Numerical Mathematics and Advanced Applications 2009

Proceedings of ENUMATH 2009, the 8th European Conference on Numerical Mathematics and Advanced Applications, Uppsala, July 2009

Bearbeitet von
Gunilla Kreiss, Per Lötstedt, Axel Målqvist, Maya Neytcheva

1st Edition. 2010. Buch. xviii, 939 S. Hardcover
ISBN 978 3 642 11794 7
Format (B x L): 15,5 x 23,5 cm
Gewicht: 1682 g

Some Numerical Approaches for Weakly Random Homogenization

Claude Le Bris

Abstract We overview a series of recent works addressing homogenization problems for some materials seen as small random perturbations of periodic materials (in a sense made precise in the body of the text). These recent works are joint works with several collaborators: Blanc (Paris 6), Lions (Collège de France), Legoll, Anantharaman, Costaouec (Ecole Nationale des Ponts et Chaussées and INRIA). The theory, developed in [C. R. Acad. Sci. Série I, 343, 717–724 (2006), Journal de Mathématiques Pures et Appliquées, 88, 34–63 (2007)], is only outlined. Next a collection of numerical appropriate approaches introduced in [Note aux Comptes Rendus de l'Académie des Sciences (2009), Thèse de l' Université Paris Est, C. R. Acad. Sci. Série I, 348, 99–103 (2010)] is presented. The theoretical considerations and the numerical tests provided here show that for the materials with only a small amount of randomness that are considered, a dedicated approach is far more efficient than a direct, stochastic approach.

1 Introduction

Multiscale approaches are increasingly popular in computational materials science. Although much effort has been devoted lately to the development of appropriate, computationally efficient approaches, there is still room for improvement, given the enormous variety of the field.

The motivation for the works summarized in the present review is contained in the following four-fold observation:

1. *A new feature that becomes ubiquitous in computational materials science is randomness*. Most of the simulations performed in the past decades, including

C. Le Bris
CERMICS, École Nationale des Ponts et Chaussées, 6 & 8, avenue Blaise Pascal, 77455 Marne-La-Vallée Cedex 2 and INRIA Rocquencourt, MICMAC project, Domaine de Voluceau, B.P. 105, 78153 Le Chesnay Cedex, France
e-mail: lebris@cermics.enpc.fr

G. Kreiss et al. (eds.), *Numerical Mathematics and Advanced Applications 2009*,
DOI 10.1007/978-3-642-11795-4_3,

the most recent development along the multiscale paradigm, consider idealized materials. Such materials are flawless, and most of the time perfectly periodic. In sharp contrast, real materials have defects, and have several characteristic length-scales that differ from one another by orders of magnitude. Their qualitative and quantitative response to environment might therefore differ a lot from the idealized scenario. Think for instance of solid materials consisting of grains, each grain being a particular assembly of monocrystals, each of them in turn possibly separated by interfaces and possibly embedding dislocations.

2. *Multiscale simulations, already computationally expensive* per se *may admittedly become prohibitively expensive in the presence of randomness.* A good example (the topic of the present review article) is random homogenization, which is *infinitely* more expensive than periodic homogenization (basically because it requires solving corrector problems posed on the entire space, see (2) and (14) below). Alternative approaches are thus interesting.
3. *The very definition of a random material is still mostly vague.* Given a microscopic picture of a material, it is indeed unclear to decide whether the microstructures are periodically repeated, whether some type of stationary ergodic character is encoded in the microstructures, or whether a much more general type of modeling should be adopted. Defining the geometric assumption that will allow to efficiently simulate the material computationally is a challenge in its own rights.
4. *In many practical situations, the random material under consideration is not far from being a periodic material.* At zero order of approximation, the material can be considered periodic, and it is only at a higher order that randomness plays a role. A good example is provided by materials that are industrially produced, where the defect of periodicity typically owes to failures in the synthesis process. See Fig. 1. Despite its smallness, the microscopic amount of randomness might affect the macroscale at order one, and it is indeed the interesting issue to quantitatively model this effect.

Considering the above, our purpose here is to outline a modeling strategy that accounts for the presence of randomness in a multiscale computation, but specifically addresses the case when the amount of randomness present in the system is small, in a sense to be made precise below. The weakly random material is thus considered as a small perturbation of a periodic material. Based on this interpretation, an efficient numerical strategy is then devised. It only aims at computing an *approximation* of the response of the material, given that the randomness is weak. But, as shown in the sequel, the strategy is computationally much less expensive than a direct stochastic approach.

The context in which we develop our approach is homogenization theory, and more precisely homogenization of simple, second order elliptic equations in divergence form with highly oscillatory coefficients. This particular case is to be thought of as a prototypical case. Although we have not developed our theory and computations for other, more general equations and settings, we are convinced that the same line of approach (namely small amount of randomness as compared to a reference periodic setting, plus expansion in the randomness amplitude, and simplified computations) can be useful in many contexts.

Fig. 1 Composite material (extracted from [18], reproduced with permission of the author): it is evident from the picture (a two-dimensional cut of a three-dimensional material) that the cross section of the fibers of the materials are not arranged periodically. On the other hand, it would not be fair to say that the material is entirely disordered. Some types of ordering, at different lengthscales, can be identified on the picture

The article is articulated as follows. Section 2 recalls some basics of the theory of periodic and stochastic homogenization, and introduces some elements on a variant recently studied by the author and collaborators. Section 3 first presents the bottom line of the approach: Taylor expanding the corrector and the homogenized matrix with respect to the small parameter measuring the amount of randomness in the system. The approach is then applied, under two different variants, to some academic cases which we hope to be representative of generic practical situations. The article concludes with Sect. 4 briefly discussing related problems and techniques.

2 Some Elements of Homogenization Theory

2.1 Periodic Homogenization

To begin with, we recall some basic ingredients of elliptic homogenization theory in the periodic setting. We refer e.g., to the monographs [4, 8, 12] for more details on homogenization theory.

We consider, in a regular domain $\mathscr{D}$ in $\mathbb{R}^d$, the problem

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

where the matrix A_{per} is symmetric 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 corrector problem associated to (1) reads, for p fixed in $\mathbb{R}^d$,

$$\begin{cases} -\mathrm{div}(A_{per}(y)(p+\nabla w_p)) = 0, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases} \tag{2}$$

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

$$\begin{aligned} [A_*]_{ij} &= \int_Q (e_i + \nabla w_{e_i}(y))^T A_{per}(y)(e_j + \nabla w_{e_j}(y))dy \\ &= \int_Q (e_i + \nabla w_{e_i}(y))^T A_{per}(y) e_j dy, \end{aligned} \tag{3}$$

where Q is the unit cube. The main result of periodic homogenization theory is that, as ε goes to zero, the solution u^ε to (1) converges to u^* solution to

$$\begin{cases} -\mathrm{div}\,[A_*\nabla u^*] = f \quad \text{in} \quad \mathscr{D}, \\ u^* = 0 \quad \text{on} \quad \partial\mathscr{D}. \end{cases} \tag{4}$$

The convergence holds in $L^2(\mathscr{D})$, and weakly in $H_0^1(\mathscr{D})$. The correctors w_{e_i} (for e_i the canonical vectors of $\mathbb{R}^d$) may then also be used to "correct" u^* in order to identify the behavior of u^ε in the strong topology $H_0^1(\mathscr{D})$. 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, take indeed p the vectors of the canonical basis of $\mathbb{R}^d$), 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.

The proof of the above result can be performed in several ways. One approach is the *energy method* by Murat and Tartar (see [14, 17]). Another possible approach is to use the notion of *two-scale convergence* introduced by G. Nguetseng and developed by G. Allaire (see [1, 15]).

2.2 Classical Random Homogenization

The present section introduces the classical *stationary ergodic setting*. We choose to present the theory in a *discrete* stationary setting, which is more appropriate for our specific purpose in the next sections. Random homogenization is more often presented in the *continuous* stationary setting. Although the two settings are different

(neither of them being an extension of the other), the modifications needed to pass from one setting to the other are tiny, and summarized in Remark 1 below.

Throughout this article, $(\Omega, \mathscr{F}, \mathbb{P})$ denotes a probability space. For any random variable $X \in L^1(\Omega, d\mathbb{P})$, we denote by $\mathbb{E}(X) = \int_\Omega X(\omega) d\mathbb{P}(\omega)$ its expectation value. We fix $d \in \mathbb{N}^*$, and assume that the group $(\mathbb{Z}^d, +)$ acts on Ω. We denote by $(\tau_k)_{k\in\mathbb{Z}^d}$ this action, and assume that it preserves the measure $\mathbb{P}$, i.e.,

$$\forall k \in \mathbb{Z}^d, \quad \forall A \in \mathscr{F}, \quad \mathbb{P}(\tau_k A) = \mathbb{P}(A). \tag{5}$$

We assume that τ is *ergodic*, that is,

$$\forall A \in \mathscr{F}, \quad \Big(\forall k \in \mathbb{Z}^d, \quad \tau_k A = A\Big) \Rightarrow (\mathbb{P}(A) = 0 \quad \text{or} \quad 1). \tag{6}$$

In addition, we define the following notion of stationarity: any $F \in L^1_{\text{loc}}(\mathbb{R}^d, L^1(\Omega))$ is said to be *stationary* if

$$\forall k \in \mathbb{Z}^d, \quad F(x + k, \omega) = F(x, \tau_k \omega) \text{ almost everywhere in } x, \text{ almost surely.} \tag{7}$$

In this setting, the ergodic theorem [13, 16] can be stated as follows:

Theorem 1 (Ergodic theorem, [13,16]). *Let $F \in L^\infty(\mathbb{R}^d, L^1(\Omega))$ be a stationary random variable in the sense of (7). For $k = (k_1, k_2, \dots k_d) \in \mathbb{R}^d$, we set $|k|_\infty = \sup_{1\le i\le d} |k_i|$. Then*

$$\frac{1}{(2N+1)^d} \sum_{|k|_\infty \le N} F(x, \tau_k \omega) \underset{N\to\infty}{\longrightarrow} \mathbb{E}(F(x, \cdot)) \quad \textit{in } L^\infty(\mathbb{R}^d), \textit{ almost surely.} \tag{8}$$

This implies that (denoting by Q the unit cube in $\mathbb{R}^d$)

$$F\left(\frac{x}{\varepsilon}, \omega\right) \overset{*}{\underset{\varepsilon\to 0}{\longrightarrow}} \mathbb{E}\Big(\int_Q F(x, \cdot) dx\Big) \quad \textit{in } L^\infty(\mathbb{R}^d), \textit{ almost surely.} \tag{9}$$

It is useful to intuitively define stationarity and ergodicity in terms of material modeling. Pick two points x and $y \neq x$ at the microscale in the material. 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 identical to that in y (considering the various realizations of the random material). In mathematical terms, the *law* of microstructures is the same at all points. 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.

Remark 1. Alternatively to the above discrete setting, it is possible to define a continuous ergodic setting, the reader might be more familiar with. We fix $d \in \mathbb{N}^*$,

and assume that the group $(\mathbb{R}^d, +)$ acts on Ω. We denote by $(\tau_x)_{x\in\mathbb{R}^d}$ this action. We assume that it preserves the measure $\mathbb{P}$, that it is ergodic, both properties being expressed using a straightforward adaptation of (5) and (6) respectively. The notion of stationarity is defined by $F(x+y,\omega) = F(x,\tau_y\omega)$, for all $y \in \mathbb{R}$, almost everywhere in $x \in \mathbb{R}$ and almost surely. To understand the difference between the discrete and the continuous settings, note for instance that a $\mathbb{Z}^d$-periodic function F is a particular case of (7), when F is assumed to be deterministic. In contrast, it is an example of the continuous setting for a *genuinely* random function F, Ω being the d dimensional torus and $\tau_x y \equiv x + y$.

In the continuous setting, the ergodic theorem [13,16] holds. The conclusions (8) and (9) are respectively replaced by:

$$\frac{1}{|B_R|}\int_{B_R} F(x,\tau_y\omega)dy \underset{R\to\infty}{\longrightarrow} \mathbb{E}\left(F(x,\cdot)\right) = \mathbb{E}(F) \quad \text{in } L^\infty(\mathbb{R}^d), \text{ almost surely,} \tag{10}$$

and

$$F\left(\frac{x}{\varepsilon},\omega\right) \overset{*}{\underset{\varepsilon\to 0}{\longrightarrow}} \mathbb{E}\left(F\right) \quad \text{in } L^\infty(\mathbb{R}^d), \text{ almost surely.} \tag{11}$$

□

We now fix $\mathscr{D}$ an open, smooth and bounded subset of $\mathbb{R}^d$, and A a square matrix of size d, which is assumed stationary in the sense defined above, and which is assumed to enjoy the classical assumptions of uniform ellipticity and boundedness. Then we consider the boundary value problem

$$\begin{cases} -\mathrm{div}\left(A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right) = f \quad \text{in} \quad \mathscr{D}, \\ u^\varepsilon = 0 \quad \text{on} \quad \partial\mathscr{D}. \end{cases} \tag{12}$$

Standard results of stochastic homogenization [4, 12] apply and allow to find the homogenized problem for problem (12). These results generalize the periodic results recalled in Sect. 2.1. The solution u^ε to (12) converges to the solution to (4) where the homogenized matrix is now defined as:

$$[A_*]_{ij} = \mathbb{E}\left(\int_Q (e_i + \nabla w_{e_i}(y,\cdot))^T A(y,\cdot)e_j\, dy\right), \tag{13}$$

where for any $p \in \mathbb{R}^d$, w_p is the solution (unique up to the addition of a (random) constant) in $\{w \in L^2_{\mathrm{loc}}(\mathbb{R}^d, L^2(\Omega)), \nabla w \in L^2_{\mathrm{unif}}(\mathbb{R}^d, L^2(\Omega))\}$ to

$$\begin{cases} -\mathrm{div}[A(y,\omega)(p + \nabla w_p(y,\omega))] = 0, \quad \text{a.s. on} \quad \mathbb{R}^d \\ \nabla w_p \quad \text{is stationary in the sense of (7),} \\ \mathbb{E}\left(\int_Q \nabla w_p(y,\cdot)\, dy\right) = 0. \end{cases} \tag{14}$$

We have used above the notation L^2_{unif} for the *uniform* L^2 space, that is the space of functions for which, say, the L^2 norm on a ball of unit size is bounded above independently from the center of the ball.

A striking difference between the stochastic setting and the periodic setting can be observed comparing (2) and (14). In the periodic case, the corrector problem is posed on a bounded domain (namely, the periodic cell Q), since the corrector w_p is periodic. In sharp contrast, the corrector problem (14) of the random case 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 $\mathbb{E}\left(\int_Q \nabla w_p(y,\cdot)\,dy\right) = 0$ in (14) is a *global* condition. It indeed equivalently reads, because of the ergodic Theorem, a.s. $-\lim_{R\longrightarrow+\infty} \frac{1}{|B_R|}\int_{B_R} \nabla w_p(y,\cdot)\,dy = 0$ 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. Truncations of problem (14) have to be considered, and the actual homogenized coefficients are only correct in the asymptotic regime. The present series of works is somehow motivated by the above observation, as already pointed out in the introduction.

Remark 2. In fact, the situation considered here is simple: it is the linear elliptic case. It is well known that, even in the periodic setting, the difficulties we mention for the random setting already arise in the periodic setting when the operator is, for instance, nonlinear. Then determining the periodic homogenized problem cannot always be reduced to a simple computation on one single periodic cell of the problem.

2.3 A Variant

A specific stochastic setting has been introduced and studied in [5, 7]. It is *not* a particular case of the classical stationary settings defined above. As briefly mentioned in the introduction, it is motivated by the consideration of random geometries (we mean, materials) that have some relation to the periodic setting. Here, the periodic setting is taken as a *reference* configuration, somewhat similarly to the classical mathematical formalization of continuum mechanics where a reference configuration is used to define the state of the material under study. Another related idea, in a completely different context, is the consideration of a reference element for finite element computations. In all cases, the real situation is seen *via* a *mapping* from the reference configuration to the actual configuration.

We fix some $\mathbb{Z}^d$-periodic, square matrix A_{per} of size d, assumed to satisfy

$$\exists \gamma > 0 / \forall \xi \in \mathbb{R}^d,\ \ \xi^T A_{per}(y)\xi \geq \gamma|\xi|^2,\ \ \text{almost everywhere in } y \in \mathbb{R}^d, \quad (15)$$

$$\forall i, j \in \{1, 2, \ldots, d\}, \quad [A_{per}]_{ij} \in L^\infty(\mathbb{R}^d). \quad (16)$$

We consider the following problem:

$$\begin{cases} -\mathrm{div}\left(A_{per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right)\nabla u^\varepsilon\right) = f \quad \text{in} \quad \mathscr{D}, \\ u^\varepsilon = 0 \quad \text{on} \quad \partial\mathscr{D}, \end{cases} \tag{17}$$

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

$$\underset{\omega\in\Omega,\, x\in\mathbb{R}^d}{\mathrm{EssInf}} \left[\det(\nabla\Phi(x,\omega))\right] = \nu > 0, \tag{18}$$

$$\underset{\omega\in\Omega,\, x\in\mathbb{R}^d}{\mathrm{EssSup}} \left(|\nabla\Phi(x,\omega)|\right) = M < \infty, \tag{19}$$

$$\nabla\Phi(x,\omega) \quad \text{is stationary in the sense of (7).} \tag{20}$$

Such a Φ is called a *random stationary diffeomorphism.*

The following result is proved in [5,7]:

Theorem 2. *Let $\mathscr{D}$ be a bounded smooth open subset of $\mathbb{R}^d$, and let $f \in H^{-1}(\mathscr{D})$. Let A_{per} be a square matrix which is $\mathbb{Z}^d$-periodic and satisfies (15) and (16). Let Φ be a random stationary diffeomorphism satisfying hypotheses (18–20). Then the solution $u^\varepsilon(x,\omega)$ to (17) satisfies the following properties:*

1. *$u^\varepsilon(x,\omega)$ converges to some $u_0(x)$ strongly in $L^2(\mathscr{D})$ and weakly in $H^1(\mathscr{D})$, almost surely;*
2. *the function u_0 is the solution to the homogenized problem:*

$$\begin{cases} -\mathrm{div}(A_*\nabla u_0) = f \quad \textit{in} \quad \mathscr{D}, \\ u_0 = 0 \quad \textit{on} \quad \partial\mathscr{D}. \end{cases} \tag{21}$$

In (21), the homogenized matrix A_* is defined by:

$$[A_*]_{ij} = \det\left(\mathbb{E}\left(\int_Q \nabla\Phi(z,\cdot)dz\right)\right)^{-1} \times \mathbb{E}\left(\int_{\Phi(Q,\cdot)} (e_i + \nabla w_{e_i}(y,\cdot))^T A_{per}(\Phi^{-1}(y,\cdot))e_j\, dy\right), \tag{22}$$

where for any $p \in \mathbb{R}^d$, w_p is the solution (unique up to the addition of a (random) constant) in $\left\{w \in L^2_{\mathrm{loc}}(\mathbb{R}^d, L^2(\Omega)), \nabla w \in L^2_{\mathrm{unif}}(\mathbb{R}^d, L^2(\Omega))\right\}$ to

$$\begin{cases} -\mathrm{div}\left[A_{per}(\Phi^{-1}(y,\omega))(p + \nabla w_p)\right] = 0, \\ w_p(y,\omega) = \tilde{w}_p(\Phi^{-1}(y,\omega),\omega), \quad \nabla\tilde{w}_p \quad \textit{is stationary in the sense of (7)}, \\ \mathbb{E}\left(\int_{\Phi(Q,\cdot)} \nabla w_p(y,\cdot)dy\right) = 0. \end{cases} \tag{23}$$

3 Numerical Approaches for an Approximation at First Order

3.1 Small Perturbations of the Periodic Setting

It has been shown in [7] that, when Φ in (17) is a perturbation of the Identity map

$$\Phi(x,\omega) = x + \eta\,\Psi(x,\omega) + O(\eta^2), \tag{24}$$

the solution to the corrector problem (23) may be developed in powers of the small parameter η. It reads $\widetilde{w}_p(x,\omega) = w_p^0(x) + \eta w_p^1(x,\omega) + O(\eta^2)$, where w_p^0 solves

$$-\operatorname{div}\left[A_{per}\,(p+\nabla w_p^0)\right] = 0, \quad w_p^0 \text{ is } Q\text{-periodic}, \tag{25}$$

and where w_p^1 solves

$$\begin{cases} -\operatorname{div}\left[A_{per}\nabla w_p^1\right] = \operatorname{div}\left[-A_{per}\nabla\Psi\nabla w_p^0 - (\nabla\Psi^T - (\operatorname{div}\Psi)\mathrm{Id})\,A_{per}\,(p+\nabla w_p^0)\right], \\ \nabla w_p^1 \text{ is stationary and } \mathbb{E}\left(\displaystyle\int_Q \nabla w_p^1\right) = 0. \end{cases} \tag{26}$$

The problem (26) in w_p^1 is random in nature, but it is in fact easy to see, taking the expectation, that $\overline{w}_p^1 = \mathbb{E}(w_p^1)$ is Q-periodic and solves the *deterministic* problem

$$\begin{aligned} &-\operatorname{div}\left[A_{per}\,\nabla\overline{w}_p^1\right] \\ &\quad = \operatorname{div}\left[-A_{per}\,\mathbb{E}(\nabla\Psi)\,\nabla w_p^0 - (\mathbb{E}(\nabla\Psi^T) - \mathbb{E}(\operatorname{div}\Psi)\mathrm{Id})\,A_{per}\,(p+\nabla w_p^0)\right]. \end{aligned} \tag{27}$$

This is useful because, on the other hand, the knowledge of w_p^0 and $\overline{w}_p^1$ suffices to obtain a first order expansion (in η) of the homogenized matrix. Define $A_{ij}^0 = \int_Q (e_i + \nabla w_{e_i}^0)^T A_{per}\,e_j$ and

$$\begin{aligned} A_{ij}^1 = &-\int_Q \mathbb{E}(\operatorname{div}\Psi)\,A_{ij}^0 + \int_Q (e_i+\nabla w_{e_i}^0)^T A_{per}\,e_j\,\mathbb{E}(\operatorname{div}\Psi) \\ &+ \int_Q \left(\nabla\overline{w}_{e_i}^1 - \mathbb{E}(\nabla\Psi)\nabla w_{e_i}^0\right)^T A_{per}\,e_j, \end{aligned}$$

we then have

$$A_* = A^0 + \eta A^1 + O(\eta^2). \tag{28}$$

As subsequently shown in [10], a similar approach can be applied to the corrector problems once *discretized* by a finite element approach. Given a mesh $\mathscr{T}_h^{(Q)}$ of Q of size h, reproduced by periodicity on $Q_N = [0,N]^d$, we define the discrete variational formulation

$$\left\{\begin{array}{l}\text{Find } \widetilde{w}_p^{h,N}(\cdot,\omega) \in V_h^{\rm per}(Q_N) \quad \text{such that, for all } \widetilde{v}_h \in V_h^{\rm per}(Q_N),\\ \displaystyle\int_{Q_N} \det(\nabla\Phi)(\nabla\widetilde{v}_h)^T(\nabla\Phi)^{-T} A_{per}\big(p + (\nabla\Phi)^{-1}\nabla\widetilde{w}_p^{h,N}(\cdot,\omega)\big) = 0 \\ \qquad\qquad \text{almost surely,}\end{array}\right. \tag{29}$$

where $V_h^{\rm per}(Q_N)$ is the set of Q_N-periodic functions that have their restriction to Q_N in a typical finite element space built from the mesh $\mathscr{T}_h^N$ (obtained by periodization). Note that the problem is formulated in terms of $\widetilde{w}_p$ (rather than w_p) because the gradient of $\widetilde{w}_p$ is stationary. The matrix

$$\begin{aligned}&\big[A_*{}^{h,N}\big]_{ij}(\omega)\\ &= \det\left(\frac{1}{|Q_N|}\int_{Q_N}\nabla\Phi\right)^{-1}\frac{1}{|Q_N|}\int_{Q_N}\det(\nabla\Phi)\big(e_i + (\nabla\Phi)^{-1}\nabla\widetilde{w}_{e_i}^{h,N}\big)^T A_{per}e_j\end{aligned} \tag{30}$$

is then considered. Using the same expansion (24) as in the above "continuous" case, a formal expansion $\widetilde{w}_p^{h,N} = w_p^{0,h,N} + \eta w_p^{1,h,N} + O(\eta^2)$ of the discrete corrector is performed and inserted in (29). The function $w_p^{0,h,N}$ is then shown to be independent of N (it is henceforth denoted $w_p^{0,h}$), while $w_p^{0,h}$ and $w_p^{1,h,N}$ are respectively solutions to

$$\begin{array}{l}\text{Find } w_p^{0,h} \in V_h^{\rm per}(Q) \text{ such that, for all } v_h \in V_h^{\rm per}(Q),\\ \displaystyle\int_Q (\nabla v_h)^T A_{per}\,(p + \nabla w_p^{0,h}) = 0,\end{array} \tag{31}$$

and

$$\left\{\begin{array}{l}\text{Find } w_p^{1,h,N}(\cdot,\omega) \in V_h^{\rm per}(Q_N) \text{ such that, for all } v_h \in V_h^{\rm per}(Q_N), \quad \text{and almost surely,}\\ \displaystyle\int_{Q_N} (\nabla v_h)^T A_{per}\,\nabla w_p^{1,h,N}\\ \qquad = \int_{Q_N}(\nabla v_h)^T\Big[A_{per}\nabla\Psi\nabla w_p^{0,h} + (\nabla\Psi^T - (\mathrm{div}\Psi)\mathrm{Id})A_{per}(p + \nabla w_p^{0,h})\Big].\end{array}\right. \tag{32}$$

Equations (31) and (32) are of course discretized formulations of (25) and (26), respectively. Similarly to what has been proven in the continuous setting in [7] (and briefly recalled above), it is possible to show that there exists a constant $C(h,N,\omega)$ such that, for η sufficiently small,

$$\eta^{-2}\left\|\nabla\widetilde{w}_p^{h,N}(\cdot,\omega) - \nabla w_p^{0,h} - \eta\nabla w_p^{1,h,N}(\cdot,\omega)\right\|_{L^2(Q_N)} \le |Q_N|^{1/2}\,C(h,N,\omega), \tag{33}$$

and

$$\eta^{-2}|A_*{}^{h,N}(\omega) - A^{0,h} - \eta A^{1,h,N}(\omega)| \le C(h,N,\omega), \tag{34}$$

where ${A_*}^{h,N}$ is defined by (30), $(A^{0,h})_{ij} = \displaystyle\int_Q \left(e_i + \nabla w_{e_i}^{0,h}\right)^T A_{per}\, e_j$ and

$$(A^{1,h,N})_{ij} = -(A^{0,h})_{ij} \frac{1}{|Q_N|} \int_{Q_N} \operatorname{div} \Psi + \frac{1}{|Q_N|} \int_{Q_N} \left(e_i + \nabla w_{e_i}^{0,h}\right)^T A_{per} e_j \operatorname{div} \Psi + \frac{1}{|Q_N|} \int_{Q_N} \left(\nabla w_{e_i}^{1,h,N} - \nabla \Psi\, \nabla w_{e_i}^{0,h}\right)^T A_{per}\, e_j.$$

Again as in the continuous setting, knowing only the expectation $\overline{w}_p^{1,h,N} = \mathbb{E}(w_p^{1,h,N})$ which solves, for all $v_h \in V_h^{\mathrm{per}}(Q_N)$,

$$\int_{Q_N} (\nabla v_h)^T A_{per}\, \nabla \overline{w}_p^{1,h,N} = \int_{Q_N} (\nabla v_h)^T \big[A_{per}\, \mathbb{E}(\nabla \Psi)\, \nabla w_p^{0,h} + \big(\mathbb{E}(\nabla \Psi)^T - \mathbb{E}(\operatorname{div} \Psi)\mathrm{Id}\big) A_{per} \left(p + \nabla w_p^{0,h}\right)\big] \tag{35}$$

is sufficient to determine the first order correction to the homogenized matrix. A simple argument shows that $\overline{w}_p^{1,h,N}$ is independent from N (it is henceforth denoted by $\overline{w}_p^{1,h}$), Q-periodic, and solution to (35) with $N = 1$, which is a converging discretization of (27) when h vanishes. The matrix $A^{1,h} = \mathbb{E}(A^{1,h,N})$ is similarly independent of N, and can be computed only using $\nabla \overline{w}_p^{1,h}$.

The question arises to know how large the (random) constant $C(h, N, \omega)$ in (34) is. Too large a constant would indeed mean that the first order expansion in η, although appealing theoretically, is useless practically to get an accurate approximation of the homogenized matrix. This is the purpose of [10] to examine this issue in a simple testcase, representative of some generality.

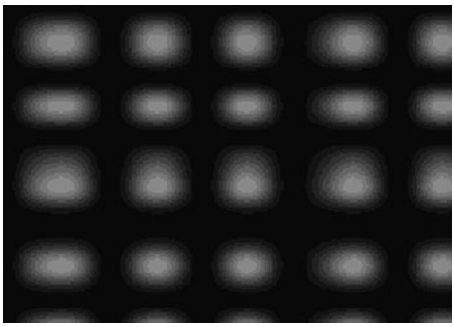
We work in dimension 2, with coordinates $x = (x_1, x_2)$, and consider two families $(X_k)_{k\in\mathbb{Z}}$ and $(Y_k)_{k\in\mathbb{Z}}$ of scalar, identically distributed, independent random variables. Their common law is the uniform law $\mathscr{U}([a, b])$ on the range $[a, b]$. We choose the diffeomorphism $\Phi(x) = x + \eta\Psi(x, \omega)$, with $\Psi(x, \omega) = (\psi_X(x_1, \omega), \psi_Y(x_2, \omega))$, where ψ_X is defined by

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

and ψ_Y is defined similarly. The periodic matrix A_{per} is defined by

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

The idea is to consider a $\mathbb{Z}^2$-periodic material, where thermal conductivity (modeled by the matrix $A_{per} \circ \Phi^{-1}$) smoothly varies from α to $\beta \le \alpha$. Conductivity is maximum at the center of the cell Q, and minimum on its boundary. Note that the map ψ_X is not stationary, but its gradient is. This is a prototypical example of



η	$(A_*{}^{h,N})_{11}$	$(e^{h,N})_{11}$
0.1	3.073 ± 0.00928	-4.233 ± 0.216
0.01	2.839 ± 0.00111	-5.009 ± 0.254
0.001	2.812 ± 0.000113	-5.104 ± 0.259
0.0001	2.809 ± 0.0000113	-5.114 ± 0.259

Fig. 2 *Left*: value of $A_{per} \circ \Phi^{-1}(x, \omega)$ for a particular random realization on the domain $Q_{N=5}$ ($\eta = 0.05$). This intuitively models a periodic structure (disks centered on a periodic lattice) slightly perturbed by a random diffeomorphism close to Identity. *Right*: values of $(A_*^{h,N})_{11}$ and $(e^{h,N})_{11}$ in function of η. All data are extracted from [10]

the setting developed in [7], which is not covered by *classical* stochastic homogenization theory since $A_{per} \circ \Phi^{-1}$ is not stationary. As shown by Fig. 2 (left) where $A_{per} \circ \Phi^{-1}(x, \omega)$ is displayed for a particular realization of the randomness, this is however a quite intuitive setting which deserves specific attention. The specific values chosen for the parameters are: $a = -2.25$, $b = 5.75$, $\alpha = 10$, and $\beta = 1$, $h = 1/3$, $N = 20$. The number of realizations is 10. The numerical results are obtained using the finite element software FreeFem++. They are displayed on the table of Fig. 2 (right). The left column shows the result obtained for the $(1, 1)$ entry of the homogenized matrix, with the interval of confidency. The right column gives the value of the error estimator

$$e^{h,N}(\omega) := \eta^{-2}\big(A_*{}^{h,N}(\omega) - A^{0,h} - \eta A^{1,h,N}(\omega)\big),$$

again for the $(1, 1)$ entry. The values found for other entries of the homogenized matrix lead to similar conclusions. Note that, for the purpose of analysis and with a view to reducing variance (see the details in [10]), we have used the random value $A^{0,h} + \eta A^{1,h,N}(\omega)$ in the right hand side of the estimator. In practice, $A^{0,h} + \eta A^{1,h}$ would be used, instead of $A^{0,h} + \eta A^{1,h,N}(\omega)$, as an approximation for $A_*{}^{h,N}$.

The conclusion is that the constant $C(h, N, \omega)$ is small (say of the order of 5 in this particular case) and that the first order approximation $A^{0,h} + \eta A^{1,h}$ of the homogenized matrix $A_*{}^{h,N}$ is thus a practically accurate numerical approach (provided the first order precision is judged satisfactory for the application considered). In terms of computational efficiency, the gain is enormous. Solving the couple of *periodic* problems (31) and (35) to respectively get $w_p^{0,h}$ and $\overline{w}_p^{1,h}$ is much less expensive than solving the original *stochastic* corrector problem (29).

3.2 Rare but Possibly Large Perturbations

We now consider a slightly different perturbative approach. It could be presented in the setting of random diffeormophisms introduced in Sect. 2.3 above, but for clarity we present it in the more classical setting of Sect. 2.2.

As above, we consider our random material as a small perturbation of a periodic material. The matrix that models its response is thus expanded as

$$A_\eta(x,\omega) = A_{per}(x) + b_\eta(x,\omega)C_{per}(x), \tag{36}$$

where, with evident notation, A_{per} is a periodic matrix modeling the unperturbed material, and where C_{per} is a periodic matrix modeling the perturbation. The amplitude of the perturbation, which used to be modeled by a *deterministic* coefficient η in the previous section, is now a scalar *random* field $b_\eta(x,\omega)$. We assume that this field satisfies

$$\|b_\eta\|_{L^\infty(Q;L^p(\Omega))} \underset{\eta\to 0}{\to} 0, \tag{37}$$

for some $1 \leq p < \infty$. For well-posedness of the problem, we also assume there exists $0 < \alpha \leq \beta$ such that for almost all $x \in \mathbb{R}^d$ and for almost all $\omega \in \Omega$,

$$\forall \xi \in \mathbb{R}^d,\ \forall \eta > 0, \quad \alpha|\xi|^2 \leq A_\eta(x,\omega)\xi\cdot\xi \quad and \quad |A_\eta(x,\omega)\xi| \leq \beta|\xi|.$$

Condition (37) states that the perturbation in (36) is small *on average*. However, it does not prevent the perturbation to be large, once in a while, because we only have $p < \infty$ (Note that the setting of the previous section corresponds to a situation where $p = \infty$). Whereas the idea underlying the setting of the previous section was *perturb the periodic material possibly often but only slightly*, the intuitive image behind the present setting is *perturb the periodic material only rarely, but then possibly largely*. The comparison of Fig. 2 (left) and Fig. 3 is self explanatory.

When the exponent p in (37) is strictly larger than one, a theory similar to that of the previous section can be developed. Assuming that $m_\eta := \|b_\eta\|_{L^\infty(Q;L^p(\Omega))} \longrightarrow 0$ as η vanishes, it may be proved, up to the extraction of a subsequence, that the homogenized tensor $A_{\eta,*}$ admits a first order expansion in terms of the small "coefficient" m_η. The coefficients are easily expressed using periodic corrector problems built from the matrices A_{per} and C_{per}. The remainder in the expansion can indeed be shown to be $o(m_\eta)$ in a certain sense and under appropriate assumptions. We refer to [2, 3] for the details. There are some cases when the expansion in fact does not converge. We now address such a case, very different in nature.

Consider the prototypical case where b_η is uniform in each cell of $\mathbb{Z}^d$ and writes

$$b_\eta(x,\omega) = \sum_{k\in\mathbb{Z}^d} \mathbf{1}_{\{Q+k\}}(x) B^k_\eta(\omega), \tag{38}$$

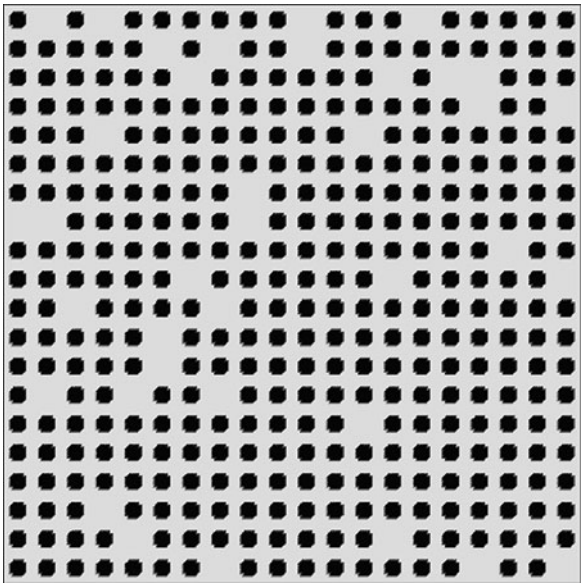


Fig. 3 A typical random realization of the Bernoulli law for the perturbed periodic material

where the B_η^k are independent identically distributed random variables. Their common law is assumed to be a Bernoulli law of parameter η. This setting satisfies condition (37) for all $p \geq 1$. The difficulty with a possible expansion in "powers" of b_η is intuitively that, a Bernoulli variable B, being valued in $\{0, 1\}$, is such that $B^p = B$ for all p. So all terms in the expansion are potentially of the same order. A different strategy is needed. We now explain an alternative, *formal* approach, for which we do not know any rigorous foundation to date. Although definite conclusions on the validity of the approach have yet to be obtained, the numerical tests we performed show its practical correctness and efficiency.

Heuristically, on the cube $Q_N = [0, N]^d$ and at order 1 in η, the probability to get the perfect periodic material (entirely modeled by the matrix A_{per}) is $(1-\eta)^{N^d} \approx 1 - N^d\eta + O(\eta^2)$, while the probability to obtain the unperturbed material on all cells except one (where the material has matrix $A_{per} + C_{per}$) is $N^d\,(1-\eta)^{N^d-1}\eta \approx N^d\eta + O(\eta^2)$. All other configurations, with more than two cells perturbed, yield contributions of orders higher than or equal to η^2. This gives the intuition that the first order correction indeed comes from the difference between the material perfectly periodic except on one cell and the perfect material itself. It is therefore claimed in [2, 3] that $A_{\eta,*} = A_{per,*} + \eta A_{1,*} + o(\eta)$ where $A_{per,*}$ is the homogenized matrix for the unperturbed periodic material and

$$A_{1,*}\, e_i = \lim_{N\to+\infty} \int_{Q_N} \Big[(A_{per} + \mathbf{1}_Q C_{per})\big(\nabla w_i^N + e_i\big) - A_{per}\,\big(\nabla w_i^0 + e_i\big)\Big], \tag{39}$$

where w_i^0 is the corrector for A_{per}, and w_i^N solves

$$\begin{aligned} &-\operatorname{div}\left(\left(A_{per}(x)+\mathbf{1}_Q C_{per}(x)\right)\left(\nabla w_i^N(x)+e_i\right)\right)=0 \\ &\text{in} \quad Q_N, \quad w_i^N \; Q_N-\text{periodic}. \end{aligned} \tag{40}$$

Note that the integral appearing in the right-hand side of (39) is *not* normalized: it a priori scales as the volume N^d of Q_N and has finite limit only because of cancellation effects between the two terms in the integrand. This is very similar in nature to the modeling of *defects* in Statistical Physics: a flawless (periodic) environment is substracted to the actual environment and acts as a normalization.

There actually exists a formal generalization of (39) that allows for recovering the setting of the previous cases. The approach of the present section therefore appears to be the most general approach to the modeling of "small" random perturbations. We again refer to [2, 3] for more details.

The approach has been tested in [3]. The matrix A_{per} is taken scalar. In each periodic cell, it has constant value 1,020 in the central circular inclusion and constant value 20 in the surrounding region. The matrix C_{per} has value $-1{,}000$ in the inclusions and 0 outside. The coefficient b_η is of the form (38), with B_η a Bernoulli variable with parameter $\eta = 0.1$. The results are shown on Fig. 4 below. On the

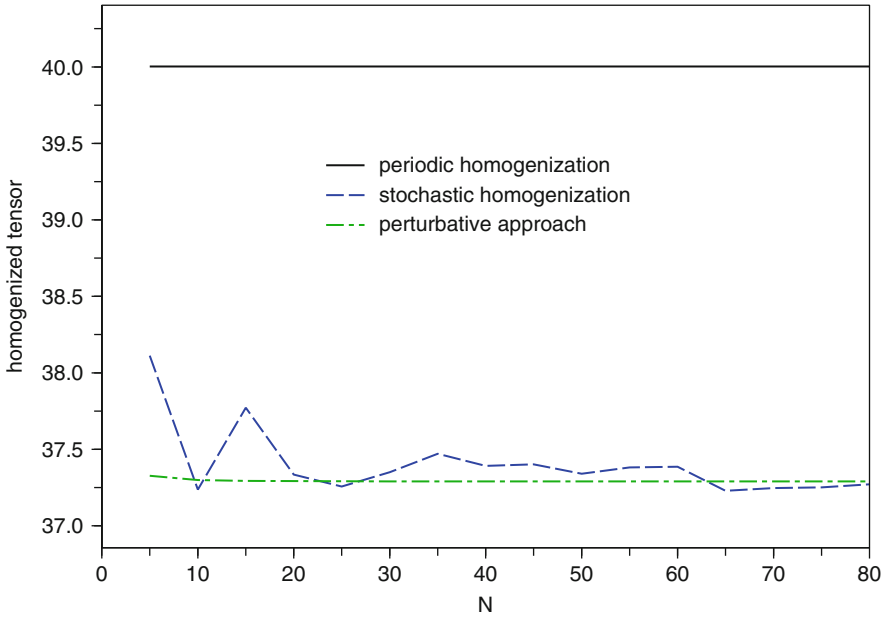


Fig. 4 Comparison of the actual random coefficient, which converges to the homogenized coefficient in the limit of large cube sizes N, (curve labelled "stochastic homogenization") with the unperturbed periodic homogenized coefficient (curve labelled "periodic homogenization") and the first order expansion (curve labelled "perturbative approach"). The asymptotic limit is almost instantaneously found by the perturbative approach

cube $Q_N = [0, N]^2$ with N increasingly large, an approximation of $A_{\eta,*}$ is directly computed. Alternatively, expression (39) is employed to calculate the first order term $A_{1,*}$ of the expansion. The values $A_{\eta,*}$ and $A_{per,*} + \eta A_{1,*}$ are then compared to one another. The process is completed for several realizations of the random material. Only a particular realization is shown on Fig. 4 but all realizations yield qualitatively similar behaviours. It is observed that, using the perturbative approach, the large N limit for cubes of size N is already very well approached for small values of N. As in the previous section, the computational efficiency of the approach is clear: solving the two periodic problems with coefficients A_{per} and $A_{per} + \mathbf{1}_Q C_{per}$ for a limited size N is much less expensive than solving the original, random corrector problem for a much larger size N.

4 Related Problems and Techniques

We conclude this article with some comments.

First, it is useful to mention that the variant of stochastic homogenization described in Sect. 2.3 has originally been introduced in [6, 7] for an apparently different context, related to atomistic modeling of materials and the limit of atomistic models to derive models for continuum mechanics. Although the two topics of Atomistic to Continuum limits and homogenization of partial differential equations look different at first sight, they actually share similarities, as two sides of the general paradigm of change of scales.

Second, the set of techniques presented above is specific to the case of periodic settings slightly perturbed by random perturbations. Although we believe this allows to treat many situations, the situation where randomness is intense is still, of course, of major interest. In that case, there seems to be no hope of simplifying the problem. A corrector problem of the type (14) (or of the type (23) when random diffeomorphisms are employed), posed on the entire ambient space, needs to be solved, for each vector p of the canonical basis. And, the average giving the homogenized matrix needs then to be computed. As in any situation where randomness is present, numerical practice shows that variance issues come into the picture and complicate the already huge computational task. A companion article [11] presents some techniques recently introduced to improve the efficiency of computations of homogenization problems that require the solution of corrector problems posed on the entire space.

Acknowledgements The work of the author is partially supported by ONR under contract Grant 00014-09-1-0470.

References

1. G. Allaire, *Homogenization and two-scale convergence*, SIAM J. Math. Anal., 23 (6), pp 1482–1518, 1992
2. A. Anantharaman, Thèse de l' Université Paris Est, Ecole des Ponts
3. A. Anantharaman, C. Le Bris, *Homogénéisation d'un matériau périodique faiblement perturbé aléatoirement*, [Homogenization of a weakly randomly perturbed periodic material], C. R., Math., Acad. Sci. Paris 348, No. 9–10, 529–534, 2010
4. A. Bensoussan, J. L. Lions, G. Papanicolaou, **Asymptotic analysis for periodic structures**, Studies in Mathematics and its Applications, 5. North-Holland, Amsterdam-New York, 1978
5. X. Blanc, C. Le Bris, 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, pp 717–724, 2006
6. X. Blanc, C. Le Bris, P.-L. Lions, *The energy of some microscopic stochastic lattices*, Arch. Rat. Mech. Anal., 184, pp 303–339, 2007
7. X. Blanc, C. Le Bris, P.-L. Lions, *Stochastic homogenization and random lattices*, Journal de Mathématiques Pures et Appliquées, 88, pp 34–63, 2007
8. D. Cioranescu, P. Donato, **An introduction to homogenization.** Oxford Lecture Series in Mathematics and its Applications, 17. The Clarendon Press, Oxford University Press, New York, 1999
9. R. Costaouec, Thèse de l' Université Paris Est, Ecole des Ponts
10. R. Costaouec, C. Le Bris, 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, pp 99–103, 2010
11. R. Costaouec, C. Le Bris, F. Legoll, *Variance reduction in stochastic homogenization: proof of concept, using antithetic variables*, Bol. Soc. Esp. Mat. Apl., 50, pp 9–27, 2010
12. V. V. Jikov, S. M. Kozlov, O. A. Oleinik, **Homogenization of differential operators and integral functionals**. Springer, Berlin, 1994
13. U. Krengel, **Ergodic theorems**, de Gruyter Studies in Mathematics, vol. 6, de Gruyter, 1985
14. F. Murat, *Compacité par compensation*, Ann. Scuola Norm. Sup. Pisa. Cl. Sci. 5 (4) pp 485–507, 1978
15. G. Nguetseng, *A general convergence result for a functional related to the theory of homogenization*, SIAM J. Math. Anal. 20 (3), pp 608–623, 1989
16. A. N. Shiryaev, **Probability**, Graduate Texts in Mathematics, vol. 95, Springer, Berlin, 1984
17. L. Tartar, *Compensated compactness and applications to partial differential equations,* Nonlinear analysis and mechanics: Heriot–Watt Symposium, Vol. IV, pp. 136–212, Res. Notes in Math., 39, Pitman, MA, 1979
18. M. Thomas, *Propriétés thermiques de matériaux composites : caractérisation expérimentale et approche microstructurale*, [Thermal properties of composite materials: experimental characterization and microstructural approach], Thèse de l' Université de Nantes, Laboratoire de Thermocinétique, CNRS - UMR 6607, 2008