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Multiscale materials science: a mathematical approach to the role of defects and uncertainty

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**6. AUTHOR(S)**

Le Bris, Claude; Legoll, Frederic; Minvielle, William

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Ecole Nationale des Ponts et Chaussees
6 et 8 avenue Blaise Pascal, Cite Descartes, Champs sur Marne
77 455 Marne la Vallee Cedex 2, FRANCE

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**14. ABSTRACT**

We focus on developing affordable numerical methods in the context of stochastic homogenization. Our aim is to compute the homogenized coefficients that represent the behavior of the material at a macroscopic scale. Such computations are usually very expensive. To decrease their cost, we consider a variance reduction technique, namely the control variate technique, and numerically demonstrate its efficiency. We also address questions related to non-periodic modelling of multiscale materials. A typical example is that of a periodic material with a superimposed defect in one periodic cell.

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Mathematical approaches for materials science, Stochastic homogenization, Variance reduction, Defects, Parameter identification

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École des Ponts
ParisTech

Direction de la Recherche

N/Réf. : DR/PC/15-051

Carolina GARCIA-OLMEDO
☎+33 164 15 3646
✉carolina.garcia-olmedo@enpc.fr

Defense Technical Information Center
8725 John J Kingman Road Ste 0944
Fort Belvoir
VA 22060-6218
USA

Champs-sur-Marne, the 17th April 2015

**SUBJECT: N00014-12-10383 – Multiscale materials science : a mathematical approach to the role of defects and uncertainty - Reports**

Dear Sir, Madame

Our project "Multiscale materials science : a mathematical approach to the role of defects and uncertainty" was concluded the 31st March 2015.

As request on the Award Modification, you will find enclosed the following reports:

- Final Technical Report with SF298

Should you have any question, please do not hesitate to contact us.

Yours faithfully,

Carolina GARCIA-OLMEDO

*Chargée d'affaires et développement de la recherche partenariale*

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DESCARTES
CHAMPS SUR MARNE, 77420
FR

13b. CAGE: FAUU2
13c. EDI/EFT NUMBER:

14. REMITTANCE ADDRESS (IF DIFFERENT FROM BLOCK 13):
Same as block #13

13d. BUSINESS OFFICE CONTACT: CAROLINA GARCIA-OLMEDO
13e. TELEPHONE NUMBER: () +33 164 15 364
13f. EMAIL ADDRESS: carolina.garcia-olmedo@enpc.fr

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|---|---|---|---|
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| OBLIGATED BY THIS ACTION: | $10,700.00 | $.00 | $10,700.00 |
| TOTAL OBLIGATED ON AWARD: | $10,700.00 | $.00 | $10,700.00 |
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20a. PRINCIPAL INVESTIGATOR/RECIPIENT TECHNICAL REPRESENTATIVE:
CLAUDE LE BRIS
20b. TELEPHONE NUMBER: () +33 164 15 35
20c. EMAIL ADDRESS: lebris@cermics.enpc.fr

21. TECHNICAL REPRESENTATIVE
21a. NAME: Reza Malek-Madani
21b. CODE: ONR 311
21c. ADDRESS:
Office of Naval Research
875 North Randolph Street
Arlington, VA 22203-1995
21d. TELEPHONE NUMBER: (703) 696-0195
21e. EMAIL ADDRESS: MALEKMR@ONR.NAVY.MIL

22. AWARDING OFFICE CONTACT
22a. NAME: Elizabeth Ford
22b. CODE: ONR BD025
22c. ADDRESS:
Office of Naval Research
875 North Randolph Street
Arlington, VA 22203-1995
22d. TELEPHONE NUMBER: (703) 696-2576
22e. EMAIL ADDRESS: FORDE@ONR.NAVY.MIL

23a. ADMINISTRATIVE OFFICE:
ONR REG BOSTON N62879
495 SUMMER STREET ROOM 627
BOSTON, MA 02210-2109
PHONE: (617) 753-3283
FAX: (617) 753-4605
23b. CODE: N62879

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DFAS COLUMB-NAVY ACQ HQ0251
COLUMBUS, OH 43213
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Office of Naval Research
ATTN: ONR BDCC
One Liberty Center
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27. SPECIAL INSTRUCTIONS:

28. DELEGATIONS: The administration duties listed below have been delegated to the administrative office (block 23a). Upon request the awarding office contact (block 22) will make their full text available. Please direct questions to the contacts @: http://www.onr.navy.mil/Contracts-Grants/Regional-Contacts.aspx

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DOCUMENT

The following documents may be found at:
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UAAC Acceptance C November 2003
UAWA Award A November 2003
Foreign Research Grant February 2011

30. OPTIONS OPTION NO. AMOUNT PERIOD

(1)
(2)
(3)
(4)

31. REPORTS: The following reports must be submitted to the indicated addressees, in the indicated quantities, within 90 days following the expiration or termination of the project. Final Technical Reports must have a SF298, Report Documentation Page, accompanying them. Unless otherwise stated in the award/modification, complete Block 12a of the SF298 as follows: "Approved for Public Release; distribution is Unlimited".

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| Defense Technical Information Center<br>8725 John J Kingman Road Ste 0944<br>Fort Belvoir, VA 22060-6218 | Final Technical Report with SF298<br>Interim Research Performance Report (As Required) with SF298 | 1<br>1 |
| See block #26a | Report of Inventions and Subcontracts - DD 882<br>Final Technical Report with SF298 | 1<br>1 |
| Naval Research Laboratory<br>ATTN: CODE 5596<br>4555 Overlook Avenue SW<br>Washington, DC 20375-5320 | Final Technical Report | 1 |

| 32. FOR THE RECIPIENT | | 33. FOR THE UNITED STATES OF AMERICA | |
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| 32a. SIGNATURE OF PERSON AUTHORIZED TO SIGN<br>N/A - SIGNATURE NOT REQUIRED ON THIS AWARD | | 33a. SIGNATURE OF AWARDING OFFICER<br>Elizabeth Ford | |
| 32b. NAME AND TITLE OF SIGNER | 32c. DATE SIGNED | 33b. NAME AND TITLE OF AWARD OFFICER<br>Elizabeth Ford | 33c. DATE SIGNED<br>15-FEB-12 |

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Contract N00014-12-1-0383

# Multiscale materials science: a mathematical approach to the role of defects and uncertainty

Report to the Office of Naval Research

C. Le Bris, F. Legoll and W. Minvielle

March 2015

# Contents

# 1 Introduction

We report here on the work performed during the three years (April 1st, 2012 - March 31st, 2015) of the contract N00014-12-1-0383 on *Multiscale materials science: a mathematical approach to the role of defects and uncertainty.*

The presence of numerous length-scales in material science problems represents a daunting challenge for numerical simulation. Quantifying the effects of defects, and more generally any uncertainty arising from data, discretization, and the mechanical model for an associated numerical method has become an increasingly important aspect of multiscale analysis. Uncertainty in materials science problems assumes various forms, and includes defects in crystals, impurities or heterogeneities in continuous media, ... Our aim is to develop new mathematical and numerical tools, including probabilistic approaches, to address the current challenging problems of interest in materials science.

In this report, we first focus on developping *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, while affordable approaches do not rest upon a sound mathematical theoretical setting.

Our aim is to compute the effective or homogenized coefficients that represent the behavior of the material at a macroscopic scale. In a first part (see Section 2), we give a very brief overview of classical results of stochastic homogenization theory. Then we explain why such results lead to *practical* difficulties. In particular, though the effective properties of the material considered here are *deterministic*, their approximations require solving partial differential equations with *random* coefficients posed on large domains. This induces very expensive computations.

In Section 3, we consider one possible technique to decrease the cost of such computations, namely the control variate technique. This variance reduction technique, which is based on using a surrogate model, is classical, and has already been successfully applied in other scientific fields. We show here that it can also be used in the general framework of stochastic homogenization. In our case, the surrogate model that we use is inspired by a defect-type theory, where a perfect periodic material is perturbed by rare defects. This model has been introduced in [9] in the context of weakly random models. Here, we address the fully random case, and show that the perturbative approach proposed in [9, 11] can be turned into an efficient control variable. When the perturbation is not small, the perturbative approach, although not accurate, is good enough to reduce the variance of a complete computation. For a large class of initial highly oscillatory coefficients, the resulting approach yields a significantly more precise estimation of the properties of the effective material, *at equal computational cost*, than Monte Carlo approaches or other variance reduction approaches that we have previously

adapted to the homogenization setting.

In Section 4, we address questions related to non-periodic modelling of multiscale materials. Random modelling is indeed a standard modelling response to situations when the idealized, say periodic, modelling is inappropriate. It is however commonly admitted, and observed in practice, that random modelling leads to possibly prohibitively computationally expensive problems. There is a definite theoretical and practical interest in generalizing modelling of perfect materials in directions different from the random paradigm.

Within the current contract, we have investigated this idea, which has not been explored in the previous ONR grant. The general approach, that we describe in Section 4, consists in approximating at the fine scale the solution to an elliptic equation with oscillatory coefficient when this coefficient consists of a "nice" function (say periodic) which is perturbed by a local defect. To date, the questions that have been investigated are essentially of a theoretical nature. They yet give rise to an associated numerical endeavour, that is now on the horizon.

In Section 5, we also investigate a research direction that has not been explored in the previous ONR grant. All models that involve a random parameter require (at least a partial, and most often a complete) knowledge of the distribution of this random parameter. Now, access to this distribution is practically 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. Put differently, 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*. The parameter identification problem that we consider in Section 5 exactly fits in this preliminary step.

The works described below have been performed (jointly or separately) by Claude Le Bris (PI), Frédéric Legoll (Co-PI) and William Minvielle (Ph.D. student).

# 2 Basics of stochastic homogenization

*[A detailed presentation can be read in [8, 14].]*

For the sake of completeness, and to fix notations, we give here a very brief overview of classical results of stochastic homogenization theory. The reader familiar with stochastic homogenization can proceed directly to our contributions, detailed in Sections 3, 4 and 5.

Stochastic homogenization is best understood in the light of the easiest context of homogenization: *periodic homogenization*. This is the reason why we begin by 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 [17, 19, 22] for more details on homogenization theory, and to the review article [8], where we addressed some computational challenges in numerical stochastic homogenization. A super elementary introduction is contained in [15].

## 2.1 Periodic homogenization

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

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

where the matrix $A_{\text{per}}$ 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 $\mathbb{R}^d$,

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

It has a unique solution up to the addition of a constant. Then, the *homogenized* matrix $A^\star$ is such that, for any $p \in \mathbb{R}^d$,

$$A^\star\, p = \int_Q A_{\text{per}}(y)\left(p + \nabla w_p(y)\right) dy,$$

where $Q = (0,1)^d$ is the unit cube. The main result of periodic homogenization theory is that, as $\varepsilon$ goes to zero, the solution $u^\varepsilon$ to (1) converges to $u^\star$ solution to

$$\begin{cases} -\text{div}\left[A^\star \nabla u^\star\right] = f \quad \text{in} \quad \mathcal{D}, \\ u^\star = 0 \quad \text{on} \quad \partial\mathcal{D}. \end{cases} \tag{3}$$

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

The practical interest of the approach is evident. No small scale $\varepsilon$ is present in the homogenized problem (3). 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 $\varepsilon$ small. A direct attack of problem (1) would require taking a meshsize smaller than $\varepsilon$. The difficulty has been circumvented. Of course, many improvements and alternatives exist in the literature.

## 2.2 Stochastic homogenization

Stochastic homogenization has a mathematical setting that is more involved than that of the periodic case.

We consider the theoretical setting of *stationary ergodic homogenization*, with a *discrete* shift operator, which 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 *probability law* of the microstructures is the same. This is *stationarity*. On the other hand, *ergodicity* means that considering all the points in the material is equivalent to fixing a point $x$ in this material and considering all the possible microstructures present there.

Consider now the problem

$$\begin{cases} -\mathrm{div}\left(A\left(\dfrac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right) = f \quad \text{in} \quad \mathcal{D}, \\ u^\varepsilon = 0 \quad \text{on} \quad \partial\mathcal{D}, \end{cases} \tag{4}$$

where the matrix $A$, encoding the properties of the material, is assumed to be stationary (or, equivalently, statistically homogeneous). The solution $u^\varepsilon$ to (4) converges, when $\varepsilon \to 0$, to the solution $u^\star$ to (3) where the homogenized matrix is now given, for any $p \in \mathbb{R}^d$, by

$$A^\star p = \mathbb{E}\left(\int_Q A(y,\cdot)\left(p + \nabla w_p(y,\cdot)\right) dy\right), \tag{5}$$

and the corrector problem now reads

$$\begin{cases} -\mathrm{div}\left[A(y,\omega)\left(p + \nabla w_p(y,\omega)\right)\right] = 0 \quad \text{in} \quad \mathbb{R}^d, \\ \nabla w_p \text{ is stationary}, \quad \mathbb{E}\left(\displaystyle\int_Q \nabla w_p(y,\cdot)\, dy\right) = 0. \end{cases} \tag{6}$$

A striking difference between the stochastic setting and the periodic setting can be observed comparing (2) and (6). In the periodic setting, the corrector problem is posed on a *bounded* domain, namely the periodic cell $Q$. In sharp contrast, the corrector problem (6) 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 fact that the random corrector problem is posed on the entire space has far reaching consequences for numerical practice. In particular, this is the reason why standard methods available in the literature often lead to very costly computations, a fact which in turn motivates our work.

# 3 Variance reduction techniques for stochastic homogenization

*[Work expanded in [6].]*

## 3.1 The direct numerical approach

Practical approximations of the homogenized matrix in random homogenization are not easily obtained, owing to the fact that the corrector problem (6) is set on the entire space. In

practice, truncations have to be considered, and the exact homogenized coefficients are only obtained in the asymptotic regime.

In practice, the matrix $A^\star$ is indeed approximated by $A_N^\star(\omega)$ defined by

$$\forall p \in \mathbb{R}^d, \quad A_N^\star(\omega)\, p = \frac{1}{|Q_N|} \int_{Q_N} A(y,\omega) \left(p + \nabla w_p^N(y,\omega)\right) dy, \tag{7}$$

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

$$\begin{cases} -\text{div}\left[A(\cdot,\omega)\left(p + \nabla w_p^N(\cdot,\omega)\right)\right] = 0 \quad \text{on} \quad \mathbb{R}^d, \\ w_p^N(\cdot,\omega) \text{ is } Q_N\text{-periodic.} \end{cases} \tag{8}$$

Although $A^\star$ itself is a deterministic object, its practical approximation $A_N^\star$ is random, for all $N$ finite. It is only in the limit of infinitely large domains $Q_N$ that the deterministic value is attained. It has indeed been shown in [18, Theorem 1] that $\lim_{N\to\infty} A_N^\star(\omega) = A^\star$.

We now remark that the error can be decomposed as

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

where the first term is a statistical error and the second term is a bias (systematic error). We focus here on the *statistical error*, and propose approaches yielding better approximations of $\mathbb{E}\left[A_N^\star\right]$, for a given truncated domain $Q_N$. Optimal estimates on the variance of $A_N^\star$ have been established in [23, Theorem 1.3 and Proposition 1.4]. See also [20, Theorem 1]. In these works, it has been noted that the systematic error is much smaller than the statistical error, in the sense that the latter decays with a slower rate with respect to $N$ than the former. These results are consistent with numerical observations. For large values of $N$, the statistical error (that we address here) is therefore dominating over the systematic error. There is thus a definite practical interest to focus on that error and design approaches to reduce it, as we do here.

To approximate $\mathbb{E}\left[A_N^\star\right]$, a standard way is the Monte Carlo method. We give ourselves a set of $M$ independent copies (or realizations) $(A^m)_{1\le m\le M}$ of the random coefficient $A$. The corresponding truncated problems (8) are solved, which provides us with a sequence of independent and identically distributed homogenized matrices $A_N^{\star,m}(\omega)$, defined, for any $p \in \mathbb{R}^d$, by

$$A_N^{\star,m}(\omega)\, p = \frac{1}{|Q_N|} \int_{Q_N} A^m(\cdot,\omega) \ \left(p + \nabla w_p^{N,m}(\cdot,\omega)\right),$$

where $w_p^{N,m}$ is the solution to the corrector problem (8) associated to $A^m$. Then we define the empirical mean

$$\mu_M\left(A_N^\star\right) = \frac{1}{M} \sum_{m=1}^{M} A_N^{\star,m}. \tag{9}$$

Since the matrices $A_N^\star$ are i.i.d., the strong law of large numbers applies:

$$\mu_M\left(A_N^\star\right)(\omega) \underset{M\to+\infty}{\longrightarrow} \mathbb{E}\left(A_N^\star\right) \text{ almost surely.}$$

The central limit theorem then yields, for any component $1 \leq i, j \leq d$,

$$\sqrt{M}\left(\mu_M\left([A_N^\star]_{ij}\right) - \mathbb{E}\left([A_N^\star]_{ij}\right)\right) \xrightarrow[M\to+\infty]{\mathcal{L}} \sqrt{\mathbb{V}\mathrm{ar}\left([A_N^\star]_{ij}\right)}\,\mathcal{N}(0,1), \tag{10}$$

where the convergence holds in law, and $\mathcal{N}(0,1)$ denotes the standard Gaussian law. From (10) it is commonly admitted that the exact mean $\mathbb{E}\left([A_N^\star]_{ij}\right)$ lies in the confidence interval

$$\left[\mu_M\left([A_N^\star]_{ij}\right) - 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}\left([A_N^\star]_{ij}\right)}}{\sqrt{M}}\ ,\ \mu_M\left([A_N^\star]_{ij}\right) + 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}\left([A_N^\star]_{ij}\right)}}{\sqrt{M}}\right].$$

The value $\mu_M\left([A_N^\star]_{ij}\right)$ is thus, for both $M$ and $N$ sufficiently large, often adopted as an approximation of the exact value $[A^\star]_{ij}$. The overall computation described above is thus very expensive, because each realization requires a new solution to the problem (8) of presumably large a size since $N$ is taken large.

In the sequel, we show that, using a control variate approach, we can design a practical approach that, for any finite $N$, allows to compute a better approximation of $\mathbb{E}\left[A_N^\star\right]$ than (9). Otherwise stated, for an equal computational cost, we obtain a more accurate (i.e. with a smaller confidence interval) approximation.

We detail in Section 3.2 the general principle of the approach, and show how to apply it to the homogenization setting in Sections 3.3 and 3.4. We next collect our numerical results in Section 3.5 and our theoretical results in Section 3.6.

## 3.2 The control variate technique: general principle

Before applying the approach to our specific setting, we briefly describe here the control variate approach in a general context. Considering a random variable $X$, our aim is to compute its expectation $\mathbb{E}(X)$. In the sequel, we will use that approach for the random variable $(A_N^\star(\omega))_{ij}$, for any entry $1 \leq i, j \leq d$.

As pointed out above, a first possibility is to resort to $M$ i.i.d. realizations of $X$, denoted $X^m(\omega)$ for $1 \leq m \leq M$. The expectation is then approximated by the Monte Carlo empirical mean

$$I_M^{\mathrm{MC}} = \frac{1}{M}\sum_{m=1}^{M} X^m(\omega)$$

and we know that, with a probability equal to 95 %, $\mathbb{E}\left[X\right]$ lies in the confidence interval

$$\left[I_M^{\mathrm{MC}} - 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}\left[X\right]}}{\sqrt{M}}, I_M^{\mathrm{MC}} + 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}\left[X\right]}}{\sqrt{M}}\right]. \tag{11}$$

To reduce the variance of the estimation, consider now a random variable $Y$, the expectation of which is analytically known. Then, for any deterministic parameter $\rho$ to be fixed later, we consider the *controlled variable*

$$D_\rho(\omega) = X(\omega) - \rho\Big(Y(\omega) - \mathbb{E}[Y]\Big). \tag{12}$$

Since $\mathbb{E}[Y]$ is known exactly, sampling realizations of $D_\rho$ amounts to sampling realizations of $X$ and $Y$. We obviously have $\mathbb{E}[D_\rho] = \mathbb{E}[X]$. To approximate $\mathbb{E}[X]$, the control variate approach consists in performing a standard Monte Carlo approximation on $D_\rho$. We hence consider $M$ i.i.d. realizations of $D_\rho$, denoted $D_\rho^m(\omega)$, introduce the empirical mean

$$I_M^{\mathrm{CV}} = \frac{1}{M}\sum_{m=1}^{M} D_\rho^m(\omega) = \frac{1}{M}\sum_{m=1}^{M}\left[X^m(\omega) - \rho\Big(Y^m(\omega) - \mathbb{E}[Y]\Big)\right],$$

and write that, with a probability equal to 95 %, $\mathbb{E}[D_\rho] = \mathbb{E}[X]$ lies in the confidence interval

$$\left[I_M^{\mathrm{CV}} - 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}[D_\rho]}}{\sqrt{M}}, I_M^{\mathrm{CV}} + 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}[D_\rho]}}{\sqrt{M}}\right]. \tag{13}$$

If $\rho$ and $Y$ are such that $\mathbb{V}\mathrm{ar}[D_\rho] < \mathbb{V}\mathrm{ar}[X]$, then the width of the above confidence interval is smaller than that of (11), and hence we have built a more accurate approximation of $\mathbb{E}[X]$.

The choice of $Y$ is problem-dependent and is discussed below in our specific context (see Section 3.4). Assuming for now that $Y$ is given, we detail here the classical rationale and technique employed to choose $\rho$ in (12). We wish to pick $\rho$ such that the variance of $D_\rho$ is minimal. Writing that

$$\mathbb{V}\mathrm{ar}[D_\rho] = \mathbb{V}\mathrm{ar}[X] - 2\rho\mathbb{C}\mathrm{ov}[X,Y] + \rho^2\mathbb{V}\mathrm{ar}[Y],$$

we see that the optimal value of $\rho$ reads

$$\rho^\star = \mathrm{argmin}\ \mathbb{V}\mathrm{ar}[D_\rho] = \frac{\mathbb{C}\mathrm{ov}[X,Y]}{\mathbb{V}\mathrm{ar}[Y]}. \tag{14}$$

For this choice, we have, using the Cauchy-Schwarz inequality,

$$\mathbb{V}\mathrm{ar}[D_{\rho^\star}] = \mathbb{V}\mathrm{ar}[X]\left(1 - \frac{(\mathbb{C}\mathrm{ov}[X,Y])^2}{\mathbb{V}\mathrm{ar}[X]\mathbb{V}\mathrm{ar}[Y]}\right) \leq \mathbb{V}\mathrm{ar}[X].$$

We thus observe that, for any choice of $Y$, we can choose $\rho$ such that the variance of $D_\rho$ is indeed smaller than that of $X$. Of course, the ratio of variances $\dfrac{\mathbb{V}\mathrm{ar}[D_{\rho^\star}]}{\mathbb{V}\mathrm{ar}[X]}$, which is directly related to the gain in accuracy, depends on $Y$, and more precisely on the value of $\dfrac{(\mathbb{C}\mathrm{ov}[X,Y])^2}{\mathbb{V}\mathrm{ar}[X]\mathbb{V}\mathrm{ar}[Y]}$. The larger the correlation between $X$ and $Y$, the better. In particular, we see that the control variable $Y$ needs to be *random*.

In practice, we do not have access to the optimal value (14), which involves exact expectations. One possibility (which is the one we adopt here) is to replace (14) by the empirical estimator

$$\rho^\star \approx \rho^\star_{\mathrm{emp}}(\omega) := \frac{\sum_{m=1}^{M}\left(X^m(\omega) - \mu_M(X)\right)\left(Y^m(\omega) - \mathbb{E}[Y]\right)}{\sum_{m=1}^{M}(Y^m(\omega) - \mathbb{E}[Y])^2}, \tag{15}$$

where $\mu_M(X) = \dfrac{1}{M}\displaystyle\sum_{m=1}^{M} X^m(\omega)$. This choice corresponds to minimizing with respect to $\rho$ the empirical variance of $D_\rho$ defined as $\dfrac{1}{M}\displaystyle\sum_{m=1}^{M}\big(D_\rho^m(\omega) - \mu_M(X)\big)^2$, where $D_\rho^m(\omega) = X^m(\omega) - \rho\Big(Y^m(\omega) - \mathbb{E}[Y]\Big)$. The expectation $\mathbb{E}(X)$ is then approximated by

$$I_M^{\mathrm{CV}} = \frac{1}{M}\sum_{m=1}^{M}\Big[X^m(\omega) - \rho^\star_{\mathrm{emp}}(\omega)\Big(Y^m(\omega) - \mathbb{E}[Y]\Big)\Big].$$

## 3.3 A weakly random setting: rare defects in a periodic structure

As pointed out in the introduction, the surrogate model that we use to build our controlled variable is inspired by a defect-type model, introduced in [9, 10, 11] in the context of weakly random models, and which we describe now.

### 3.3.1 Presentation of the model

Assume that, in (4), the random matrix $A$ is of the form

$$A(x,\omega) = A_\eta(x,\omega) = A_{\mathrm{per}}(x) + b_\eta(x,\omega)\Big(C_{\mathrm{per}}(x) - A_{\mathrm{per}}(x)\Big) \tag{16}$$

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

$$b_\eta(x,\omega) = \sum_{k\in\mathbb{Z}^d} \mathbf{1}_{Q+k}(x) B_k^\eta(\omega), \tag{17}$$

where $(B_k^\eta)_{k\in\mathbb{Z}^d}$ are i.i.d. scalar random variables. We furthermore assume that $B_k^\eta$ follows a Bernoulli law of parameter $\eta \in (0,1)$:

$$\mathbb{P}(B_k^\eta = 1) = \eta, \quad \mathbb{P}(B_k^\eta = 0) = 1-\eta. \tag{18}$$

In each cell $Q+k$, the field $A$ is equal to $A_{\mathrm{per}}$ with the probability $1-\eta$, and equal to $C_{\mathrm{per}}$ with the probability $\eta$. When $\eta$ is small, then (16)–(17)–(18) models a periodic material (described by $A_{\mathrm{per}}$) that is randomly perturbed (and then described by $C_{\mathrm{per}}$). The perturbation is rare when $\eta$ is small (therefore the material is described by $A_{\mathrm{per}}$ "most of the time"), and thus it can be considered as a defect. However, the perturbation $C_{\mathrm{per}} - A_{\mathrm{per}}$ is not small. We refer to [11] for practical examples motivating this framework.

On Fig. 1, we show two realizations of the field $A_\eta(x,\omega)$ (on the domain $Q_N$ for $N = 20$) for some specific choices of $A_{\mathrm{per}}$ and $C_{\mathrm{per}}$ (see [11, Fig. 4.2] for more details). On the right part of that figure, we set $\eta = 0.4$, which is close to the value $\eta = 1/2$, when defects are as frequent as non-defects.

Note that specifying $A_\eta(x,\omega)$ on $Q_N$ simply amounts to specifying the values of $B_k^\eta(\omega)$ for all $k$ such that $k + Q \subset Q_N$.

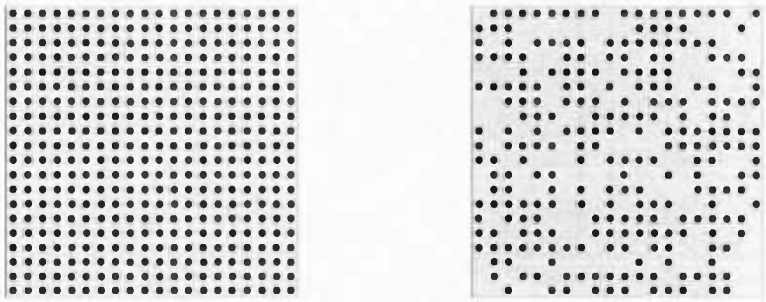

Figure 1: Two instances of material (16). Left ($\eta = 0$): perfect material with circular inclusions located on a periodic network. Right ($\eta = 0.4$): perturbed material (each inclusion is deleted with a probability equal to 0.4).

### 3.3.2 Weakly-random homogenization result

Consider the model (16)–(17)–(18). The random variable $B_k^\eta(\omega)$ can take only two values, 0 or 1. Therefore, on the domain $Q_N$, there are only a finite number of realizations of $A_\eta(x,\omega)$. The realizations with the highest probabilities are as follows.

With probability $(1-\eta)^{|Q_N|}$, there are no defects in $Q_N$, and the realization actually corresponds to the perfect periodic situation. We introduce the periodic corrector $w_p^0$, solution to

$$-\mathrm{div}\left(A_{\mathrm{per}}\left(p+\nabla w_p^0\right)\right)=0, \qquad w_p^0 \text{ is } Q\text{-periodic}, \tag{19}$$

and the associated matrix $A^\star_{\mathrm{per}}$, obtained by periodic homogenization:

$$\forall p\in\mathbb{R}^d, \quad A^\star_{\mathrm{per}}\, p=\int_Q A_{\mathrm{per}}\left(p+\nabla w_p^0\right). \tag{20}$$

With probability $\eta(1-\eta)^{|Q_N|-1}$, there is a unique defect in $Q_N$, located, say, in the cell $k+Q$ (see Fig. 2). Let us define

$$A_1^k = A_{\mathrm{per}} + 1_{k+Q}\Big(C_{\mathrm{per}} - A_{\mathrm{per}}\Big), \tag{21}$$

the associated corrector $w_p^{1,k,N}$, solution to

$$-\mathrm{div}\left(A_1^k\left(p+\nabla w_p^{1,k,N}\right)\right)=0, \qquad w_p^{1,k,N} \text{ is } Q_N\text{-periodic}, \tag{22}$$

and the homogenized matrix $A^\star_{1,k,N}$, given by

$$\forall p\in\mathbb{R}^d, \quad A^\star_{1,k,N}\, p=\frac{1}{|Q_N|}\int_{Q_N} A_1^k\left(p+\nabla w_p^{1,k,N}\right). \tag{23}$$

With probability $\eta^2(1-\eta)^{|Q_N|-2}$, there are two defects in $Q_N$, located, say, in the cells $k+Q$ and $l+Q$ (see Fig. 2). Let us define

$$A_2^{k,l} = A_{\mathrm{per}} + \Big(1_{k+Q}+1_{l+Q}\Big)\Big(C_{\mathrm{per}} - A_{\mathrm{per}}\Big), \tag{24}$$

the associated corrector $w_p^{2,k,l,N}$, solution to

$$-\mathrm{div}\left(A_2^{k,l}\left(p+\nabla w_p^{2,k,l,N}\right)\right)=0, \qquad w_p^{2,k,l,N} \text{ is } Q_N\text{-periodic}, \tag{25}$$

and the homogenized matrix $A^\star_{2,k,l,N}$, given by

$$\forall p\in\mathbb{R}^d, \quad A^\star_{2,k,l,N}\,p=\frac{1}{|Q_N|}\int_{Q_N}A_2^{k,l}\left(p+\nabla w_p^{2,k,l,N}\right). \tag{26}$$

All the other configurations (with three defects or more) have a smaller probability.

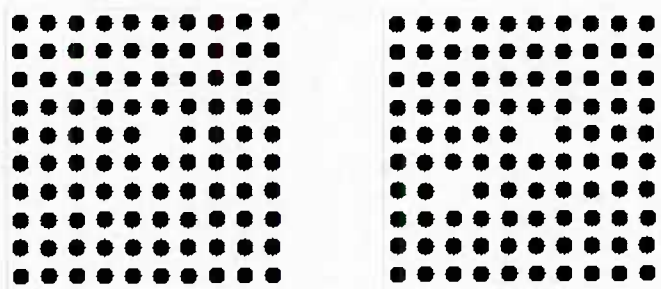

Figure 2: Left: material modelled by $A_1^k$, with a single defect. Right: material modelled by $A_2^{k,l}$, with two defects.

As formally shown in [11, Section 3.2], we then have the following result, for any given $N$:

$$\mathbb{E}\left[A^\star_{\eta,N}\right]=A^\star_{\rm per}+\eta\overline{A}_1^N+\eta^2\overline{A}_2^N+O(\eta^3), \tag{27}$$

where $A^\star_{\rm per}$ is given by (20) and

$$\begin{aligned}\overline{A}_1^N &= \sum_{k\in\mathcal{I}_N}\left(A^\star_{1,k,N}-A^\star_{\rm per}\right),\\ \overline{A}_2^N &= \frac{1}{2}\sum_{k,l\in\mathcal{I}_N,k\neq l}\left(A^\star_{2,k,l,N}-A^\star_{1,k,N}-A^\star_{1,l,N}+A^\star_{\rm per}\right),\end{aligned}$$

where

$$\mathcal{I}_N:=\left\{k\in\mathbb{Z}^d;\ Q+k\subset Q_N\right\}.$$

We note that

$$\overline{A}_1^N=\sum_{k\in\mathcal{I}_N}\overline{A}_{1\,\rm def}^{k,N}, \quad \text{and} \quad \overline{A}_2^N=\frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,l\neq k}\overline{A}_{2\,\rm def}^{k,l,N}, \tag{28}$$

where $\overline{A}_{1\,\rm def}^{k,N}$ (resp. $\overline{A}_{2\,\rm def}^{k,l,N}$) is the "marginal contribution" to the homogenized matrix from a configuration with a single defect in $k+Q$ (resp. two defects in $k+Q$ and $l+Q$):

$$\overline{A}_{1\,\rm def}^{k,N} = A^\star_{1,k,N}-A^\star_{\rm per}, \tag{29}$$

$$\overline{A}_{2\,\rm def}^{k,l,N} = A^\star_{2,k,l,N}-A^\star_{1,k,N}-A^\star_{1,l,N}+A^\star_{\rm per}. \tag{30}$$

We refer to [11] for illustrative numerical results.

Due to periodic boundary conditions (22), that are reminiscent of the periodic boundary conditions in (8), we have that

$$A^\star_{1,k,N} \text{ does not depend on } k. \tag{31}$$

Likewise, $A^\star_{2,k,l,N}$ depends only on $k-l$. Thus, there is only *one* problem (22) to be solved (say for $k=0$). Likewise, there are $|\mathcal{I}_N|-1$ problems (25) to be solved (say for $k=0$ and $l\neq 0$), and not $|\mathcal{I}_N|$ ($|\mathcal{I}_N|-1$). Noticing that (25) is a problem parameterized by $l$, the authors of [16] have shown how to use a Reduced Basis approach to further speed-up the computation of $\overline{A}_2^N$. In practice, one can still obtain a good approximation of $\overline{A}_2^N$ without solving all the $|\mathcal{I}_N|-1$ problems (25).

## 3.4 Application to stochastic homogenization

We now introduce, for the model (16)–(17)–(18), a control variate approach. Our aim is now to address the regime when $\eta$ is *not* close to 0 or 1 (the approximation (27) is therefore not accurate enough). Recall also that, in view of the discussion of Section 3.2, we need a *random* surrogate model to build our controlled variable. In what follows, we first build an approximate model based on configurations with a single defect (see Section 3.4.1), and next turn to building a better approximate model that also uses configurations with two defects (see Section 3.4.2). As will be seen below, this second approximate model not only depends on the quantity of defects, but also on their geometry, that is on where the defects are located in $Q_N$.

Numerical results obtained with these approaches are collected in Section 3.5. On the particular test-case at hand, we will observe (see Fig. 5 below) that the approach using the single defects provides a variance reduction ratio close to 6, while the approach using single defects and pairs of defects provides a gain roughly 6 times larger (here of the order of 40).

### 3.4.1 A first-order model

Recall (see (16)–(17)) that

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

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

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

where $(B_k^\eta)_{k\in\mathbb{Z}^d}$ are i.i.d. scalar random variables. Introduce

$$A_1^{\eta,N}(\omega) = \sum_{k\in\mathcal{I}_N} B_k^\eta(\omega)\, \overline{A}_{1\,\rm def}^{k,N}, \tag{32}$$

where $\overline{A}_{1\,\rm def}^{k,N}$, defined by (29), is the "marginal contribution" to the homogenized matrix coming from the configuration with a single defect located in $k+Q$. In view of (28), we notice that

$$\mathbb{E}\left[A_1^{\eta,N}\right] = \sum_{k\in\mathcal{I}_N} \mathbb{E}\left[B_k^\eta\right] \overline{A}_{1\,\rm def}^{k,N} = \eta \sum_{k\in\mathcal{I}_N} \overline{A}_{1\,\rm def}^{k,N} = \eta \overline{A}_1^N,$$

which is the first order correction in the expansion (27). When $\eta$ is small, the expectation of $A^\star_{\text{per}} + A_1^{\eta,N}(\omega)$ is a good approximation of the expectation of $A^\star_{\eta,N}(\omega)$, accurate up to an error of the order of $\eta^2$. Thus $A^\star_{\text{per}} + A_1^{\eta,N}(\omega)$ is a good surrogate model for $A^\star_{\eta,N}(\omega)$. Following (12), we now introduce our controlled variable as

$$\begin{aligned} D_\rho^{1,\eta}(\omega) &= A^\star_{\eta,N}(\omega) - \rho\left(A^\star_{\text{per}} + A_1^{\eta,N}(\omega) - \mathbb{E}\left[A^\star_{\text{per}} + A_1^{\eta,N}\right]\right) \\ &= A^\star_{\eta,N}(\omega) - \rho\left(A_1^{\eta,N}(\omega) - \eta \overline{A}_1^N\right). \end{aligned} \tag{33}$$

In view of (32), (29) and (31), we recast (33) as

$$D_\rho^{1,\eta}(\omega) = A^\star_{\eta,N}(\omega) - \rho\left[\left(\sum_{k\in\mathcal{I}_N} B_k^\eta(\omega)\right) - \eta\,|\mathcal{I}_N|\right] \overline{A}^{0,N}_{1\,\text{def}}. \tag{34}$$

**Remark 1** *Note that, in* (34), $A^\star_{\eta,N}(\omega)$ *and* $\sum_{k\in\mathcal{I}_N} B_k^\eta(\omega)$ *are correlated. Indeed, in practice, we start by drawing a realization of the random variables* $B_\eta^k(\omega)$ *for all* $k \in \mathcal{I}_N$. *This determines first* $\sum_{k\in\mathcal{I}_N} B_k^\eta(\omega)$, *and second the field* $A(x,\omega)$ *on* $Q_N$, *from which we compute the associated* $A^\star_{\eta,N}(\omega)$ *following* (7)–(8). *The fact that* $A^\star_{\eta,N}(\omega)$ *and* $\sum_{k\in\mathcal{I}_N} B_k^\eta(\omega)$ *are correlated is important in view of variance reduction, as explained in Section 3.2.*

Computing $M$ realizations of $D_\rho^{1,\eta}(\omega)$ therefore amounts to:

- (offline stage) determine $\overline{A}^{0,N}_{1\,\text{def}}$ by solving the problem (19)–(20) on $Q$ and solving only once the problem (22)–(23) on $Q_N$ (say for $k = 0$), and
- (online stage) solve $M$ corrector problems (7)–(8) on $Q_N$ (for $M$ i.i.d. realizations of $A$ on $Q_N$), and evaluate $D_\rho^{1,\eta}(\omega)$ according to (34).

Let $\mathcal{C}_N$ denote the cost to solve a single corrector problem on $Q_N$. The Monte Carlo empirical estimator and the Control Variate empirical estimator, defined respectively by

$$I_M^{\text{MC}} = \frac{1}{M}\sum_{m=1}^M A^{\star,m}_{\eta,N}(\omega) \quad \text{and} \quad I_M^{\text{CV}} = \frac{1}{M}\sum_{m=1}^M D_\rho^{1,\eta,m}(\omega),$$

therefore share the same cost ($M\,\mathcal{C}_N$ for the former, $(1+M)\,\mathcal{C}_N$ for the latter). We are now left with choosing $\rho$ in (33) to minimize the variance of any entry $\left(D_\rho^{1,\eta}\right)_{ij}$, $1 \le i,j \le d$. Note that $\rho$ therefore depends on $ij$. This parameter $\rho$ is in practice chosen according to (15).

### 3.4.2 A second-order model

We now introduce a more refined approach, that not only takes into account the contributions from single defects (through $\overline{A}^{k,N}_{1\,\text{def}}$, see (32)) but also contributions from pairs of defects. To that aim, we introduce

$$A_2^{\eta,N}(\omega) = \frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\,l\neq k} B_k^\eta(\omega)\,B_l^\eta(\omega)\,\overline{A}^{k,l,N}_{2\,\text{def}}, \tag{35}$$

where $\overline{A}^{k,l,N}_{2\,\mathrm{def}}$, defined by (30), is the "marginal contribution" to the homogenized matrix associated to the configuration with two defects located in $k+Q$ and $l+Q$. In view of (28), we notice that

$$\mathbb{E}\left[A_2^{\eta,N}\right] = \frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\,l\neq k}\mathbb{E}\left[B_k^\eta\,B_l^\eta\right]\overline{A}^{k,l,N}_{2\,\mathrm{def}} = \frac{\eta^2}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\,l\neq k}\overline{A}^{k,l,N}_{2\,\mathrm{def}} = \eta^2\overline{A}_2^N,$$

which is the second order correction in the expansion (27). When $\eta$ is small, the expectation of $A^\star_{\mathrm{per}} + A_1^{\eta,N}(\omega) + A_2^{\eta,N}(\omega)$ is a good approximation of the expectation of $A^\star_{\eta,N}(\omega)$, accurate up to an error of the order of $\eta^3$.

In a way similar to (33), we now introduce our second-order controlled variable as

$$D^{2,\eta}_{\rho_1,\rho_2}(\omega) = A^\star_{\eta,N}(\omega) - \rho_1\left(A_1^{\eta,N}(\omega) - \eta\overline{A}_1^N\right) - \rho_2\left(A_2^{\eta,N}(\omega) - \eta^2\overline{A}_2^N\right). \tag{36}$$

We have introduced two deterministic parameters $\rho_1$ and $\rho_2$, which need not be equal. For any choice of these parameters, we have $\mathbb{E}\left[D^{2,\eta}_{\rho_1,\rho_2}\right] = \mathbb{E}\left[A^\star_{\eta,N}\right]$.

To evaluate (36), we first have to precompute the deterministic matrices

$$\overline{A}^{k,N}_{1\,\mathrm{def}} = \overline{A}^{0,N}_{1\,\mathrm{def}} \quad \text{and} \quad \overline{A}^{k,l,N}_{2\,\mathrm{def}} = \overline{A}^{0,l-k,N}_{2\,\mathrm{def}}.$$

Computing $M$ realizations of $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$ therefore amounts to:

- offline stage: (i) determine $\overline{A}^{0,N}_{1\,\mathrm{def}}$ by solving the problem (19)–(20) on $Q$ and by solving only once the problem (22)–(23) on $Q_N$ (say for $k=0$); (ii) determine $\overline{A}^{0,l,N}_{2\,\mathrm{def}}$ by solving $|\mathcal{I}_N|-1$ problems (25)–(26) on $Q_N$ (for $k=0$ and $l\in\mathcal{I}_N$, $l\neq 0$).
- online stage: solve $M$ corrector problems (7)–(8) on $Q_N$ (for $M$ i.i.d. realizations of $A$ on $Q_N$), and evaluate $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$ according to (36).

Questions related to the cost of evaluating $\overline{A}^{0,l,N}_{2\,\mathrm{def}}$ are discussed below.

Notice that, in the above construction, we have considered as reference configuration the defect-free material, i.e. that for $\eta = 0$. Since, in the regime we focus on, $\eta$ is not small, there is no reason to favor the defect-free configuration ($\eta = 0$) rather than the full defect configuration ($\eta = 1$), which corresponds to the periodic matrix $C_{\mathrm{per}}$. We therefore introduce (compare with (29))

$$\overline{C}^{k,N}_{1\,\mathrm{def}} = C^\star_{1,k,N} - C^\star_{\mathrm{per}},$$

where $C^\star_{1,k,N}$ is the homogenized matrix corresponding to a unique defect with respect to the periodic configuration $C_{\mathrm{per}}$ (compare with (21), (22) and (23)):

$$\forall p\in\mathbb{R}^d,\quad C^\star_{1,k,N}\,p = \frac{1}{|Q_N|}\int_{Q_N} C_1^k\left(p+\nabla v_p^{1,k,N}\right), \tag{37}$$

where, for any $p$, the corrector $v_p^{1,k,N}$ is a solution to

$$-\mathrm{div}\left(C_1^k\left(p+\nabla v_p^{1,k,N}\right)\right) = 0, \qquad v_p^{1,k,N} \text{ is } Q_N\text{-periodic},$$

where $C_1^k = C_{\rm per} - 1_{k+Q}\Big(C_{\rm per} - A_{\rm per}\Big)$. Likewise, we introduce the second order correction (compare with (30)):

$$\overline{C}_{2\,\rm def}^{k,l,N} = C_{2,k,l,N}^\star - C_{1,k,N}^\star - C_{1,l,N}^\star + C_{\rm per}^\star, \tag{38}$$

where $C_{1,k,N}^\star$ is defined by (37) and $C_{2,k,l,N}^\star$ is defined by (compare with (24), (25) and (26)):

$$\forall p \in \mathbb{R}^d, \quad C_{2,k,l,N}^\star\, p = \frac{1}{|Q_N|}\int_{Q_N} C_2^{k,l}\left(p + \nabla v_p^{2,k,l,N}\right), \tag{39}$$

where, for any $p \in \mathbb{R}^d$, the corrector $v_p^{2,k,l,N}$ is a solution to

$$-\mathrm{div}\left(C_2^{k,l}\left(p + \nabla v_p^{2,k,l,N}\right)\right) = 0, \qquad v_p^{2,k,l,N} \text{ is } Q_N\text{-periodic},$$

where $C_2^{k,l} = C_{\rm per} - \Big(1_{k+Q} + 1_{l+Q}\Big)\Big(C_{\rm per} - A_{\rm per}\Big)$. As in (35), we introduce

$$C_2^{\eta,N}(\omega) = \frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\, l\neq k}\Big(1 - B_k^\eta(\omega)\Big)\Big(1 - B_l^\eta(\omega)\Big)\,\overline{C}_{2\,\rm def}^{k,l,N}, \tag{40}$$

where $\overline{C}_{2\,\rm def}^{k,l,N}$ is defined by (38). Its expectation reads

$$\begin{aligned}\overline{C}_2^{\eta,N} := \mathbb{E}\left[C_2^{\eta,N}\right] &= \frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\, l\neq k}\mathbb{E}\left[\left(1 - B_k^\eta\right)\left(1 - B_l^\eta\right)\right]\overline{C}_{2\,\rm def}^{k,l,N} \\ &= \frac{1}{2}\sum_{k\in\mathcal{I}_N}\sum_{l\in\mathcal{I}_N,\, l\neq k}(1-\eta)^2\,\overline{C}_{2\,\rm def}^{k,l,N}.\end{aligned}$$

We eventually introduce the controlled variable (compare with (36))

$$\begin{aligned}D_{\rho_1,\rho_2,\rho_3}^{3,\eta}(\omega) = A_{\eta,N}^\star(\omega) &- \rho_1\left(A_1^{\eta,N}(\omega) - \eta\overline{A}_1^N\right) \\ &- \rho_2\left(A_2^{\eta,N}(\omega) - \eta^2\overline{A}_2^N\right) - \rho_3\left(C_2^{\eta,N}(\omega) - \overline{C}_2^{\eta,N}\right).\end{aligned} \tag{41}$$

Consider now a specific entry $1 \le i,j \le d$ of the homogenized matrix. The control variate approach consists in approximating $\mathbb{E}\left[\left(A_{\eta,N}^\star\right)_{ij}\right]$ by considering a Monte Carlo estimator for $\mathbb{E}\left[\left(D_{\rho_1,\rho_2,\rho_3}^{3,\eta}\right)_{ij}\right]$. The deterministic parameters $\rho_1$, $\rho_2$ and $\rho_3$ are ideally chosen to minimize the variance of $\left(D_{\rho_1,\rho_2,\rho_3}^{3,\eta}(\omega)\right)_{ij}$. They depend on $ij$ and are the solution of the following $3\times 3$ linear system (we drop the subscript $i,j$ for conciseness):

$$\begin{aligned}\mathbb{V}\mathrm{ar}[A_1^{\eta,N}]\rho_1 + \mathbb{C}\mathrm{ov}[A_1^{\eta,N}, A_2^{\eta,N}]\rho_2 + \mathbb{C}\mathrm{ov}[A_1^{\eta,N}, C_2^{\eta,N}]\rho_3 &= \mathbb{C}\mathrm{ov}[A_{\eta,N}^\star, A_1^{\eta,N}] \\ \mathbb{C}\mathrm{ov}[A_2^{\eta,N}, A_1^{\eta,N}]\rho_1 + \mathbb{V}\mathrm{ar}[A_2^{\eta,N}]\rho_2 + \mathbb{C}\mathrm{ov}[A_2^{\eta,N}, C_2^{\eta,N}]\rho_3 &= \mathbb{C}\mathrm{ov}[A_{\eta,N}^\star, A_2^{\eta,N}] \\ \mathbb{C}\mathrm{ov}[C_2^{\eta,N}, A_1^{\eta,N}]\rho_1 + \mathbb{C}\mathrm{ov}[C_2^{\eta,N}, A_2^{\eta,N}]\rho_2 + \mathbb{V}\mathrm{ar}[C_2^{\eta,N}]\rho_3 &= \mathbb{C}\mathrm{ov}[A_{\eta,N}^\star, C_2^{\eta,N}]\end{aligned}$$

depending on the covariances between the entries $ij$ of $A_{\eta,N}^\star$, $A_1^{\eta,N}$, $A_2^{\eta,N}$ and $C_2^{\eta,N}$. In practice, these covariances are approximated by empirical estimators, as explained in Section 3.2.

In practice, computing the matrices $\overline{A}_{2\,\mathrm{def}}^{0,l,N}$ (and likewise $\overline{C}_{2\,\mathrm{def}}^{0,l,N}$) is rather expensive (because each problem is set on the large domain $Q_N$, and the number of these problems increases when $N$ increases). It is therefore useful to approximate them using the Reduced Basis strategy introduced in [16], which dramatically decreases the computational cost. The procedure is essentially as follows. We first solve the single defect problem (22) for $k = 0$, and solve (25) for a limited number of locations of the defect pairs, say $k = 0$ and $l$ close to $k$. On the basis of these computations, we are then in position to obtain very efficient approximations of the matrices $\overline{A}_{2\,\mathrm{def}}^{0,l,N}$ for all $l \in \mathcal{I}_N$, $l \neq 0$. Evaluating (35) is thus inexpensive. Thus, up to a limited offline cost (i.e. the cost for solving the few problems (25) that we have to consider), the Monte Carlo empirical estimator and the Control Variate empirical estimator, defined respectively by

$$I_M^{\mathrm{MC}} = \frac{1}{M}\sum_{m=1}^{M} A_{\eta,N}^{\star,m}(\omega) \quad \text{and} \quad I_M^{\mathrm{CV}} := \frac{1}{M}\sum_{m=1}^{M} D_{\rho_1,\rho_2,\rho_3}^{3,\eta,m}(\omega),$$

share the same cost.

**Remark 2** *In sharp contrast to the first order control variable, the second order control variable not only depends on the number of defects in the materials, i.e.* $\sum_{k\in\mathcal{I}_N} B_k^{\eta}(\omega)$, *but also on their location. The specific geometry of the materials, which is ignored in* (34), *is taken into account in* (41).

In the sequel, we demonstrate numerically the efficiency of the approach (see e.g. Figure 5 below), before giving some theoretical arguments proving that variance is indeed reduced.

## 3.5 Numerical experiments

We now apply the methodology described above to some two-dimensional model material for which the field $A$ is of the form (16)–(17)–(18) (see Fig. 3). We choose

$$A_{\mathrm{per}}(x) = \alpha \mathrm{Id}_2 \quad \text{and} \quad C_{\mathrm{per}}(x) = \beta \mathrm{Id}_2,$$

with $\alpha = 3$ and $\beta = 23$ (similar qualitative conclusions are obtained with other generic values). All variances are estimated on the basis of $M = 100$ independent realizations. All the correctors problems have been solved using FreeFEM++ [21], on a mesh of size $h = 0.2$, using P1 finite elements. We present here some numerical results, and refer to [6] for additional results.

On Fig. 4, we plot as a function of $\eta \in (0, 1)$ three quantities:

- the first entry of the matrix $\mathbb{E}\left[A_{\eta,N}^{\star}\right]$ (obtained in practice by an expensive Monte Carlo estimation);
- the weakly stochastic approximation (27), which is an approximation of $\mathbb{E}\left[A_{\eta,N}^{\star}\right]$ with an error of the order of $O(\eta^3)$;
- the weakly stochastic approximation obtained in the regime $(1-\eta) \ll 1$, which is an approximation of $\mathbb{E}\left[A_{\eta,N}^{\star}\right]$ with an error of the order of $O\big((1-\eta)^3\big)$.

Figure 3: A typical realization of the checkerboard test-case with $\eta = 1/2$.

We work with $N = 10$, and the following observations are also valid for larger values of $N$. We see on Fig. 4 that, when $\eta \leq 0.4$, the deterministic expansion (27) is a very accurate approximation of $\mathbb{E}\left[\left(A^{\star}_{\eta,N}\right)_{11}\right]$. This approximation is inexpensive to compute. The same observation holds in the regime $\eta \geq 0.7$, where the deterministic expansion around $\eta = 1$ provides a satisfying approximation. However, we note that none of the two weakly stochastic expansions are accurate when $0.4 \leq \eta \leq 0.7$. In that regime, one has to compute $\mathbb{E}\left[\left(A^{\star}_{\eta,N}\right)_{11}\right]$ by considering several realizations of (7)–(8). In that regime, considering a variance reduction approach is useful.

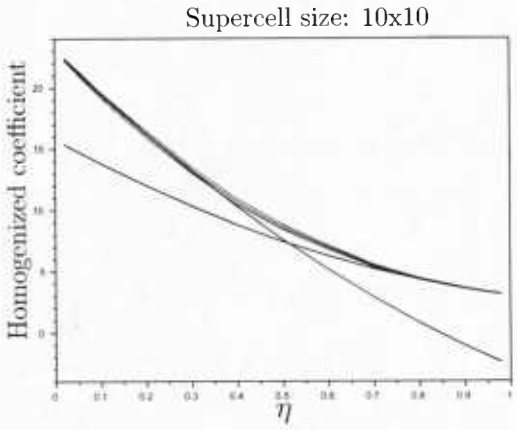


Figure 4: $\mathbb{E}\left[\left(A^{\star}_{\eta,N}\right)_{11}\right]$ as a function of $\eta$, for $N = 10$. Black curves: weakly stochastic approximations. Blue curve: Monte Carlo standard estimator.

In the regime we have identified, we show on Fig. 5 the ratios of variance

$$R_{\eta,N} = \frac{\mathbb{V}\mathrm{ar}\Big(\left[A^{\star}_{\eta,N}\right]_{11}\Big)}{\mathbb{V}\mathrm{ar}(D)}, \tag{42}$$

where $D$ is either the first-order controlled variable $D^{1,\eta}_{\rho}(\omega)$ defined by (33), or the second-order controlled variable $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$ defined by (36), or the controlled variable $D^{3,\eta}_{\rho_1,\rho_2,\rho_3}(\omega)$

defined by (41). The parameter $\rho$ (resp. $(\rho_1, \rho_2)$ and $(\rho_1, \rho_2, \rho_3)$) is chosen to minimize the empirical variance of the estimator (see Section 3.2).

**Remark 3** *The second-order controlled variable $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$ defined by (36) is built by considering $A_{\rm per}$ as the reference. One could alternatively build a second-order controlled variable considering $C_{\rm per}$ as the reference. Numerical results obtained with such a controlled variable are similar to those obtained with $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$ (results not shown).*

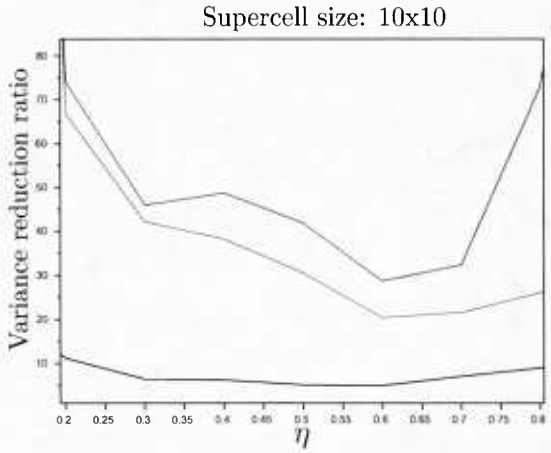


Figure 5: Ratio $R_{\eta,N}$ defined by (42) as a function of $\eta$ ($N = 10$). Black curve: controlled variable $D^{1,\eta}_{\rho}(\omega)$. Red curve: controlled variable $D^{2,\eta}_{\rho_1,\rho_2}(\omega)$. Blue curve: controlled variable $D^{3,\eta}_{\rho_1,\rho_2,\rho_3}(\omega)$.

We observe on Fig. 5 that, for $\eta = 1/2$, the approach using the first-order controlled variable (33) provides a variance reduction ratio (42) close to 6. This gain is close to the gain obtained using an antithetic variable approach (see [13, Table 2]). In contrast, when using the controlled variable (41) taking into account first order and second order corrections with respect to both the cases $\eta = 0$ and $\eta = 1$, we obtain a gain close to 40.

We now investigate how the gain depends on the size of the domain $Q_N$. To that aim, we show on Table 1 the ratio (42) as a function of $N$, for $\eta = 1/2$. We observe that the gain is essentially independent of $N$.

| | $N = 6$ | $N = 10$ | $N = 20$ | $N = 30$ | $N = 50$ |
|---|---|---|---|---|---|
| First order | 7.57 | 5.18 | 6.55 | 8.51 | 7.34 |
| Second order | 35.9 | 41.8 | 37.6 | 35.6 | 40.4 |

Table 1: Ratio $R_{\eta,N}$ defined by (42) as a function of $N$ ($\eta = 1/2$). First order: controlled variable $D^{1,\eta}_{\rho}(\omega)$. Second order: controlled variable $D^{3,\eta}_{\rho_1,\rho_2,\rho_3}(\omega)$.

We eventually plot on Fig. 6 the confidence intervals obtained for the Monte Carlo approach and the Control Variate approach based on (41). The latter confidence interval width is dramatically smaller than the former.

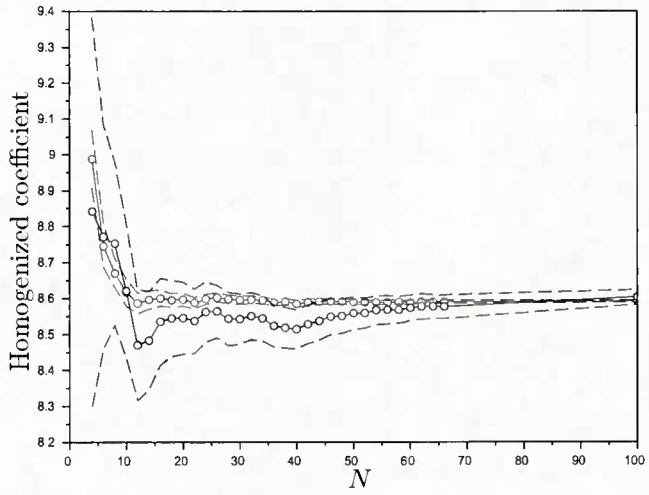


Figure 6: Estimation of $\mathbb{E}\left(\left[A^{\star}_{\eta,N}\right]_{11}\right)$ as a function of $N$. Blue: standard Monte-Carlo estimator. Red: Control Variate estimator based on (41). In both cases, estimators are built using $M = 100$ i.i.d. realizations.

The numerical results presented above have been exposed in details in [6]. They clearly demonstrate, from a numerical perspective, the efficiency of the approach.

## 3.6 Theoretical validation

In [6], we have given arguments that guarantee the efficiency of the method in the one dimensional case. We have also provided there elements of theoretical analysis in higher dimensional settings. We review here the main results that we have obtained.

### 3.6.1 One-dimensional case

In the one-dimensional case, we have the following result:

**Proposition 1** *Consider the model* (16)–(17)–(18) *in the one-dimensional case. Let* $A^{\star}_{\eta,N}$ *be the apparent homogenized matrix defined by* (7)–(8) *and* $D^{1,\eta}_{\rho}$ *be the first-order controlled variable defined by* (33). *Then*

$$\mathbb{V}ar(A^{\star}_{\eta,N}) = \frac{C}{N} + O\left(\frac{1}{N^2}\right)$$

*and, for the optimal value of the deterministic parameter* $\rho$,

$$\min_{\rho} \mathbb{V}ar\left(D^{1,\eta}_{\rho}\right) = \mathbb{V}ar\left(D^{1,\eta}_{\rho^{\star}}\right) = O\left(\frac{1}{N^2}\right).$$

*Let* $D^{3,\eta}_{\rho_1,\rho_2,\rho_3}(\omega)$ *be the second-order controlled variable defined by* (41). *For the optimal value of the deterministic parameters* $\rho_1$, $\rho_2$ *and* $\rho_3$, *we have*

$$\min_{\rho_1,\rho_2,\rho_3} \mathbb{V}ar\left(D^{3,\eta}_{\rho_1,\rho_2,\rho_3}\right) = O\left(\frac{1}{N^3}\right).$$

Using the control variate approach based on the first-order model (resp. second order model), the variance is thus improved by at least one order (resp. two orders) in terms of $N$. Note in particular that, in the above results, we have not assumed $\eta$ to be small.

### 3.6.2 Multi-dimensional case

In the multi-dimensional case, our theoretical results cover the regime $\eta \ll 1$. This is *not* the regime we wish to address with our approach. Obtaining theoretical results in the general case is still an open question. Note that the numerical experiments of Section 3.5 have been perfored in the regime of interest when weakly stochastic approximations (based on the asymptotics $\eta \ll 1$) do not yield accurate results.

Consider any entry $ij$ of the homogenized matrix. The estimation of $\mathbb{E}\left[\left(A^\star_{\eta,N}\right)_{ij}\right]$ can be done by a Monte Carlo empirical mean on $\left(A^\star_{\eta,N}(\omega)\right)_{ij}$, $\left(D^{1,\eta}_{\rho}(\omega)\right)_{ij}$ (see Section 3.4.1) or $\left(D^{2,\eta}_{\rho_1,\rho_2}(\omega)\right)_{ij}$ (see Section 3.4.2).

**Proposition 2** *For any entry $ij$ of the homogenized matrix, we have*

$$\mathbb{V}ar\left[\left(A^\star_{\eta,N}\right)_{ij}\right] = O(\eta), \quad \mathbb{V}ar\left[\left(D^{1,\eta}_{\rho=1}\right)_{ij}\right] = O(\eta^2), \quad \mathbb{V}ar\left[\left(D^{2,\eta}_{\rho_1=\rho_2=1}\right)_{ij}\right] = O(\eta^3).$$

We thus see that, by using the first-order (resp. the second order) surrogate model, the variance is improved by at least one order (resp. two orders) in terms of $\eta$.

# 4 Homogenization approach for the numerical simulation of periodic microstructures with defects

*[Work expanded in [12, 1, 2, 3].]*

The homogenization of (deterministic) non-periodic systems is a well-known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc and P.-L. Lions, C. Le Bris has introduced a possible theory, giving rise to a numerical approach, for the simulation of multiscale non-periodic systems. The theoretical considerations are based on earlier works by the same authors (derivation of an algebra of functions appropriate to formalize a theory of homogenization). The numerical endeavour that is on the horizon is completely new.

The general approach consists in approximating at the fine scale the solution to an elliptic equation with oscillatory coefficient when this coefficient consists of a "nice" function which is, in some sense to be made precise, perturbed. A typical example is that of a periodic material (where the period is small with respect to the size of the sample, so that there exists a separation of scales between the microstructure and the macrostructure), with a superimposed defect in *one* (or "a few") periodic cells. The equation of interest is

$$-\mathrm{div}\left[\left[A_{\mathrm{per}}\left(\frac{x}{\varepsilon}\right) + B_{\mathrm{def}}\left(\frac{x}{\varepsilon}\right)\right]\nabla u_\varepsilon\right] = f \text{ in } \Omega, \tag{43}$$

where the perturbation $B_{\rm def}$ is localized (in the sense that $B_{\rm def}$ vanishes at infinity), while $A_{\rm per}$ encodes the perfect, periodic medium. From the macroscopic standpoint, the overall behavior might, or not, be the same as that of a perfect periodic material. Anyhow, close to the defect (close to the "support" of $B_{\rm def}$), the response is of course very different from that of the perfect material.

We aim at developing numerical approaches able to efficiently and accurately capture this local difference. In terms of material science, this is of course of paramount importance: material failure indeed often occurs close to defects.

The approach is based on the determination of a *local profile*, solution to an equation similar to the corrector equation (2) in classical homogenization. In the case (43) with $B_{\rm def} \in L^2(\mathbb{R}^d)$ (an assumption which somehow formalizes the fact that $B_{\rm def}$ vanishes at infinity), this equation is

$$-\mathrm{div}\left[\left(A_{\rm per} + B_{\rm def}\right)\left(p + \nabla w_p\right)\right] = 0 \text{ in } \mathbb{R}^d,$$

where $p$ is any fixed vector in $\mathbb{R}^d$. The well-posedness of that equation, in various functional settings depending upon the nature of the perturbation, is a theoretical issue that has now been investigated and solved, for several prototypical situations: local perturbation, two different periodic structures separated by a common interface, ...

The theoretical results obtained to date are being collected in the series of publications [12, 1, 2]. The work [12] also contains preliminary numerical simulations, in the case $B_{\rm def} \in L^2(\mathbb{R}^d)$. The review article [3] presents the various approaches within a more general perspective.

The purpose is now to consider cases closer to actual local defects in materials (such as dislocations) and also to put all this in action as a general numerical approach on cases of actual practical relevance.

# 5 A parameter identification problem in stochastic homogenization

*[Work expanded in [7].]*

Consider the highly oscillatory equation (4), where the matrix $A$ is assumed to be random and stationary. We have seen in Section 2.2 that this problem admits the homogenized limit (3). Random homogenization theory actually provides formulas to compute the homogenized matrix $A^\star$, see (5)–(6). We thus have at our disposal a procedure to compute macroscopic quantities if we know the microscopic quantities, and to solve the so-called *forward problem*. However, in practice, given a heterogeneous materials, it is a difficult question to decide on the law of the microscopic physical properties, i.e. on the probability law of $A(x,\omega)$. On the other hand, macroscopic quantities are more easily accessible. It is thus of interest to consider the *inverse problem*, and try to extract some information on the properties of the materials at the microscopic scale on the basis of macroscopic quantities.

Of course, homogenization is an averaging process, which filters out many features of the microscopic coefficients. There is thus no hope to recover a full information about the microstructure (in our case, the *probability distribution* of $A(x,\omega)$) from the only knowledge of macroscopic quantities such as $A^\star$. We adopt here a more restricted objective. We assume a functional form for the distribution of the microscopic field (namely, a Weibull distribution,

see Section 5.1 below) and aim at recovering the *parameters* of that microscopic law of the basis of macroscopic quantities. This question belongs to the wide family of inverse problems. However, the mutiscale context brings in some specificities. We refer to [24] for a review article on inverse problems in such a multiscale context.

## 5.1 The microscopic model

We consider here a problem written at the fine scale as a finite difference problem (rather than as the partial differential equation (4)). The motivation for this choice is related to the particular application (transport phenomena in porous media, modelled as a lattice of channels) we have in mind. However, our approach is not specific to discrete elliptic equations. It could also be applied for problems modelled by continuous elliptic partial differential equations (PDEs) with random, highly oscillatory coefficients, such as (4).

For the sake of completeness, we detail here the homogenization result in the setting of discrete elliptic equations, which is in essence the same as that recalled in Section 2.2.

Let $\mathcal{D}$ be a bounded domain of $\mathbb{R}^d$ and $f \in C^0(\overline{\mathcal{D}})$. Let $A$ be the random stationary matrix field given by

$$\forall x \in \mathbb{Z}^d, \quad A(x,\omega) = \mathrm{diag}\Big(a_1(x,\omega),\dots,a_d(x,\omega)\Big), \tag{44}$$

where the *conductances* $\{a_i(x,\cdot)\}_{1\le i\le d,\ x\in\mathbb{Z}^d}$ form an i.i.d. sequence of random variables. Let $u_\varepsilon$ be the unique solution to

$$\nabla_\varepsilon^\star\big[A(x/\varepsilon,\omega)\nabla_\varepsilon u_\varepsilon(x,\omega)\big] = f(x) \ \text{ in } \mathcal{D}\cap\varepsilon\mathbb{Z}^d, \qquad u_\varepsilon(x,\omega) = 0 \text{ in } (\mathbb{R}^d\setminus\mathcal{D})\cap\varepsilon\mathbb{Z}^d, \tag{45}$$

where the discrete gradient $\nabla_\varepsilon$ (resp. the discrete divergence $\nabla_\varepsilon^\star$) is defined, for any function $v$ defined on the lattice $\varepsilon\mathbb{Z}^d$, by

$$(\nabla_\varepsilon v)(x) = \frac{1}{\varepsilon}\begin{pmatrix} v(x+\varepsilon e_1)-v(x) \\ \vdots \\ v(x+\varepsilon e_d)-v(x)\end{pmatrix}$$

and

$$-(\nabla_\varepsilon^\star v)(x) = \sum_{i=1}^d \frac{v_i(x)-v_i(x-\varepsilon e_i)}{\varepsilon}.$$

The equation (45) plays here the role, in the current setting, of (4).

When $\varepsilon$ goes to 0, $u_\varepsilon$ converges to some homogenized function $u^\star$, solution to the (continuous) partial differential equation (3), where the homogenized matrix $A^\star$ is given as follows:

$$\forall p\in\mathbb{R}^d, \quad A^\star p = \mathbb{E}\big[A(x,\cdot)(p+\nabla w_p(x,\cdot))\big] \tag{46}$$

where, for any $p\in\mathbb{R}^d$, the *corrector* $w_p$ is the unique (up to the addition of a constant) solution to

$$\begin{cases} -\nabla^\star\Big[A(\cdot,\omega)\big(p+\nabla w_p(\cdot,\omega)\big)\Big] = 0 \text{ in } \mathbb{Z}^d, \\ \nabla w_p \text{ is stationary}, \\ \forall x\in\mathbb{Z}^d, \quad \mathbb{E}[\nabla w_p(x,\cdot)] = 0. \end{cases} \tag{47}$$

The expressions (46)–(47) play here the role, in the current setting, of the expressions (5)–(6).

As in the continuous case described in Section 2.2, the corrector problem (47) is untractable in practice, since it is posed in the entire lattice $\mathbb{Z}^d$. Approximations are therefore in order. The standard procedure amounts to considering finite boxes as in Section 3.1. For any $N$, we denote by $Q_N$ the finite box $\{0,\dots,N\}^d$. The *truncated corrector* $w_p^N(\cdot,\omega)$ is defined on $Q_N$ as the solution to

$$\begin{cases} -\nabla^\star\Big[A(\cdot,\omega)\big(p+\nabla w_p^N(\cdot,\omega)\big)\Big] = 0 \text{ in } Q_N, \\ w_p^N(\cdot,\omega) \text{ is } Q_N\text{-periodic.} \end{cases} \tag{48}$$

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

$$\forall p\in\mathbb{R}^d, \quad A_N^\star(\omega)p = \frac{1}{|Q_N|}\sum_{x\in Q_N} A(x,\omega)\big(p+\nabla w_p^N(x,\omega)\big). \tag{49}$$

In the sequel, we assume that the conductances $\{a_i(x,\omega)\}_{x\in\mathbb{Z}^d,\,1\le i\le d}$ (entering the microscopic field $A$, see (44)) form an i.i.d. sequence of random variables that are distributed according to the Weibull law of parameter $(\lambda,k)$. We recall that such random variables are positive, with a probability density that reads (see Figure 7)

$$\forall r>0, \qquad f(r;k,\lambda) = \frac{k}{\lambda}\left(\frac{r}{\lambda}\right)^{k-1}\exp\left(-(r/\lambda)^k\right).$$

In practice, a Weibull distribution is generated as follows. Let $u(\omega)$ be a random variable uniformly distributed in $[0,1]$. Then

$$a(\omega) = \lambda\Big[-\ln(1-u(\omega))\Big]^{1/k} \tag{50}$$

is distributed according to the Weibull law of parameter $(\lambda,k)$.

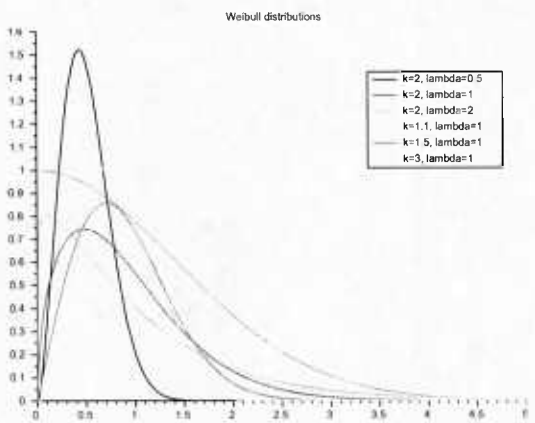


Figure 7: Examples of Weibull distributions.

## 5.2 Forward and inverse problems

The forward (direct) problem can be phrased as follows: given the parameters $(\lambda,k)$ of the Weibull law of the microscopic field $A(\cdot,\omega)$, compute

- the macroscopic (homogenized) permeability $\mathbb{E}[A_N^\star]$,
- its relative variance

$$\mathbb{V}\mathrm{arR}[A_N^\star] = \frac{\mathbb{V}\mathrm{ar}[A_N^\star]}{(\mathbb{E}[A_N^\star])^2}.$$

The inverse problem we consider here is the following. Given the quantities $\mathbb{E}[A_N^\star]$ and $\mathbb{V}\mathrm{arR}[A_N^\star]$, we wish to find parameters $(\lambda, k)$ consistent with these observations. The reason why we choose $\mathbb{E}[A_N^\star]$ and $\mathbb{V}\mathrm{arR}[A_N^\star]$ as input parameters is discussed below.

Ideally, the inverse problem can be formulated as follows. Consider the functional

$$F_N(\lambda, k) = \left(\frac{\mathbb{E}[A_N^\star(\lambda, k)]}{A_{\mathrm{obs}}^\star} - 1\right)^2 + \left(\frac{\mathbb{V}\mathrm{arR}[A_N^\star(\lambda, k)]}{V_{\mathrm{obs}}} - 1\right)^2,$$

where

$$A_{\mathrm{obs}}^\star = \mathbb{E}[A_N^\star(\lambda_{\mathrm{obs}}, k_{\mathrm{obs}})]$$

is the observed macroscopic permeability, while

$$V_{\mathrm{obs}} = \mathbb{V}\mathrm{arR}[A_N^\star(\lambda_{\mathrm{obs}}, k_{\mathrm{obs}})]$$

is the observed relative variance. We consider the problem

$$\inf_{\lambda,k} F_N(\lambda, k)$$

and we obviously see that $(\lambda_{\mathrm{obs}}, k_{\mathrm{obs}})$ is a minimizer of the above problem. Furthermore, we have the following result (see [7]):

**Lemma 1** *Consider the one-dimensional setting $d = 1$, and set*

$$F_\infty(\lambda, k) = \lim_{N\to\infty} F_N(\lambda, k).$$

*Then $F_\infty(\lambda, k)$ has a* unique *minimizer, which is $(\lambda_{\mathrm{obs}}, k_{\mathrm{obs}})$.*

The above result motivates our choice of the expectation and the relative variance as input observations. It shows that, although homogenization is an averaging process which filters out many features of the microscopic coefficients, our two macroscopic input observations are enough to characterize the two parameters of the microscopic probability distribution.

In practice, the expectations in $F_N$ are approximated by empirical estimators:

$$\mathbb{E}[A_N^\star(\lambda, k)] \approx A_{N,M}^\star(\lambda, k; \omega) := \frac{1}{M}\sum_{m=1}^{M} A_{N,m}^\star(\omega, \lambda, k)$$

and likewise for $\mathbb{V}\mathrm{arR}[A_N^\star(\lambda, k)]$, which is approximated by $V_{N,M}(\lambda, k; \omega)$. A practical formulation is hence to consider the optimization problem

$$\inf_{\lambda,k} F_{N,M}(\lambda, k; \omega), \tag{51}$$

where

$$F_{N,M}(\lambda, k; \omega) = \left(\frac{A_{N,M}^\star(\lambda, k; \omega)}{A_{\mathrm{obs}}^\star} - 1\right)^2 + \left(\frac{V_{N,M}(\lambda, k; \omega)}{V_{\mathrm{obs}}} - 1\right)^2,$$

where the observed values are given by $A_{\mathrm{obs}}^\star = A_{N,M}^\star(\lambda_{\mathrm{obs}}, k_{\mathrm{obs}}; \overline{\omega})$ and likewise for $V_{\mathrm{obs}}$.

## 5.3 Algorithm and numerical results

To address the optimization problem (51), recall that, in view of (44) and (50), the microscopic field can be written as

$$A(\cdot,\omega) = \mathcal{A}\Big(\lambda, k, \{u_k(\omega)\}_{k\in\mathbb{Z}^d}\Big), \tag{52}$$

where $u_k(\omega)$ are i.i.d. random variables uniformly distributed in $(0,1)$, and where $\mathcal{A}$ is a *deterministic* function, the derivatives of which (with respect to $\lambda$ and $k$) are easy to compute.

By computing the derivatives of (48) and (49) with respect to $\lambda$ and $k$, one can easily compute the first and second derivatives of $A^\star_N(\lambda,k;\omega)$. It is thus possible to use a Newton algorithm to solve (51).

On Figure 8, we show the numerical results that we have obtained on a two-dimensional problem, with the parameters $N = 10$ and $M = 30$. We proceed as follows. We pick some target values $\lambda_{\rm obs}$ and $k_{\rm obs}$, pick some fixed $\overline{\omega} \in \Omega$, and solve the forward problem for these values, thereby generating synthetic observed values $A^\star_{\rm obs} = A^\star_{N,M}(\lambda_{\rm obs}, k_{\rm obs}, \overline{\omega})$ and $V_{\rm obs}$. We next repeat the following procedure:

1. we generate microstructures $A(x,\omega)$ at the fine scale which are independent of those used to compute the observed values $A^\star_{\rm obs}$ and $V_{\rm obs}$.
2. we solve the optimization problem (51) using a Newton algorithm, starting from an initial guess 10% off the reference value $(\lambda_{\rm obs}, k_{\rm obs})$.
3. we thereby identify some optimal parameters $(\lambda_{\rm opt}(\omega), k_{\rm opt}(\omega))$.

We repeat the above procedure many times in order to obtain several i.i.d. realizations of the optimal parameters $(\lambda_{\rm opt}(\omega), k_{\rm opt}(\omega))$, from which we build the histograms shown on Figure 8. We see that, despite the limited values of $N$ and $M$, we obtain a meaningful estimation of the exact parameters $(\lambda_{\rm obs}, k_{\rm obs})$.

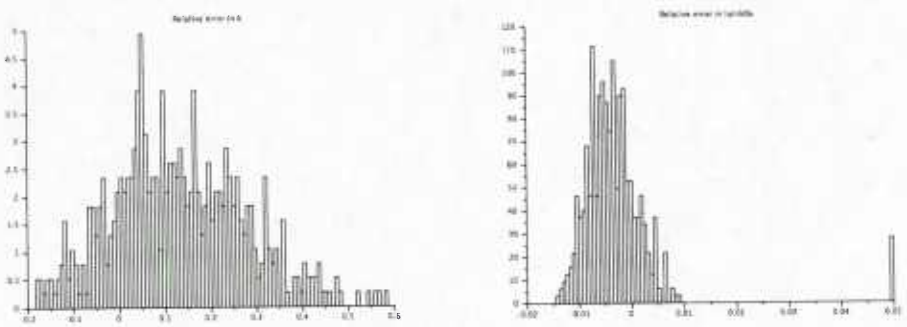

Figure 8: Left: histogram of $\dfrac{k_{\rm opt}(\omega) - k_{\rm obs}}{k_{\rm obs}}$. Right: histogram of $\dfrac{\lambda_{\rm opt}(\omega) - \lambda_{\rm obs}}{\lambda_{\rm obs}}$.

**Remark 4** *Our approach is not specific to Weibull laws. It can be used for other distribution laws with parameters $\theta$. What we need is that the random field $A(x,\omega)$ used at the microscopic scale can be written as*

$$A(x,\omega) = \mathcal{F}\Big(u(x,\omega),\theta\Big)$$

*where $u(x,\omega)$ is a field of random variables that are uniformly distributed and $\mathcal{F}$ smoothly depends on the parameters $\theta$ (see (52) in our particular case). Computing the derivatives of the microscopic random field $A(x,\omega)$ (and next of the macroscopic, homogenized quantities) with respect to $\theta$ is then easy. Our motivation for choosing Weibull laws comes from physical reasons: based on experimental results, it appears to be a reasonable choice.*

# 6 Conclusions

The series of works presented in this report has contributed to provide more efficient numerical methods for the simulation of random heterogeneous materials.

First, in some previous works (see [13] and subsequent works), funded by an earlier ONR grant, we have demonstrated the feasibility of using variance reduction techniques in the context of stochastic homogenization. We used there the antithetic variable approach. We have shown in Section 3 that it is as well possible to use other variance reduction approaches, such as control variate approaches, that involve the construction of *reduced models* in this particular context. This technique is less generic than the antithetic variable approach, but provides better results. Ongoing efforts are focused on the development of yet another technique, based on the a priori selection of "representative" microstructures [4]. This selection step is inexpensive in comparison to the overall computational cost. The corrector problem (8) is next solved only for these "better" microstructures.

Of course, considering other problems than the linear equation (4) (such as nonlinear problems, ...) is also of interest. In [5], we have considered a nonlinear, convex homogenization problem, and we have shown that the technique of antithetic variables, considered in [13] for linear problems, can also be used in that nonlinear context, with similar results.

Second, we have started to develop homogenization approaches for the numerical simulation of periodic microstructures with defects (see Section 4). This theory gives rise to completely new numerical approaches. Numerical results have already been obtained for some classes of defects. These questions have not been explored in the previous ONR grant. Our purpose now is to consider cases closer to actual local defects in materials.

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