\sin^2(\pi y)\,\mathrm{Id}_2$$

and

$$C_{\rm per}(x,y) = -100 \sum_{k\in\mathbb{Z}^2} \mathbf{1}_{Q+k}(x,y)\sin^2(\pi x)\sin^2(\pi y)\,\mathrm{Id}_2.$$

In line with Figure 1, this test case represents a material with constant properties, reinforced by a periodic lattice of circular inclusions. Loosely speaking, the perturbation consists in randomly eliminating some fibers. See Figure 2 for a particular realization of the material.

In the sequel, we focus on the first entry $[A_N^\star]_{11}$ of the homogenized matrix. We thus set $p = e_1$ in (14), (15) and (16). These corrector problems are numerically solved using a mesh of size $h = 1/10$. Qualitatively similar conclusions are obtained with the other entries.

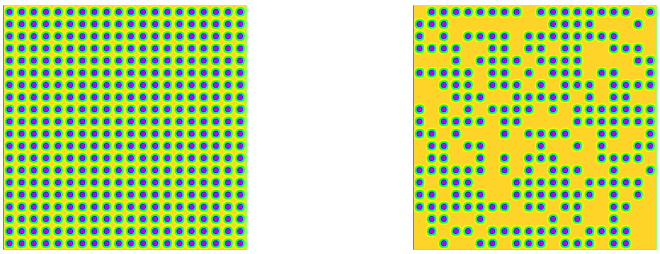

Figure 2: Left: the perfect (periodic) material. Right: a realization of the material with some defects.

4.2 Difficulties

In [6], we propose to use a Reduced Basis approach to speed-up the computation of the family of problems (16) parameterized by s, the weak form of which is

$$\forall v \in H^1_{\text{per}}(\mathbb{R}^d), \quad a(w_p^{2,s,N}, v; s) = b_p(v), \tag{17}$$

where

$$a(u, v; s) := \int_{Q_N} (\nabla v)^T \, A_2^{1,s} \, \nabla u \quad \text{and} \quad b_p(v) := \int_{Q_N} (\nabla v)^T \, A_2^{1,s} \, p.$$

The Reduced Basis approach (see [13] for a presentation of the method in the stochastic case) can be understood as a way to approximate the set of functions

$$\mathcal{E} := \left\{ w_p^{2,s,N}, 1 \leq s \leq N^d - 1 \right\}$$

by an element in the space

$$X_M = \text{Span}\{w_p^{2,s_m,N}, 1 \leq m \leq M\}, \tag{18}$$

for some well-chosen values of s_m, $1 \leq s_m \leq N^d - 1$. This approach is efficient if we can choose a *small* value for the dimension M of X_M, while maintaining accuracy.

Once X_M has been defined, we approximate the solution of (17) using a standard Galerkin approximation on X_M: we approximate $w_p^{2,s,N}$ by $w_p^{2,s,N,M} \in X_M$, solution to

$$\forall v_M \in X_M, \quad a(w_p^{2,s,N,M}, v_M; s) = b_p(v_M). \tag{19}$$

The construction of X_M is performed beforehand by computing the solution of (17) for some values of the parameter s. The set of appropriate parameters $\{s_m\}_{1\leq m\leq M}$ is selected using a standard procedure, called the Greedy procedure. The Reduced Basis approach is expected to be efficient because M is small (the problem (19) is hence posed in a low-dimensional space, and thus easy to solve) and because there are $N^d - 1$ problems (17) to be solved.

Blindly applied to the family of problems (17), the Reduced Basis approach is not efficient, because we would have to take M of the order of N^d. The reason is the following. We first compute the solution of the problem (17) for all the different values of the parameter s, and then proceed with a Proper Orthogonal Decomposition of the family $\left(w_p^{2,s,N}\right)_{1\leq s\leq N^2-1}$ for the H^1 scalar product. We then look at the decay of the spectrum, which is shown on Figure 3. We observe no decay of the spectrum, which indicates that the functions $w_p^{2,s,N}$ are linearly independent. There is no good structure in that family, and therefore we would need to choose M of the order of N^d to accurately approximate the functions in $\mathcal{E}$ by an element in X_M. There is thus no speed-up. The appropriate way of applying the Reduced Basis approach is described in Section 4.3.1.

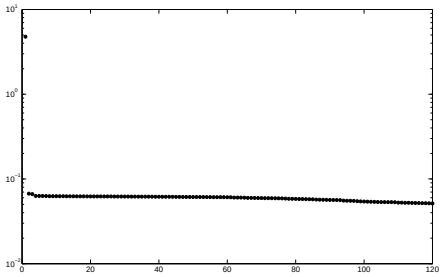

Figure 3: POD (using the H^1 scalar product) of the family $\left(w_p^{2,s,N}\right)_{1\leq s\leq N^2-1}$, for $N = 11$.

A second difficulty is that the Reduced Basis approach requires an *a posteriori* error estimator, both to select the appropriate values of s_m in (18), and to assess the quality of the final outcome. In our particular context, because of the specificities of our problem, the computation of the classical error estimator turns out to be prohibitively expensive. We describe in Section 4.3.2 a way to circumvent this difficulty.

4.3 Adjustment of the Reduced Basis approach

In this section, we show how to address the two difficulties underlined above.

4.3.1 Building a family of functions with a good structure

We have seen above that there is no good structure in the family of functions $w_p^{2,s,N}$. In this section, we rewrite these functions as linear combinations of the functions $\left(\overline{w}_p^{2,s,N}\right)_{1\leq s\leq N^d-1}$ and $\left(\widetilde{w}_p^{2,s,N}\right)_{1\leq s\leq N^d-1}$ defined below. The interest is that these two latter families have a good structure.

To build these good families, we begin by introducing

$$\begin{aligned}\overline{w}_p^{1,N} &= w_p^{1,N} - w_p^0,\\ \overline{w}_p^{2,s,N} &= w_p^{2,s,N} - w_p^{1,N} - w_p^{1,N}(\cdot - s) + w_p^0,\end{aligned}$$

where w_p^0, $w_p^{1,N}$ and $w_p^{2,s,N}$ are defined by (14), (15) and (16), respectively. Heuristically, this amounts to subtracting the appropriate reference function from the correctors $w_p^{1,N}$ and $w_p^{2,s,N}$. One can show that $\overline{w}_p^{1,N}$ and $\overline{w}_p^{2,s,N}$ go to 0 at infinity, and are hence essentially supported in a compact domain, in contrast to $w_p^{1,N}$ and $w_p^{2,s,N}$. We see that $\overline{w}_p^{1,N}$ is solution to

$$\begin{cases} -\operatorname{div}\left(A_1\nabla\overline{w}_p^{1,N}\right) = \operatorname{div}(\mathbf{1}_Q C_{\rm per}(\nabla w_p^0 + p)),\\ \overline{w}_p^{1,N} \quad Q_N-\text{periodic},\end{cases}$$

and $\overline{w}_p^{2,s,N}$ is solution to

$$\begin{cases} -\operatorname{div}\left(A_2^{1,s}\nabla\overline{w}_p^{2,s,N}\right) = \operatorname{div}\left(\mathbf{1}_{\{Q+s\}} C_{\rm per}\nabla\overline{w}_p^{1,N}\right) + \operatorname{div}\left(\mathbf{1}_Q C_{\rm per}\nabla\overline{w}_p^{1,N}(\cdot - s)\right),\\ \overline{w}_p^{2,s,N} \quad Q_N-\text{periodic}.\end{cases} \tag{20}$$

We next use the linearity of (20), and rewrite $\overline{w}_p^{2,s,N}$ as

$$\overline{w}_p^{2,s,N} = \widehat{w}_p^{2,s,N} + \widetilde{w}_p^{2,s,N},$$

where $\widehat{w}_p^{2,s,N}$ solves

$$\begin{cases} -\operatorname{div}\left(A_2^{1,s}\nabla\widehat{w}_p^{2,s,N}\right) = \operatorname{div}\left((\mathbf{1}_{\{Q+s\}} C_{\rm per}\nabla\overline{w}_p^{1,N}\right),\\ \widehat{w}_p^{2,s,N} \quad Q_N-\text{periodic},\end{cases}$$

and $\widetilde{w}_p^{2,s,N}$ solves

$$\begin{cases} -\operatorname{div}\left(A_2^{1,s}\nabla\widetilde{w}_p^{2,s,N}\right) = \operatorname{div}\left(\mathbf{1}_Q C_{\rm per}\nabla\overline{w}_p^{1,N}(\cdot - s)\right), \\ \widetilde{w}_p^{2,s,N} \quad Q_N - \text{periodic.} \end{cases}$$

Due to the periodic boundary conditions, we have $\widetilde{w}_p^{2,s,N} = \widehat{w}_p^{2,-s,N}(\cdot - s)$. After tedious but straightforward computations, and assuming for the sake of simplicity that $A_{\rm per}$ is symmetric, we recast the matrix $A_2^{\star,N}$ defined by (13) as

$$\left(A_2^{\star,N}\right)_{ij} = \sum_{s=1}^{N^2-1}\int_{Q_N}(\mathbf{1}_Q + \mathbf{1}_{Q+s})(\nabla w_{e_j}^0 + e_j)^T C_{\rm per}\nabla\widetilde{w}_{e_i}^{2,s,N} + \int_Q (\nabla w_{e_j}^0 + e_j)^T C_{\rm per}\nabla\overline{w}_{e_i}^{1,N}(\cdot - s).$$

Only the functions $\overline{w}_p^{1,N}$ and $\left\{\widetilde{w}_p^{2,s,N}\right\}_{1\le s\le N^d-1}$ are needed to evaluate $A_2^{\star,N}$. A similar formula holds if $A_{\rm per}$ is not symmetric, up to slight modifications.

We now numerically test for the linear independence, or dependence, of the functions $\left(\overline{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$ and $\left(\widetilde{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$, with $N = 11$. There are $N^2-1 = 120$ functions is each family. We compute the POD of the family $\left(\overline{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$ and of the family $\left(\widetilde{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$, and plot in Figure 4 the 120 POD eigenvalues in decreasing order.

In contrast to Figure 3, we now observe a decay in the eigenvalues. There is a good structure in both families $\left(\widetilde{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$ and $\left(\overline{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$. Therefore, much fewer vectors are needed to approximate these families than for approximating the family $\left(w_p^{2,s,N}\right)_{1\le s\le N^2-1}$ considered in Section 4.2. Otherwise stated, we expect that the dimension of the Reduced Basis approximation space that we will need is low, in contrast to the situation of Section 4.2. Note also that the decay is somewhat stronger for the family $\left(\widetilde{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$ than for $\left(\overline{w}_p^{2,s,N}\right)_{1\le s\le N^2-1}$.

4.3.2 Modifying the error estimator

We now address the second difficulty identified at the end of Section 4.2, related to the classical *a posteriori* estimator, and suggest an alternative estimator, better suited to our context here.

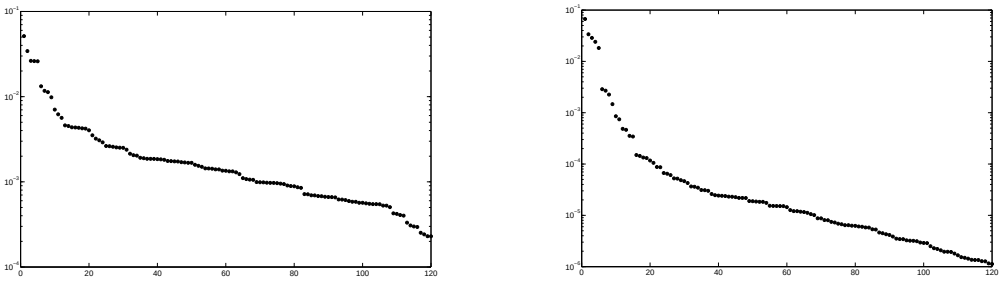

Figure 4: POD (using the H^1 scalar product) of the family $\left(\overline{w}_p^{2,s,N}\right)_{1\leq s\leq N^2-1}$ (left) and of the family $\left(\widetilde{w}_p^{2,s,N}\right)_{1\leq s\leq N^2-1}$ (right), for $N = 11$.

The idea is to use the ℓ^2 norm of the discrete residual, rather than the classical estimator, based on the norm of the dual of the residual. Let us denote $\mathcal{W}_h := \text{span}(\phi_i)$ the finite element space used to solve the problem (16), in the reference approach. We define the ith component of the discrete residual as

$$G_i^m(s) := a(w_p^{2,s,N,m}, \phi_i; s) - b_p(\phi_i),$$

where $w_p^{2,s,N,m}$ is the approximation of the solution to (16) computed using the approximation space X_m (see (19)). In the sequel, we work with the error estimator

$$\widetilde{\Delta}_m(s) := \|G^m(s)\|_{\ell^2} = \sqrt{\sum_i \left[G_i^m(s)\right]^2}.$$

The classical error estimator is denoted $\Delta_m(s)$.

4.4 Numerical results

We collect here numerical results that demonstrate the efficiency of our approach.

We first compute the relative error on $A_2^{\star,N}$ between the reference value (13) and its approximation obtained using the Reduced Basis approach, for different values of the dimension M of the approximation space X_M. In Figure 5, we plot this indicator for two components of the matrix $A_2^{\star,N}$. We observe that, for both estimators $\Delta_m(s)$ and $\widetilde{\Delta}_m(s)$, the accuracy improves rapidly with M. Choosing a value for M of the order of 20 is enough to obtain a good accuracy. Since this value is much smaller that the total number of functions

to compute, which is here $N^2 - 1 = 120$, we obtain a good computational speed-up.

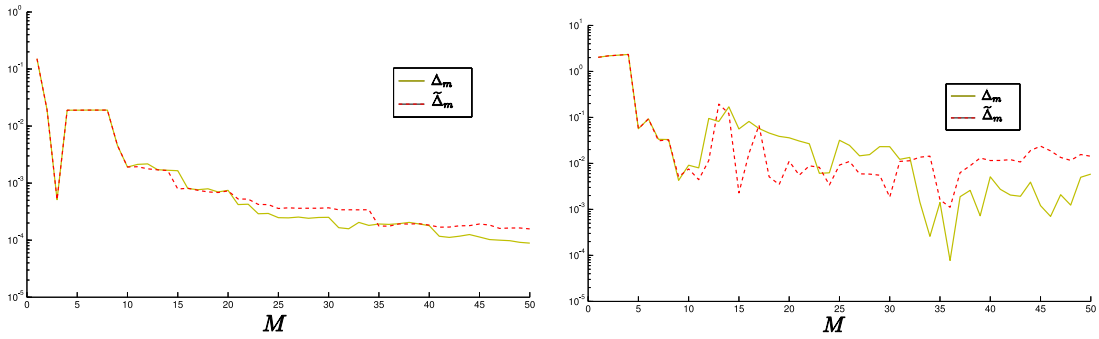

Figure 5: Relative error on $A_2^{\star,N}$ as a function of the dimension M of the Reduced Basis space X_M. Left: $(A_2^{\star,N})_{11}$. Right: $(A_2^{\star,N})_{12}$.

Next, in Figure 6, we plot the indicator

$$e(m) := \max_{1 \leq s \leq N^2-1} \left(\frac{\|\nabla w_p^{2,s,N} - \nabla w_p^{2,s,N,m}\|_{L^2(Q_N)}}{\|\nabla w_p^{2,s,N}\|_{L^2(Q_N)}} \right), \tag{21}$$

for the two Reduced Basis approaches (using the error estimators Δ_m or $\widetilde{\Delta}_m$). In both cases, we observe a significant decay of $e(m)$ as a function of m. Starting from an error of 100% with $m = 1$ (the Reduced Basis space is of dimension one), we see that the error decreases down to 2% for $M \approx 20$. As above, we hence see that a *small* value of M is sufficient to ensure accuracy, hence the computational speed-up.

On Figure 7, we show in which order the relevant cells (i.e. parameters s_m) are selected by the Greedy procedure. We compare in this matter the two error estimators. We observe that, although the actual order may vary, the two estimators provide the same set of parameters $\{s_m\}_{1 \leq m \leq M}$, both for the eight and the twenty best parameters.

5 A variant of stochastic homogenization

[Work expanded in [7].]

As announced in the previous report [3], we have considered a variant of the classical setting of stochastic homogenization, originally introduced a

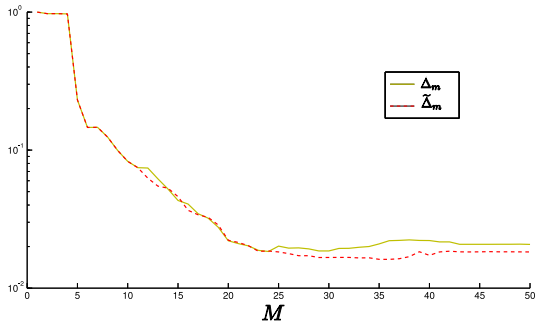

Figure 6: Relative error (21) on the two-defects correctors $w_p^{2,s,N}$. The magnitude of the residual error for large M (of the order of 2 %) is close to the Finite Element error.

		19	20	11		
	15	8	4	6	12	
	10	1		2	9	
	14	5	3	7	17	
		18	16	13		

		12	20	16		
	14	7	4	6	13	
	9	1		2	10	
	18	5	3	8	17	
		11	15	19		

Figure 7: Ordering of the cells selected by the Greedy procedure, for the two error estimators, $\Delta_m(s)$ (left) and $\widetilde{\Delta}_m(s)$ (right).

few years ago in [11, 12]. The equation under consideration is (1), where the matrix A is the composition of a periodic matrix A_{per} with a stochastic diffeomorphism Φ:

$$A\left(\frac{x}{\varepsilon},\omega\right) := A_{\text{per}}\left[\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right]. \tag{22}$$

We assume that, almost surely, the map $\Phi(\cdot,\omega)$ is a well-behaved diffeomorphism (in the sense that $\text{EssInf}_{\omega\in\Omega,x\in\mathbb{R}^d}\left(\det(\nabla\Phi(x,\omega))\right) = \nu > 0$ and $\text{EssSup}_{\omega\in\Omega,x\in\mathbb{R}^d}\left|\nabla\Phi(x,\omega)\right| = M < +\infty$), and that it satisfies

$$\nabla\Phi \text{ is stationary.} \tag{23}$$

Formally, such a setting is well suited to model materials that are periodic, in a given reference configuration. The latter is only known up to a cer-

tain randomness. Materials we have in mind are ideally periodic materials, where some random deformation has been introduced, for instance during the manufacturing process. Assumption (23) means that $\nabla\Phi$ is statistically homogeneous, i.e. the randomness is the same anywhere in the material.

The problem (1)-(22) admits a homogenized limit when ε vanishes. It is indeed shown in [11] that, under the above assumptions, $u^\varepsilon(\cdot,\omega)$ solution to (1)-(22) converges as ε goes to 0 to $u^\star$, solution to the homogenized problem (2). The homogenized matrix $A^\star$ is given by, for any $1 \leq i,j \leq d$,

$$A^\star_{ij} = \det\left(\mathbb{E}\left(\int_Q \nabla\Phi(y,\cdot)dy\right)\right)^{-1} \times \mathbb{E}\left(\int_{\Phi(Q,\cdot)} e_i^T A_{\rm per}\left(\Phi^{-1}(y,\cdot)\right)\left(e_j + \nabla w_{e_j}(y,\cdot)\right) dy\right), \quad (24)$$

where $Q = (0,1)^d$ and where, for any $p \in \mathbb{R}^d$, w_p solves the corrector problem

$$\left\{\begin{array}{l} -\mathrm{div}\left[A_{\rm per}\left(\Phi^{-1}(y,\omega)\right)\left(p + \nabla w_p(y,\omega)\right)\right] = 0 \text{ in } \mathbb{R}^d, \\ w_p(y,\omega) = \widetilde{w}_p(\Phi^{-1}(y,\omega),\omega), \quad \nabla\widetilde{w}_p \text{ is stationary}, \\ \mathbb{E}\left(\displaystyle\int_{\Phi(Q,\cdot)} \nabla w_p(y,\cdot)dy\right) = 0. \end{array}\right. \quad (25)$$

The first question we address in [7] is to precisely understand the behavior of $u^\varepsilon(x,\omega) - u^\star(x)$ when ε goes to 0, where u^ε is the solution to the highly oscillating problem and $u^\star$ the solution to the homogenized problem. In the classical random ergodic setting, the convergence of $\dfrac{u^\varepsilon(x,\omega) - u^\star(x)}{\sqrt{\varepsilon}}$ to a Gaussian process has been shown in [16, 18] for the one-dimensional case. We show in [7] a similar result, for the variant we consider here.

We have also investigated the question of how to approximate the homogenized matrix (24) in practice. Note indeed that the corrector problem (25) is posed on the entire space $\mathbb{R}^d$, and thus challenging to solve. In the classical context, described in Section 2, the corrector problem (3) is also posed on $\mathbb{R}^d$, and a standard procedure is to solve the corrector problem on a truncated domain $Q_N = (-N,N)^d$ (see (4)). The convergence of the procedure when $N \to \infty$ is given by [17, Theorem 1]. In [7], we perform a similar analysis in the context of (24)-(25). In the following, we first describe a numerical strategy to approximate the homogenized matrix $A^\star$, which was first introduced in [14]. We next provide an example of numerical results, before turning to the analysis of the approach.

Derivation of the truncated problem The weak formulation of the corrector problem (25) reads as follows (see [11]): for all $\widetilde{\psi}$ stationary, we have

$$\mathbb{E}\left(\int_{\Phi(Q,\cdot)} (\nabla\psi(y))^T A_{\rm per}\left(\Phi^{-1}(y,\omega)\right)\left(p+\nabla w_p(y,\omega)\right)dy\right)=0,$$

where $\psi=\widetilde{\psi}\circ\Phi^{-1}$. The above expression can be rewritten, after a change of variables, as

$$\mathbb{E}\left[\int_Q \det(\nabla\Phi)\left(\nabla\widetilde{\psi}\right)^T(\nabla\Phi)^{-T}A_{\rm per}\left(p+(\nabla\Phi)^{-1}\nabla\widetilde{w}_p\right)\right]=0.$$

As $\widetilde{\psi}$, $\nabla\Phi$, A_{per} and $\nabla\widetilde{w}_p$ are stationary, this equivalently reads, because of the ergodic theorem,

$$\lim_{N\to\infty}\frac{1}{|Q_N|}\int_{Q_N}\det(\nabla\Phi)\left(\nabla\widetilde{\psi}\right)^T(\nabla\Phi)^{-T}A_{\rm per}\left(p+(\nabla\Phi)^{-1}\nabla\widetilde{w}_p\right)=0.$$

At fixed N, we now define the approximate corrector $\widetilde{w}_p^N$ as the Q_N-periodic function satisfying

$$\int_{Q_N}\det(\nabla\Phi)\left(\nabla\widetilde{\psi}\right)^T(\nabla\phi)^{-T}A_{\rm per}\left(p+(\nabla\phi)^{-1}\nabla\widetilde{w}_p^N\right)=0$$

for all $\widetilde{\psi}$ Q_N-periodic, or, equivalently,

$$\left\{\begin{array}{l} -\mathrm{div}\left[\det(\nabla\Phi)(\nabla\phi)^{-T}A_{\rm per}\left(p+(\nabla\phi)^{-1}\nabla\widetilde{w}_p^N\right)\right]=0,\\ \widetilde{w}_p^N(\cdot,\omega)\text{ is }Q_N\text{-periodic.}\end{array}\right. \tag{26}$$

In turn, we approximate the homogenized matrix $A^\star$ defined by (24) by, for any $1\le i,j\le d$,

$$\begin{aligned}[A_N^\star(\omega)]_{ij}=\det\left(\frac{1}{|Q_N|}\int_{Q_N}\nabla\phi(\cdot,\omega)\right)^{-1}\times\\ \frac{1}{|Q_N|}\int_{\phi(Q_N,\omega)} e_i^T A_{\rm per}\left(\phi^{-1}(y,\omega)\right)\left(e_j+\nabla w_{e_j}^N(y,\omega)\right)dy\end{aligned} \tag{27}$$

where $w_p^N(y,\omega)=\widetilde{w}_p^N(\phi^{-1}(y,\omega),\omega)$. Note that, as is standard when approximating the homogenized matrix of stochastic elliptic problems, the approximation $A_N^\star(\omega)$ is a *random* matrix, even though the exact homogenized matrix (24) is deterministic. This is a by-product of working on the *truncated* domain Q_N rather than $\mathbb{R}^d$.

Numerical illustration Some numerical tests following our strategy (26)-(27) are reported in [2, Section 3.2]. We reproduce here some of them.

Consider the following two dimensional test-case: we give ourselves two families $(X_k)_{k\in\mathbb{Z}}$ and $(Y_k)_{k\in\mathbb{Z}}$ of i.i.d. random variables, all sharing the uniform law $\mathcal{U}([a,b])$, with $a = -2.25$ and $b = 5.75$. We then consider the diffeomorphism $\Phi(x,\omega) = 6\,x + \Psi(x,\omega)$, with $x = (x_1,x_2) \in \mathbb{R}^2$, $\Psi(x,\omega) = (\psi_X(x_1,\omega),\psi_Y(x_2,\omega))$, where

$$\psi_X(x_1,\omega) = \sum_{k\in\mathbb{Z}} 1_{[k,k+1[}(x_1)\left(\sum_{q=0}^{k-1} X_q(\omega) + 2X_k(\omega)\int_k^{x_1}\sin^2(2\pi t)\,dt\right),$$

and likewise for ψ_Y. The periodic matrix A_{per} is defined, for all $x \in Q$, by

$$A_{per}(x) = a_{\rm per}(x)\,{\rm Id}_2, \quad a_{\rm per}(x_1,x_2) = \beta + (\alpha-\beta)\sin^2(\pi x_1)\sin^2(\pi x_2),$$

with $\alpha = 10$ and $\beta = 1$. The results obtained with (26)-(27) are shown on Fig. 8. We indeed observe the convergence of our approximation as $N \to \infty$.

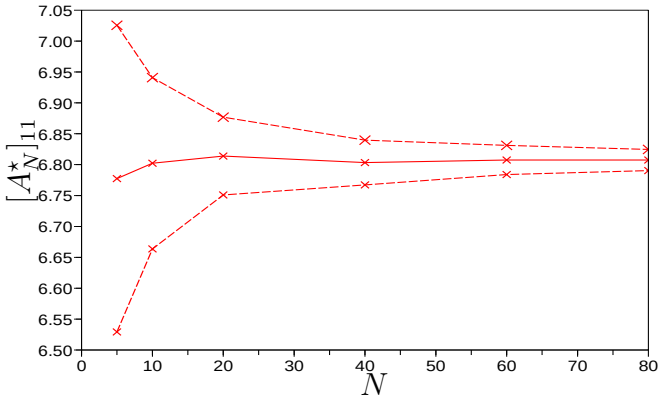

Figure 8: For any N, following (26)-(27), we compute several realizations of $A^\star_N(\omega)$, and build from these a confidence interval for $\mathbb{E}\,[(A^\star_N)_{11}]$.

Convergence of the numerical strategy In [7], we study the convergence of our approach, as $N \to \infty$. We obtained the following result, which generalizes [17, Theorem 1] (see (5) above) to the variant we consider here.

Theorem 1 *Let Φ be a diffeomorphism that satisfies* (23)*, and $A_{\rm per}$ be a periodic, coercive and bounded matrix. Then the random matrix $A_N^\star(\omega)$ defined by* (27) *converges almost surely when $N \to \infty$ to the deterministic homogenized matrix $A^\star$ defined by* (24)*.*

6 Conclusions and agenda for the third year of contract

We summarize here the directions of research we wish to pursue during the third year of contract.

A first track is to develop a MsFEM-type approach for random materials modelled by (1)-(22) (see Section 5). Our idea relies on approximating the solution to the corrector problem (25) by the periodic corrector (associated to the periodic matrix $A_{\rm per}$) composed with the random diffeomorphism Φ. The advantage of this approximation is that, for any new realization of Φ, we do not have to recompute the corrector. We have developed a MsFEM-type approach using this approximation, and have performed some preliminary numerical experiments, that yield encouraging results. More comprehensive tests are yet needed to better understand the capabilities of this approach.

A second direction concerns the use of Reduced Basis methods in a multiscale context. We have seen in Section 4 that the Reduced Basis approach can be used to speed-up the computation of the corrector problems. In the next future, we would like to apply this approach in the context of the spectral multiscale method introduced by Y. Efendiev and J. Galvis [20].

The spectral multiscale method is designed to address the highly oscillatory problem (8) in the case when the ratio between the maximum and the minimum values of A^ε is large (high contrast problem). The main idea is to complement the standard MsFEM approximation space $\mathcal{W}_h = \text{Span } \{\phi_i^\varepsilon\}$ (where ϕ_i^ε are the MsFEM basis functions, see Section 3 above) with eigenfunctions that correspond to small eigenvalues. More precisely, consider the local eigenvalue problem

$$-\text{div}\,[A^\varepsilon \nabla \psi_\ell^{\omega_i}] = \lambda_\ell \widetilde{A}^\varepsilon \psi_\ell^{\omega_i} \text{ in } \omega_i, \tag{28}$$

with homogeneous Neumann boundary conditions, where $\omega_i := \text{supp}(\phi_i^\varepsilon)$ is the support of the MsFEM highly oscillatory basis functions ϕ_i^ε and where

the weight $\widetilde{A}^\varepsilon$ is defined by $\widetilde{A}^\varepsilon = \dfrac{1}{h^2}\left(\sum_i |\nabla \phi_i^\varepsilon|^2\right) A^\varepsilon$. Note that, by definition, the first eigenvalue $\lambda_{\ell=0}$ is exactly zero, and the eigenvector $\psi_{\ell=0}^{\omega_i}$ associated to that eigenvalue is constant in ω_i. We then select the eigenvectors $\psi_\ell^{\omega_i}$ associated with an eigenvalue λ_ℓ below a certain threshold $\tau \geq 0$, and construct the so-called spectral multiscale basis functions

$$\chi_{i,\ell}^\varepsilon := \phi_i^\varepsilon \, \psi_\ell^{\omega_i}.$$

The spectral multiscale method consists in performing a Galerkin approximation of (8) on the approximation space $\mathcal{W} := \mathrm{Span}(\chi_{i,\ell}^\varepsilon)$. Note that, since $\psi_{\ell=0}^{\omega_i}$ is a constant function, the function $\chi_{i,\ell=0}^\varepsilon$ is proportional to ϕ_i^ε. Hence the space $\mathcal{W}$ contains the standard MsFEM approximation space $\mathrm{Span}(\phi_i^\varepsilon)$.

Our project is to use the Reduced Basis approach to more efficiently compute the eigenfunctions $\psi_\ell^{\omega_i}$ needed to build $\mathcal{W}$.

References

References authored by the investigators in the context of the contrat

[1] A. Anantharaman, X. Blanc and F. Legoll, *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, submitted, preprint available on `arXiv`.

[2] A. Anantharaman, R. Costaouec, C. Le Bris, F. Legoll and F. Thomines, *Introduction to numerical stochastic homogenization and the related computational challenges: some recent developments*, Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, Volume 22, 2011.

[3] C. Le Bris, F. Legoll and F. Thomines, *Multiscale problems in materials science: a mathematical approach to the role of uncertainty*, Report 2010 to the European Office of Aerospace Research and Development (EOARD), 2010.

[4] C. Le Bris, F. Legoll and F. Thomines, *Multiscale finite element approach for "weakly" random problems and related issues*, submitted, preprint available on `arXiv`.

[5] C. Le Bris, F. Legoll and F. Thomines, *Rate of convergence of a two-scale expansion for some weakly stochastic homogenization problems*, submitted, preprint available on `arXiv`.

[6] C. Le Bris and F. Thomines, *Reduced Basis method for weakly random media*, Series in Contemporary Applied Mathematics, P. G. Ciarlet and T.-T. Li Eds., Higher Education Press and World Scientific Publishing, in preparation.

[7] F. Legoll and F. Thomines, *Convergence of the residual process of a variant of stochastic homogenization in dimension one*, in preparation.

References authored by the investigators and not related to the contract

[8] A. Anantharaman and C. Le Bris, *Homogénéisation d'un matériau périodique faiblement perturbé aléatoirement [Homogenization of a weakly randomly perturbed periodic material]*, C. R. Acad. Sci. Série I, 348:529–534, 2010.

[9] A. Anantharaman and C. Le Bris, *A numerical approach related to defect-type theories for some weakly random problems in homogenization*, SIAM Multiscale Modeling & Simulation, 9(2):513-544, 2011.

[10] A. Anantharaman and C. Le Bris, *Elements of mathematical foundations for a numerical approach for weakly random homogenization problems*, Communications in Computational Physics, to appear, preprint available on `arXiv`.

[11] X. Blanc, C. Le Bris and P.-L. Lions, *Une variante de la théorie de l'homogénéisation stochastique des opérateurs elliptiques [A variant of stochastic homogenization theory for elliptic operators]*, C. R. Acad. Sci. Série I, 343:717–724, 2006.

[12] X. Blanc, C. Le Bris and P.-L. Lions, *Stochastic homogenization and random lattices*, Journal de Mathématiques Pures et Appliquées, 88:34–63, 2007.

[13] S. Boyaval, C. Le Bris, T. Lelièvre, Y. Maday, N. Nguyen, and A. Patera, *Reduced basis techniques for stochastic problems*, Archives of Computational Methods in Engineering, 17:435-454, 2010.

[14] R. Costaouec, C. Le Bris and F. Legoll, *Approximation numérique d'une classe de problèmes en homogénéisation stochastique [Numerical approximation of a class of problems in stochastic homogenization]*, C. R. Acad. Sci. Série I, 348:99–103, 2010.

[15] C. Le Bris, *Some numerical approaches for "weakly" random homogenization*, in Numerical Mathematics and Advanced Applications 2009, Proceedings of ENUMATH 2009, G. Kreiss, P. Lötstedt, A. Malqvist and M. Neytcheva Eds., pp. 29–45, Lecture Notes in Computational Science and Engineering, Springer, 2010.

General references by other authors

[16] G. Bal, J. Garnier, S. Motsch and V. Perrier, *Random integrals and correctors in homogenization*, Asymptotic Analysis, 59(1-2):1–26, 2008.

[17] A. Bourgeat and A. Piatnitski, *Approximation of effective coefficients in stochastic homogenization*, Ann I. H. Poincaré - PR, 40(2):153–165, 2004.

[18] A. Bourgeat and A. Piatnitski, *Estimates in probability of the residual between the random and the homogenized solutions of one-dimensional second-order operator*, Asymptotic Analysis, 21(3-4):303–315, 1999.

[19] W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden, *Heterogeneous multiscale methods: a review*, Comm. Comput. Phys., 2(3):367–450, 2007.

[20] Y. Efendiev, J. Galvis and X-H. Wu, *Multiscale finite element methods for high-contrast problems using local spectral basis functions*, Journal of Computational Physics, 230(4):937-955, 2011.

[21] Y.R. Efendiev, T.Y. Hou and X.-H. Wu, *Convergence of a nonconforming multiscale finite element method*, SIAM Journal on Numerical Analysis, 37(3):888–910, 2000.

Contract FA 8655-10-C-4002

Multiscale problems in materials science: a mathematical approach to the role of uncertainty

Report 2010 to the European Office of Aerospace Research and Development (EOARD)

C. Le Bris, F. Legoll, F. Thomines

October 2010

Contents

Summary

We report here on the work performed during the first year (october 2009 - october 2010) of the contract FA 8655-10-C-4002 on *Multiscale problems in materials science: a mathematical approach to the role of uncertainty*.

The bottom line of our work is to develop *affordable numerical methods* in the context of *stochastic homogenization*. Many partial differential equations of materials science indeed involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems (and the associated stochastic homogenization theory) are one instance for modelling uncertainty in continuous media. The theoretical aspects of these problems are now well-understood, at least for a large variety of situations.

On the other hand, the numerical aspects have received less attention from the mathematics community. Standard methods available in the literature often lead to very, and sometimes prohibitively, costly computations.

In this report, we first review an approach popular in particular in the computational mechanics community, which is to try and obtain *bounds* on the homogenized matrix, rather than computing it. Only computations of moderate difficulty are then required. However, we will show that, not unexpectedly, this method has strong limitations.

We will next introduce a class of materials of significant practical relevance, that of random materials where the amount of randomness is *small*. They can be considered as *stochastic perturbations of deterministic materials*, in a sense made precise below. We will adapt to such a case the well-known Multiscale Finite Element Method (MsFEM), and design a method which is much more affordable than, and as accurate as, the original method.

The works described below have been performed by Claude Le Bris (PI), Frédéric Legoll (Co-PI), and Florian Thomines (first year Ph.D. student).

1 Introduction

Many partial differential equations of materials science involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems are one of the most famous instances of mathematical uncertainty of continuous media. However, the elaborate tools and techniques of (i) mathematical probability, stochastic analysis, and (ii) numerical analysis and large-scale computing have not yet permitted practical computations. These are most often accomplished otherwise by the engineering community, using more traditional approaches. Despite definite achievements by leading experts, numerical analysis of stochastic, and more generally speaking non periodic, homogenization problems remains in its infancy.

The purpose of this report is to present the recent progress we have made during last year on this topic, with the aim *to make numerical random homogenization more practical*. Because we cannot embrace all difficulties at once, the case under consideration here is a *simple, linear, scalar second order elliptic partial differential equation in divergence form*, for which a sound

theoretical groundwork exists. We focus here on different practical computational approaches.

This report begins, in Section 2, with a brief introduction to stochastic homogenization. There is of course no novelty in such an introduction, the only purpose of which is the consistency of this report and the convenience of the reader not familiar with the theory. We will recall there why stochastic homogenization often leads to extremely expensive computations.

In Section 3, we describe a classical approach from the applied communities, which is to try and obtain *bounds* on the homogenized matrix, rather than computing it. The computational gain is evident. We will report on some numerical experiments. Such experiments are likely to not be new. But they at least show, quantitatively and qualitatively, the strong limitations of such an approach.

As pointed out above, random homogenization for general stochastic materials is very costly. Yet, it turns out that it is possible to identify classes of materials of significant practical relevance, where stochastic homogenization theory and practice can be reduced to more affordable, less computationally demanding problems. These materials are neither periodic (because such an oversimplifying assumption is rarely met in practice), nor fully stochastic. They can be considered as an intermediate case, that of *stochastic perturbations of deterministic (possibly periodic) materials*. The case when the tensor describing the properties of the material is the sum of a periodic term and a small random term is an instance of such an approach. In Section 4, we show that we can adapt to that particular setting the well-known Multiscale Finite Element Method (MsFEM), which is designed to directly address the highly oscillating elliptic problem, rather than studying the limit problem when the typical small lengthscale goes to 0. This method has been initially proposed for deterministic problems [24, 21, 22, 14], and has been recently adapted to the stochastic setting [18]. It then leads to extremely intensive computations. We show in the sequel that, if the problem is only weakly stochastic, then it is possible to design a method as accurate as the original MsFEM, with a much smaller computational cost. As we explain below, this method is accurate provided the stochastic perturbation is indeed small.

We collect in Section 5 some conclusions about the work performed so far, and future directions for the next two years of contract.

2 Basics of stochastic homogenization

[Detailed presentation can be read in [1].]

Stochastic homogenization is best understood in the light of the easiest context of homogenization: *periodic* homogenization. This is the reason why we begin with Section 2.1 laying some groundwork in the periodic context, before turning to stochastic homogenization *per se* in Section 2.2.

We refer to, *e.g.*, the monographs [15, 19, 25] for more details on homogenization theory, and to the review article [1] that we wrote, addressing some computational challenges in numerical stochastic homogenization. A super elementary introduction is contained in [13].

In this section, we present classical results of the literature. The reader familiar with stochastic homogenization can proceed directly to our contributions, detailed in Sections 3 and 4.

2.1 Periodic homogenization

For consistency, we recall here some basic ingredients of elliptic homogenization theory in the periodic setting. We consider, in a regular bounded domain $\mathcal{D}$ in $\mathbb{R}^d$, the problem

$$\left\{ \begin{array}{l} -\mathrm{div}\left[A_{per}\left(\dfrac{x}{\varepsilon}\right)\nabla u^\varepsilon\right] = f \quad \text{in} \quad \mathcal{D}, \\ u^\varepsilon = 0 \quad \text{on} \quad \partial\mathcal{D}, \end{array} \right. \tag{1}$$

where the matrix A_{per} is symmetric definite positive and $\mathbb{Z}^d$-periodic. We manipulate for simplicity *symmetric* matrices, but the discussion carries over to non symmetric matrices up to slight modifications.

The microscopic problem associated to (1), called the *corrector problem* in the terminology of homogenization theory, reads, for p fixed in $\mathbb{R}^d$,

$$\left\{ \begin{array}{l} -\mathrm{div}\left(A_{per}(y)\left(p+\nabla w_p\right)\right) = 0 \quad \text{in} \quad \mathbb{R}^d, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{array} \right. \tag{2}$$

It has a unique solution up to the addition of a constant. Then, the *homogenized* coefficients read

$$[A^\star]_{ij} = \int_Q \left(e_i + \nabla w_{e_i}(y)\right)^T A_{per}(y) e_j dy, \tag{3}$$

where Q is the unit cube, and where w_{e_i} denotes the solution to (2) for $p = e_i$, with e_i the canonical vectors of $\mathbb{R}^d$. The main result of periodic homogenization theory is that, as ε goes to zero, the solution u^ε to (1) converges to $u^\star$ solution to

$$\begin{cases} -\text{div}\left[A^\star \nabla u^\star\right] = f \quad \text{in} \quad \mathcal{D}, \\ u^\star = 0 \quad \text{on} \quad \partial\mathcal{D}. \end{cases} \tag{4}$$

Several other convergences on various products involving $A_{per}\left(\frac{x}{\varepsilon}\right)$ and u^ε also hold. All this is well documented.

The practical interest of the approach is evident. No small scale ε is present in the homogenized problem (4). At the price of only computing d periodic problems (2) (as many problems as dimensions in the ambient space) the solution to problem (1) can be efficiently approached for ε small. A direct attack of problem (1) would require taking a meshsize smaller than ε. The difficulty has been circumvented. Of course, many improvements and alternatives exist in the literature.

2.2 Stochastic homogenization

The mathematical setting of stochastic homogenization is more involved than that of the periodic case.

We put ourselves in the usual probability theoretic setting for *stationary ergodic homogenization*, with the exception that our notion of stationarity is *discrete*. It intuitively means the following. Pick two points x and $y \neq x$ at the microscale in the material and assume $y = x + k$ with $k \in \mathbb{Z}^d$. The particular local environment seen from x (that is, the microstructure present at x) is generically different from what is seen from y (that is, the microstructure present at y). However, the *average* local environment in x is assumed to be identical to that in y (considering the various realizations of the random material). In mathematical terms, the *law* of microstructures is the same. This is *stationarity*. On the other hand, *ergodicity* means that considering all the points in the material amounts to fixing a point x in this material and considering all the possible microstructures present there.

2.2.1 Main result

With the same setting as that described for periodic homogenization, we may now briefly describe the main result of stochastic homogenization. The

solution u^ε to the boundary value problem

$$\begin{cases} -\mathrm{div}\left(A\left(\dfrac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right) = f \quad \text{in} \quad \mathcal{D}, \\ u^\varepsilon = 0 \quad \text{on} \quad \partial\mathcal{D}, \end{cases} \tag{5}$$

converges, when $\varepsilon \to 0$, to the solution $u^\star$ of (4) where the homogenized matrix is now

$$[A^\star]_{ij} = \mathbb{E}\left(\int_Q \left(e_i + \nabla w_{e_i}(y,\cdot)\right)^T A\left(y,\cdot\right) e_j \, dy\right). \tag{6}$$

The corrector problem now reads

$$\begin{cases} -\mathrm{div}\left[A\left(y,\omega\right)\left(p + \nabla w_p(y,\omega)\right)\right] = 0 \quad \text{on} \quad \mathbb{R}^d, \\ \nabla w_p \quad \text{is stationary}, \quad \mathbb{E}\left(\displaystyle\int_Q \nabla w_p(y,\cdot)\, dy\right) = 0. \end{cases} \tag{7}$$

A striking difference between the stochastic setting and the periodic setting can be observed comparing (2) and (7). In the periodic setting, the corrector problem is posed on a *bounded* domain, namely the periodic cell Q. In sharp contrast, the corrector problem (7) of the random setting is posed on the *whole space* $\mathbb{R}^d$, and cannot be reduced to a problem posed on a bounded domain. The reason is, condition $\mathbb{E}\left(\displaystyle\int_Q \nabla w_p(y,\cdot)\, dy\right) = 0$ in (7) is a *global* condition. It indeed equivalently reads, because of the ergodic theorem, $\lim\limits_{R\longrightarrow+\infty} \dfrac{1}{|B_R|}\displaystyle\int_{B_R} \nabla w_p(y,\cdot)\, dy = 0$ for any sequence of balls B_R of radii R.

The fact that the random corrector problem is posed on the entire space has far reaching consequences for numerical practice. Actually, this is probably the main source of all the *practical difficulties* of stochastic homogenization.

2.2.2 The direct numerical approach

Practical approximations of the homogenized problem in random homogenization are not easily obtained, owing to the fact that the corrector problem (7) is set on the entire space. In practice, truncations have to be considered, and the actual homogenized coefficients are only obtained in the asymptotic regime.

Let us now be more explicit. In practice, the matrix $A^\star$ is approximated by the matrix

$$[A_N^\star]_{ij}(\omega) = \frac{1}{|Q_N|}\int_{Q_N} \left(e_i + \nabla w_{e_i}^N(y,\omega)\right)^T A(y,\omega)\left(e_j + \nabla w_{e_j}^N(y,\omega)\right) dy, \quad (8)$$

which is in turn obtained by solving the corrector problem on a *truncated* domain, say the cube $Q_N = (-N,N)^d \subset \mathbb{R}^d$:

$$\left\{\begin{array}{l} -\mathrm{div}\left(A(\cdot,\omega)\left(p + \nabla w_p^N(\cdot,\omega)\right)\right) = 0 \quad \text{on} \quad \mathbb{R}^d, \\ w_p^N(\cdot,\omega) \text{ is } Q_N\text{-periodic.} \end{array}\right. \quad (9)$$

Although $A^\star$ itself is a deterministic object, its practical approximation $A_N^\star$ is random. It is only in the limit of infinitely large domains Q_N that the deterministic value is attained (the convergence $\lim_{N\to\infty} A_N^\star(\omega) = A^\star$ has been shown in [16, Theorem 1]).

At fixed N, the approximate homogenized matrix $A_N^\star$ is random: a set of M independent realizations of the random coefficient A are therefore considered. The corresponding truncated problems (9) are solved, and an empirical mean of the truncated coefficients (8) is inferred. This empirical mean only agrees with the theoretical mean value of the truncated coefficient within a margin of error which is given by the central limit theorem (in terms of M). For a sufficiently large truncation size N, this truncated value is admittedly the exact value of the coefficient. The overall computation described above is thus very expensive, because each realization requires a new solution to the problem (9) of presumably large a size since N is taken large.

3 Bounds for homogenization

[Work expanded in [1].]

Given the above computational workload, practitioners, especially scientists from the applied communities (computational mechanics, ...), sometimes choose to avoid computing actual homogenized equations and concentrate on *bounds* on the homogenized matrices $A^\star$. In [1], we have carefully studied this approach, which has some (strong, as will be seen below) limitations.

We consider here the specific case of composite materials consisting of only two phases. We denote by A and B the associated matrix coefficients, modelling the properties of the phases. We also fix the average volume fraction θ of the phase A. For simplicity, we assume here that θ is uniform over the whole material. The problem is to find all possible homogenized materials, that is, mathematically, matrices $A^\star$, that can be attained homogenizing such phases A and B with the volume fraction θ.

In this specific case, some bounds on the homogenized coefficients may be established. Here, we present one example of such bounds (actually the most famous one). The case we consider is a scalar equation of the type (1) with a matrix coefficient $A^\varepsilon(x)$ that needs not be periodic, nor stationary ergodic, and that reads

$$A^\varepsilon(x) = \chi^\varepsilon(x)A + (1 - \chi^\varepsilon(x))B$$

where $\chi^\varepsilon(x)$ is the caracteristic function of phase A. Obtaining estimates on $A^\star$ without being in position to explicitly compute $A^\star$ at a reasonable computational price is the whole interest of the approach by "bounds".

3.1 The Hashin-Shtrikman bounds

Based on the density of the matrices obtained by periodic homogenization in the set of matrices obtained by arbitrary homogenization, it is possible to derive the following *Hashin-Shtrikman bounds* on $A^\star$. In the sequel, we assume $B \geq A$.

Under the above assumptions, any homogenized matrix $A^\star$ satisfies the upper bound

$$A^\star p \cdot p \leq Bp \cdot p + \theta \min_{\eta \in \mathbb{R}^d} \left[2p \cdot \eta + (B - A)^{-1}\eta \cdot \eta + (1 - \theta)h(\eta) \right] \qquad (10)$$

for any $p \in \mathbb{R}^d$, where $h(\eta)$ is defined by

$$h(\eta) = \min_{k \in \mathbb{Z}^d, k \neq 0} \frac{|\eta \cdot k|^2}{Bk \cdot k}.$$

Similarly, any homogenized matrix $A^\star$ satisfies the lower bound

$$A^\star p \cdot p \geq Ap \cdot p + (1 - \theta) \max_{\eta \in \mathbb{R}^d} \left[2p \cdot \eta - (B - A)^{-1}\eta \cdot \eta - \theta g(\eta) \right], \qquad (11)$$

where $g(\eta)$ is defined by

$$g(\eta) = \max_{k \in \mathbb{Z}^d, k \neq 0} \frac{|\eta \cdot k|^2}{Ak \cdot k}.$$

Furthermore, the upper bound can always be attained: for any $p \in \mathbb{R}^d$, there exists a function χ, $\mathbb{Z}^d$-periodic and that generally depends on p, such that for the matrix $A_p^\star$ obtained by periodic homogenization of

$$A(\frac{x}{\varepsilon}) = \chi(\frac{x}{\varepsilon})A + (1 - \chi(\frac{x}{\varepsilon}))B,$$

the inequality (10) becomes an equality (see *e.g.* [30]). Likewise, the lower bound (11) can always be attained. We have summarized in [1, Section 2.3.2] a proof of the Hashin Shtrikman bounds.

Remark 1 *Besides the Hashin-Shtrikman bounds, many other estimates have been proposed, such as the dilute approximation, the self-consistent method [31] and the Mori Tanaka methods [28]. They are all based on the fact that the problem of a single inclusion in an infinite material (Eshelby problem) is analytically solvable [23]. Similarly to the Hashin-Shtrikman bounds, the spatial distribution of the phases is not taken into account in these other bounds. The accuracy of these estimates and bounds strongly depends on the contrast between A and B and the volume fraction θ as shown on Figure 1 below.*

3.2 Numerical illustration

We consider a two-phase composite with A and B. We denote by a the scalar conductivity of A (respectively b the conductivity of B) with $a < b$. We denote by d the dimension, and by θ the volume fraction of A.

We consider the case of the random checkerboard, for which the exact homogenized matrix is known: $A^\star = a^\star \, \mathrm{Id} = \sqrt{\mathrm{ab}} \, \mathrm{Id}$. In this simple case, the different bounds and estimates have an analytical form: the homogenized coefficient $a^\star$ is bounded from below by the harmonic mean (often called the Reuss bound) and from above by the arithmetic mean (often called the Voigt bound):

$$\frac{1}{\theta/a + (1-\theta)/b} \leq a^\star \leq \theta a + (1-\theta)b.$$

These bounds are also called Wiener Bounds or Paul bounds. In this case, the Hashin-Shtrikman bounds detailed above read (see *e.g.* [25, page 188]):

$$a\left(1+\frac{d(1-\theta)(b-a)}{da+\theta(b-a)}\right) \leq a^\star \leq b\left(1-\frac{d\theta(b-a)}{db+(1-\theta)(a-b)}\right),$$

and the Self-Consistent model leads to an estimate λ_{eff} of the effective conductivity $a^\star$ defined implicitly (see [26]) by

$$\theta\frac{a-\lambda_{\text{eff}}}{a+2\lambda_{\text{eff}}}+(1-\theta)\frac{b-\lambda_{\text{eff}}}{b+2\lambda_{\text{eff}}}=0.$$

On Figure 1 we plot these bounds and estimates for different values of the contrast, defined by b/a, for $a=1$. Note that in this case, by construction, the volume fraction for any a and b is $\theta=1/2$. In Tab. 1, we collect the values of all these bounds and estimates, for the particular case $a=1$ and $b=10$.

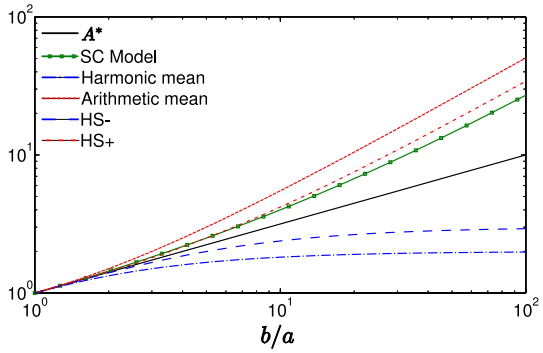

Figure 1: Different bounds for the checkerboard test case.

$A^\star$	Harmonic	HS-	SC Model	HS+	Arithmetic
3.16	1.81	2.38	4.00	4.19	5.50

Table 1: Values of bounds and estimate for a contrast of $b/a=10$.

We verify that, for the critical volume fraction $\theta=0.5$, even for a contrast which is not extremely large ($a=1$ and $b=10$), the range of homogenized matrix atteignable, given by the Hashin-Shtrikman bounds, is *wide*. In such a case, the spatial distribution of phases, which is not taken into account on

the bounds, is certainly important. Note also that a typical case for real-world composites is more challenging than the case above, since the contrast is usually larger (of the order 100 rather than 10) and the volume fraction is similar.

Our numerical example therefore shows that, in many cases, *the Hashin Shtrikman bounds cannot provide accurate estimates of the homogenized matrix*. For a contrast of 10, the error between the bounds and $A^\star$ is larger than 25 %. For a contrast of 100, the upper bound is three times as large as the actual homogenized value, which is itself three times as large as the lower bound. *There is therefore a need for developing efficient numerical methods that provide more accurate results.*

4 A weakly-stochastic MsFEM approach

[Work expanded in [3].]

In this section, we show how the Multiscale Finite Element Method (MsFEM) can be adapted to the stochastic setting. We refer to [20] for a review on the MsFEM approach. Let us recall here that this method is designed to directly address the original problem (namely (5) in the case of interest here), keeping ε at its fixed value, rather than studying the limit problem when $\varepsilon \to 0$ (as we do in Section 2, going from (5) to (4)). Another interest of this method is that it does not require any explicit formula for the homogenized tensor (such as (2)-(3), or (6)-(7)), which are not always available. More details and comprehensive numerical tests are published in [3]. See also [4].

4.1 MsFEM approaches

For consistency and to set our notation, we briefly review the classical, deterministic setting for MsFEM approaches. We next turn to the stochastic setting. We consider problem (1), which we reproduce here for convenience,

$$\left\{ \begin{array}{rcll} -\mathrm{div}(A^\varepsilon(x)\nabla u^\varepsilon(x)) & = & f(x) & \text{in } \mathcal{D}, \\ u^\varepsilon & = & 0 & \text{on } \partial\mathcal{D}, \end{array} \right. \tag{12}$$

where A^ε is a symmetric matrix satisfying the standard coercivity and boundedness conditions. Note that the approach is not restricted to the periodic setting, so we do not assume that $A^\varepsilon(x) = A(x/\varepsilon)$ for a periodic matrix A.

As recalled above, we wish here to keep ε fixed at a (small) given value. The MsFEM approach consists in performing a variational approximation of (12) where the basis functions are defined *numerically* and *encode the fast oscillations* present in (12). In the sequel we will argue on the variational formulation of (12):

$$\text{Find } u^\varepsilon \in H^1_0(\mathcal{D}) \text{ such that}, \quad \forall v \in H^1_0(\mathcal{D}), \quad \mathcal{A}_\varepsilon(u^\varepsilon, v) = b(v), \tag{13}$$

where

$$\mathcal{A}_\varepsilon(u,v) = \sum_{i,j} \int_{\mathcal{D}} A^\varepsilon_{ij}(x) \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} dx \quad \text{and} \quad b(v) = \int_{\mathcal{D}} f\, v\, dx.$$

We introduce a classical P1 discretization of the domain $\mathcal{D}$, with L nodes, and denote ϕ^0_i, $i = 1, \ldots, L$, the basis functions.

Definition of the MsFEM basis functions Several definitions of the basis functions have been proposed in the literature (see *e.g.* [24, 21, 22, 14]). They give rise to different methods. In the following, we present one of these methods. We consider the problem

$$\left\{ \begin{array}{rl} -\text{div}(A^\varepsilon(x) \nabla \phi_i^{\varepsilon,\mathbf{K}}) & = 0 \quad \text{in } \mathbf{K} \\ \phi_i^{\varepsilon,\mathbf{K}} & = \phi_i^0|_{\mathbf{K}} \quad \text{on } \partial\mathbf{K}. \end{array} \right. \tag{14}$$

Note the similarity between (14) and the corrector problem (2). Note also that the problems (14), indexed by $\mathbf{K}$, are all independent from one another. They can hence be solved in parallel, using a discretization adapted to the small scale ε.

Macro scale problem We now introduce the finite dimensional space

$$\mathcal{W}_h := \text{span}\left\{\phi_i^\varepsilon,\ i = 1, \ldots, L\right\},$$

where ϕ_i^ε is such that $\phi_i^\varepsilon|_{\mathbf{K}} = \phi_i^{\varepsilon,\mathbf{K}}$ for all $\mathbf{K}$, and proceed with a standard Galerkin approximation of (13) using $\mathcal{W}_h$:

$$\text{Find } u_h^\varepsilon \in \mathcal{W}_h \text{ such that}, \quad \forall v \in \mathcal{W}_h, \quad \mathcal{A}_\varepsilon(u_h^\varepsilon, v) = b(v). \tag{15}$$

The dimension of $\mathcal{W}_h$ is equal to L: the formulation (15) hence requires solving a linear system with only a limited number of degrees of freedom.

Numerical illustration In order to illustrate the MsFEM approach, we solve (12) in a one dimensional setting with

$$A^\varepsilon(x) = 5 + 50 \sin^2\left(\frac{\pi x}{\varepsilon}\right),$$

on the domain $\mathcal{D} = (0,1)$, with $\varepsilon = 0.025$ and $f = 1000$. We subdivide the interval $(0,1)$ in $L = 10$ elements. On Figure 2, we plot the MsFEM basis functions in a reference element and the MsFEM solution u_h^ε.

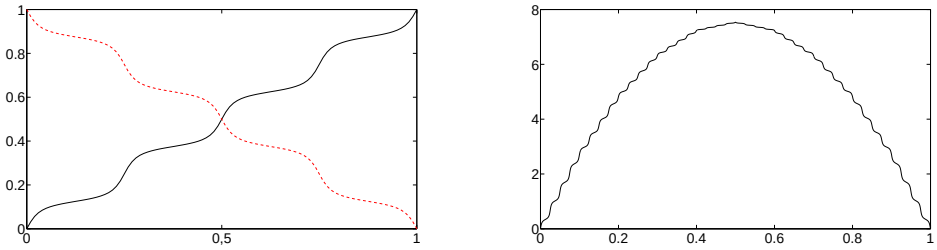

Figure 2: Left: Multiscale basis functions $\phi^{\varepsilon,\mathbf{K}}$ in the reference element. Right: MsFEM solution u_h^ε in the domain $(0,1)$.

Natural adaptation to the stochastic setting When applied to the stochastic problem

$$\left\{ \begin{array}{rcl} -\mathrm{div}(A^\varepsilon(x,\omega)\nabla u^\varepsilon(x,\omega)) & = & f(x) \quad \text{in } \mathcal{D}, \\ u^\varepsilon & = & 0 \quad \text{on } \partial\mathcal{D}, \end{array} \right. \tag{16}$$

where the practical issue is to build an estimate of the mean $\mathbb{E}(u^\varepsilon(x,\cdot))$ using a Monte-Carlo simulation method, the natural adaptation of the MsFEM method is the following: for each random realization m, first construct a MsFEM basis and next solve the macroscale problem. This approach requires a significantly large number of computations, since, for each realization, a new basis of oscillating functions is built, and a problem at the macroscale is solved. Such an approach has been described and analyzed in *e.g.* [18].

4.2 A weakly stochastic setting

As seen above, considering general random materials lead to extremely expensive computations. The question arises to know whether this general random context is really relevant, and whether adequate modifications can lead

to substantial improvements. Our line of thought here is based on the following two-fold observation: classical random homogenization is costly but perhaps, in a number of situations, not necessary. Many materials, albeit not deterministic, are not totally random. Some of them can be considered as a perturbation of a deterministic material. The homogenized behaviour should expectedly be close to that of the underlying deterministic material (and thus tractable from the practical viewpoint), up to an error depending on the amount of randomness present.

Model We introduce and study here a specific model for a randomly perturbed deterministic material (we refer to [12] for a quick overview of this setting, and some of the associated numerical techniques, and to [1] for a more comprehensive review of our contributions along these ideas). We are interested in the following elliptic problem

$$\left\{ \begin{array}{rcl} -\mathrm{div}\left(A_\eta^\varepsilon(x,\omega)\,\nabla u_\eta^\varepsilon\right) &=& f(x) \quad \text{in } \mathcal{D} \subset \mathbb{R}^d, \\ u_\eta^\varepsilon &=& 0 \quad \text{on } \partial\mathcal{D}, \end{array} \right. \tag{17}$$

that is (16) with

$$A^\varepsilon(x,\omega) \equiv A_\eta^\varepsilon(x,\omega) = A_0^\varepsilon(x) + \eta A_1^\varepsilon(x,\omega), \tag{18}$$

where $\eta \in \mathbb{R}$ is a *small* parameter, A_0^ε is a deterministic matrix uniformly elliptic and bounded, and $A_1^\varepsilon(x,\omega)$ is a bounded matrix. The matrix A_η^ε is hence a *perturbation* of the deterministic matrix A_0^ε.

Remark 2 *The above setting is of course* one *possible setting where the theory may be developed. Other forms of random perturbations of deterministic (possibly periodic) problems could also be addressed. See e.g. [5, 6, 7, 8] and the review article [1].*

In the case (18), a MsFEM method alternative to the one presented in Section 4.1 can be proposed. The idea is to compute the MsFEM basis functions only *once*, with the *deterministic part* of the matrix A_η^ε and next to perform Monte-Carlo realizations only for the macro scale problems. We refer to [3] for all the details.

As above, we hence first solve (14), with $A^\varepsilon \equiv A_0^\varepsilon$, and build the finite dimensional space

$$\mathcal{W}_h := \mathrm{span}\left\{\phi_i^\varepsilon,\ i = 1, \ldots, L\right\}.$$

We next proceed with a standard Galerkin approximation of (17) using $\mathcal{W}_h$: for each $m \in \{1, \ldots, M\}$, we consider a realization $A_\eta^{\varepsilon,m}(\cdot,\omega)$ and compute $u^m(\cdot,\omega) \in \mathcal{W}_h$ such that

$$\forall v \in \mathcal{W}_h, \ \sum_{i,j} \int_{\mathcal{D}} (A_\eta^{\varepsilon,m})_{ij}(x,\omega) \frac{\partial u^m}{\partial x_i}(x,\omega) \frac{\partial v}{\partial x_j}(x)\, dx = \int_{\mathcal{D}} f(x)\, v(x)\, dx. \quad (19)$$

Since the MsFEM basis functions are only computed once, a large computational gain is expected, and this is indeed the case.

Numerical studies We now estimate the performance of the approach. To this aim, we compare the solution of the above approach with the solution of the direct approach (of Section 4.1) and, for reference, the solution to (17) obtained using a finite element method with a mesh size adapted to the small scale ε. Our estimators are built as follows:

$$e(u_1, u_2) = \mathbb{E}\left(\frac{||u_1 - u_2||_N}{||u_2||_N} \right), \quad (20)$$

where N is the norm used, u_1 and u_2 are the solutions obtained with any two different methods. The expectation is in turn computed using a Monte-Carlo method. Considering M realizations $\{X_m(\omega)\}_{1 \le m \le M}$ of a random variable (here $X(\omega) = \dfrac{||u_1(\cdot,\omega) - u_2(\cdot,\omega)||_N}{||u_2(\cdot,\omega)||_N}$), we compute the empirical mean μ_M and the empirical standard deviation σ_M as

$$\begin{aligned} \mu_M(X) &= \frac{1}{M} \sum_{m=1}^{M} X_m(\omega), \\ \sigma_M^2(X) &= \frac{1}{M-1} \sum_{m=1}^{M} \left(X_m(\omega) - \mu_M(X) \right)^2. \end{aligned}$$

As a classical consequence of the Central Limit Theorem, it is commonly admitted that $\mathbb{E}(X)$ satisfies

$$|\mathbb{E}(X) - \mu_M(X)| \le 1.96\, \frac{\sigma_M(X)}{\sqrt{M}}.$$

We consider the following numerical example. Let $(X_{k,l})_{(k,l)\in\mathbb{Z}^2}$ denote a sequence of independent, identically distributed scalar random variables uniformly distributed over the interval $[0, 1]$. We define the random conductivity

matrix as

$$A_\eta^\varepsilon(x,y,\omega) = \sum_{(k,l)\in\mathbb{Z}^2} \mathbf{1}_{(k,k+1]}(\frac{x}{\varepsilon})\mathbf{1}_{(l,l+1]}(\frac{y}{\varepsilon}) \left(\frac{2+P\sin(2\pi x/\varepsilon)}{2+P\sin(2\pi y/\varepsilon)} + \frac{2+\sin(2\pi y/\varepsilon)}{2+P\sin(2\pi x/\varepsilon)}\right)(1+\eta X_{k,l}(\omega))\,\mathrm{Id}_2,$$

with the parameters $P = 1.8$ and $\varepsilon = 0.025$. Then we compute u_{ref} solution to (17) on the domain $\mathcal{D} = (0,1)^2$, with $f \equiv 1$. Let u_M and u_S be its approximation by the general MsFEM approach (of Section 4.1) and the weakly-stochastic MsFEM approach described above, respectively. The numerical parameters for the computation are determined using an empirical study of convergence. We used for the reference solution a fine mesh of size $h_f = \varepsilon/40$. The MsFEM basis functions are computed in each element $\mathbf{K}$ using a mesh of size $h_M = \varepsilon/80$. The coarse mesh size is $H = 1/30$. We consider $M = 30$ realizations.

We report in Tables 2 and 3 the estimator (20), along with its confidence interval, for the norms $H^1(\mathcal{D})$ and $L^2(\mathcal{D})$, respectively.

η	$e(u_M, u_{ref})$	$e(u_S, u_{ref})$	$e(u_S, u_M)$
1	8.12 ± 0.19	17.37 ± 0.78	15.51 ± 0.87
0.1	7.17 ± 0.02	7.62 ± 0.07	2.56 ± 0.10
0.01	7.15 ± 0.002	7.28 ± 0.007	1.39 ± 0.002

Table 2: $H^1(\mathcal{D})$ error (in %).

η	$e(u_M, u_{ref})$	$e(u_S, u_{ref})$	$e(u_S, u_M)$
1	0.56 ± 0.08	1.69 ± 0.49	1.47 ± 0.50
0.1	0.54 ± 0.01	0.57 ± 0.06	0.20 ± 0.07
0.01	0.53 ± 0.001	0.62 ± 0.005	0.11 ± 0.003

Table 3: $L^2(\mathcal{D})$ error (in %).

We observe that, when η is small (here, $\eta \leq 0.1$), the alternative approach provides a function u_S that is an approximation of u_{ref} as accurate as u_M. Recall that, since the MsFEM basis has only been computed once, the cost for obtaining an empirical approximation of $\mathbb{E}(u_S)$ is much smaller than that

for obtaining the corresponding empirical estimator of $\mathbb{E}(u_M)$. This demonstrates the efficiency of the approach. As expected, when η is not small (say $\eta \approx 1$), the accuracy of the solution u_S computed with the alternative approach proposed here decreases.

Elements of proof In [3], we have analyzed the method introduced here in the one-dimensional setting (see also [4]). For the sake of analysis, we assume that the highly oscillating coefficient reads $a_\eta^\varepsilon(x,\omega) = a_\eta\left(\frac{x}{\varepsilon},\omega\right)$, where a_η satisfies the standard assumption of stochastic homogenization (see Section 2.2). The problem (17) now reads

$$\left\{ \begin{array}{l} -\dfrac{d}{dx}\left(a_\eta\left(\dfrac{x}{\varepsilon},\omega\right)\dfrac{d}{dx}u_\eta^\varepsilon(x,\omega)\right) = f(x) \quad \text{in } (0,1), \\ u_\eta^\varepsilon(0,\omega) = u_\eta^\varepsilon(1,\omega) = 0. \end{array} \right. \tag{21}$$

We assume that the randomness is *small*, in the sense (see (18)) that

$$a_\eta(x,\omega) = a_{per}(x) + \eta\, a_1(x,\omega), \tag{22}$$

where a_{per} is a deterministic, periodic function and η is a *small* deterministic parameter.

In [3], we have bounded from above the difference between $u_\eta^\star$, the solution to the homogenized equation (4), and the weakly-stochastic MsFEM solution, in the following sense. For a given realization of the random coefficient $a_\eta(x,\omega)$, let $u(\cdot,\omega)$ be the weakly-stochastic MsFEM solution, that solves (19). By construction, this solution is a linear combination of the highly oscillating basis functions:

$$u(x,\omega) = \sum_{i=1}^{L} U_i(\omega)\phi_i^\varepsilon(x).$$

Let $v_{\text{w}-\text{MsFEM}}(x,\omega)$ be the associated representation in terms of standard P1 basis functions:

$$v_{\text{w}-\text{MsFEM}}(x,\omega) = \sum_{i=1}^{L} U_i(\omega)\phi_i^0(x).$$

We have the following estimate:

$$\|u_\eta^\star - v_{\text{w}-\text{MsFEM}}(\cdot,\omega)\|_{H^1(0,1)} \leq C\left(h + \frac{\varepsilon}{h} + \eta\sigma_h^\varepsilon(\omega) + \eta^2\mathcal{C}(\eta)\right) \tag{23}$$

where C is a deterministic constant, independent of h, ε and η, and $\mathcal{C}(\eta)$ is a deterministic function, bounded when $\eta \to 0$. In the above bound, $\sigma_h^\varepsilon(\omega)$ is a random number, independent of η, that depends on ε, h and the random term $a_1(x,\omega)$ in (22).

Let us comment on (23). Assume that $\eta = 0$, i.e. the problem (21) is a periodic problem. Then our method is identical to the standard deterministic MsFEM method, and we recover from (23) the classical bound known in that case, namely

$$\|u_\eta^\star - v_{\mathrm{MsFEM}}\|_{H^1(0,1)} \leq C\left(h + \frac{\varepsilon}{h}\right).$$

Assume now that a_1 is deterministic. Then our method is not exactly the MsFEM method, since we do not take into account a_1 to build the highly oscillating basis functions. In that case, $\sigma_h^\varepsilon(\omega)$ turns out to vanish, and we infer from (23) that

$$\|u_\eta^\star - v_{\mathrm{w-MsFEM}}\|_{H^1(0,1)} \leq C\left(h + \frac{\varepsilon}{h} + \eta^2\mathcal{C}(\eta)\right).$$

We hence observe that, provided the term neglected to build the basis functions is small (namely $\eta \ll 1$), we obtain a similar accuracy as with the standard MsFEM method.

A similar conclusion holds in the general case (22). Note also that the bound (23) is valid for any realization ω of the randomness. It is therefore a more precise result than a bound on the expectation of the error, where all random realizations are averaged. For instance, the bound (23) allows to understand what is the probability distribution of the error.

5 Conclusions and plan for the following years

In this report, we have first reviewed an approach to obtain bounds (here, the Hashin-Shtrikman bounds) on the homogenized matrix. This approach only involves computations of moderate difficulty. However, we have outlined the strong limitations of such a strategy. In some cases, the difference between the lower and upper bounds is indeed very large. The obtained estimations are then inaccurate. This motivates the development of efficient numerical methods that provide more accurate results.

To this aim, we have focused on weakly stochastic materials, for which we successfully adapted the well-known Multiscale Finite Element Method (MsFEM). We have proposed a method with a much smaller computational cost

than the original MsFEM in the stochastic setting. Provided the stochastic perturbation is indeed small, the method we propose is as accurate as the original one.

We summarize now the directions of research we wish to pursue during the following years.

A variant of classical random homogenization In the short term, our aim is to study a particular setting for stochastic homogenization, which is not the classical setting described in Section 2.2 (where the random coefficient A in (5) is stationary). The setting we wish to study is the case when the random coefficient is the composition of a standard deterministic and periodic function $A_{\rm per}$ with a stochastic diffeomorphism:

$$A^\varepsilon(x,\omega) = A_{\rm per}\left[\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right] \tag{24}$$

where, for any random realization ω, the application $x \mapsto \Phi(x,\omega)$ is a diffeomorphism. Formally, such a setting models a microstructure that is periodic, in a given reference configuration. The latter is only known up to a certain randomness. Materials we have in mind are ideally periodic materials, where some random deformation has been introduced, for instance during the manufacturing process. Othewise stated, these are periodic materials seen through random glasses! This setting has been initially introduced in [9], where the homogenized problem is identified.

An interesting question in that context is that of numerical discretization. In the classical context, a standard procedure is to solve the corrector problem on a truncated domain (see (8) and (9)). The convergence of the procedure is given by [16, Theorem 1]. We currently work on a similar analysis in the context of (24) (see [2]).

A more theoretical question is to precisely understand the behaviour of $u^\varepsilon(x,\omega) - u^\star(x)$ when ε goes to 0, where u^ε is the solution of the highly oscillating problem and $u^\star$ the solution of the homogenized problem. In the classical setting, and in the one-dimensional case, the convergence of $\varepsilon^{-1/2}(u^\varepsilon(x,\omega) - u^\star(x))$ to a Gaussian process has been shown in [17]. This question, in the context of (24), is addressed in [2].

The setting (24) is in general not a weakly stochastic setting, as the amount of randomness present in Φ may be large. Yet, in the case when the diffeomorphism Φ is close to the identity, namely

$$\Phi(x,\omega) = x + \eta\Psi(x,\omega) + O(\eta^2) \tag{25}$$

for a small deterministic parameter η, the amount of randomness turns out to be small. This case is thus another instance of randomly perturbed deterministic materials (recall Section 4.2, where we introduced another weakly stochastic setting, and Remark 2, where we pointed out other weakly stochastic settings). The case (24)-(25) has been studied in [10, 11].

A Fast Fourier Transform approach In the course of our investigations, we have identified the following tracks of research, which are closely related to the research directions of the contract.

First, in the periodic homogenization setting recalled in Section 2.1, a method based on Fast Fourier Transform has been proposed in [29, 27]. The idea is as follows. Let A_0 be a constant symmetric positive matrix. The corrector problem (2) is equivalent to

$$\begin{cases} -\mathrm{div}\left(A_0\left(p+\nabla w_p\right)\right) = \mathrm{div}\left(\left(A_{per}(y)-A_0\right)\left(p+\nabla w_p\right)\right) & \text{in} \quad \mathbb{R}^d, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases}$$

The idea of [29, 27] is to solve this problem iteratively. Knowing the iterate w_p^k at iteration k, the next iterate w_p^{k+1} is defined as the unique solution to

$$\begin{cases} -\mathrm{div}\left(A_0\left(p+\nabla w_p^{k+1}\right)\right) = \mathrm{div}\left(\left(A_{per}(y)-A_0\right)\left(p+\nabla w_p^{k}\right)\right) & \text{in} \quad \mathbb{R}^d, \\ w_p^{k+1} \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases}$$

As A_0 is a tensor independent of y (in contrast to $A_{per}(y)$), the above problem can be solved very efficiently using a Fourier transform. Hence, rather than solving (2), we are left with solving many times a simpler problem.

Our aim is to compare this iterative method with the standard method, in term of efficiency. The choice of A_0 is most probably of paramount importance, since the convergence rate (and also the fact that the iterations in k converge or not) depends on it. We have already run some preliminary tests with this method, but definite conclusions are yet to be obtained.

Second, in the context of stochastic homogenization, approaches using some decomposition of the random matrix $A(x,\omega)$ in (5) would be worthwhile to investigate.

References

References authored by the investigators in the context of the contract

[1] A. Anantharaman, R. Costaouec, C. Le Bris, F. Legoll and F. Thomines, *Introduction to numerical stochastic homogenization and the related computational challenges: some recent developments*, Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, submitted.

[2] R. Costaouec, F. Legoll and F. Thomines, *Approximation of effective coefficients for a variant of classical random homogenization*, in preparation.

[3] C. Le Bris, F. Legoll and F. Thomines, *Multiscale FEM for weakly random problems and related issues*, preprint.

[4] F. Thomines, Thèse de l'Université Paris Est, Ecole des Ponts ParisTech, in preparation.

References authored by the investigators and scientifically related to the contract

[5] A. Anantharaman and C. Le Bris, *Homogénéisation d'un matériau périodique faiblement perturbé aléatoirement [Homogenization of a weakly randomly perturbed periodic material]*, C. R. Acad. Sci. Série I, 348:529–534, 2010.

[6] A. Anantharaman and C. Le Bris, *A numerical approach related to defect-type theories for some weakly random problems in homogenization*, SIAM Multiscale Modeling & Simulation, submitted, `http://arxiv.org/abs/1005.3910`

[7] A. Anantharaman and C. Le Bris, *Elements of mathematical foundations for a numerical approach for weakly random homogenization problems*, Communications in Computational Physics, submitted, `http://arxiv.org/abs/1005.3922`

[8] X. Blanc, R. Costaouec, C. Le Bris and F. Legoll, *Variance reduction in stochastic homogenization using antithetic variables*, Markov Processes and Related Fields, submitted.

[9] X. Blanc, C. Le Bris and P.-L. Lions, *Une variante de la théorie de l'homogénéisation stochastique des opérateurs elliptiques [A variant of stochastic homogenization theory for elliptic operators]*, C. R. Acad. Sci. Série I, 343:717–724, 2006.

[10] X. Blanc, C. Le Bris and P.-L. Lions, *Stochastic homogenization and random lattices*, Journal de Mathématiques Pures et Appliquées, 88:34–63, 2007.

[11] R. Costaouec, C. Le Bris and F. Legoll, *Approximation numérique d'une classe de problèmes en homogénéisation stochastique [Numerical approximation of a class of problems in stochastic homogenization]*, C. R. Acad. Sci. Série I, 348:99–103, 2010.

[12] C. Le Bris, *Some numerical approaches for "weakly" random homogenization*, Proceedings of ENUMATH 2009, Springer Lecture Notes in Computational Science and Engineering, in press.

[13] C. Le Bris, *A selection of mathematical topics in multiscale sciences*, Proceedings of the XIV Jacques-Louis Lions Spanish-French School, 6-10 September 2010, Publications of the University of La Coroña, to appear.

General references by other authors

[14] G. Allaire and R. Brizzi, *A multiscale finite element method for numerical homogenization*, Multiscale Modeling & Simulation, 4(3):790–812, 2005.

[15] A. Bensoussan, J.-L. Lions and G. Papanicolaou, **Asymptotic analysis for periodic structures**, Studies in Mathematics and its Applications, 5. North-Holland Publishing Co., Amsterdam-New York, 1978.

[16] A. Bourgeat and A. Piatnitski, *Approximation of effective coefficients in stochastic homogenization*, Ann I. H. Poincaré - PR, 40(2):153–165, 2004.

[17] A. Bourgeat and A. Piatnitski, *Estimates in probability of the residual between the random and the homogenized solutions of one-dimensional second-order operator*, Asymptotic Analysis, 21(3-4):303–315, 1999.

[18] Z. Chen and T.Y. Savchuk, *Analysis of the multiscale finite element method for nonlinear and random homogenization problems*, SIAM Journal on Numerical Analysis, 46(1):260–279, 2008.

[19] D. Cioranescu and P. Donato, **An introduction to homogenization**. Oxford Lecture Series in Mathematics and its Applications, 17. The Clarendon Press, Oxford University Press, New York, 1999.

[20] Y. Efendiev and T. Hou, **Multiscale Finite Element method**, Theory and applications. Surveys and Tutorials in the Applied Mathematical Sciences, 4. Springer, New York, 2009.

[21] Y.R. Efendiev, T.Y. Hou and X.-H. Wu, *Convergence of a nonconforming multiscale finite element method*, SIAM Journal on Numerical Analysis, 37(3):888–910, 2000.

[22] Y.R. Efendiev, T.Y. Hou and V. Ginting, *Multiscale finite element methods for nonlinear problems and their applications*, Communications in Mathematical Sciences, 2(4):553–589, 2004.

[23] J.D. Eshelby, *The determination of the elastic field of an ellipsoidal inclusion, and related problems*, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, 241(1226):376–396, 1957.

[24] T.Y. Hou and X.-H. Wu, *A multiscale finite element method for elliptic problems in composite materials and porous media*, Journal of Computational Physics, 134(1):169–189, 1997.

[25] V.V. Jikov, S.M. Kozlov and O.A. Oleinik, **Homogenization of differential operators and integral functionals**, Springer-Verlag, 1994.

[26] T. Kanit, S. Forest, I. Galliet, V. Mounoury and D. Jeulin, *Determination of the size of the representative volume element for random composites: statistical and numerical approach*, International Journal of Solids and Structures, 40(13-14):3647–3679, 2003.

[27] J.C. Michel, H. Moulinec and P. Suquet, *Effective properties of composite materials with periodic microstructure: a computational approach*, Comput. Methods Appl. Mech. Engrg., 172:109–143, 1999.

[28] T. Mori and K. Tanaka, *Average stress in matrix and average elastic energy of materials with misfitting inclusions*, Acta Metallurgica, 21(5):571–574, 1973.

[29] H. Moulinec and P. Suquet, *A numerical method for computing the overall response of nonlinear composites with complex microstructure*, Comput. Methods Appl. Mech. Engrg., 157:69–94, 1998.

[30] L. Tartar, *Estimations fines des coefficients homogénéisés*, in *Ennio De Giorgi colloquium (Paris, 1983)*, volume 125 of *Res. Notes in Math.*, pages 168–187. Pitman, Boston, MA, 1985.

[31] J.R. Willis, *Bounds and self-consistent estimates for the overall properties of anisotropic composites*, Journal of the Mechanics and Physics of Solids, 25(3):185–202, 1977.