A Numerical Study of the Convergence in Stochastic Homogenization

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Abstract. There are a lot of works on how to compute the effective characteristics of random composite media, but behind all these computations there are no indications on how they are related to the rigorous methods of stochastic homogenization. The definition of a random medium is also often unclear. In this paper we partly fill in this gap and present numerical results where this relation is clear. Moreover, we compare these results with other frequently used methods.

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1. Introduction

In this paper we compare some different methods of computing the homogenized (or effective) conductivity of composite materials. In particular, we will consider composites where one phase is included in another continuous phase.

When one assumes that the inclusions are periodically distributed, there are well-known rigorous mathematical results which tell how to compute the effective properties of different composite media, see e.g. [6] and [13]. The effective properties are expressed in terms of a solution of a problem over one cell of periodicity. This solution can be computed by some numerical method, see e.g. Section 3.2.

In the case when the inclusions are randomly distributed there are also mathematical homogenization results on how to (almost surely) compute the effective properties in terms of a solution of an auxiliary problem. Since this auxiliary problem is stated in an abstract probability space it is not

possible to find this solution by any numerical method. However, in [1], it was proved how to find a converging sequence of approximations, which can be numerically computed.

There are a lot of works on how to compute the effective characteristics of random composite media but behind all these computations there is no indication on how they are related to the rigorous methods of stochastic homogenization. The definition of a random media is also often unclear.

The main goal of this paper is to apply the results in [1] to compute effective properties of some examples of random composite media. Moreover, we compare these results with other methods frequently used in the literature.

The paper is organized in the following way: In Section 2 give some preliminary results concerning the theory of stochastic homogeneous fields. In Section 3 we present some results from stochastic homogenization. In particular, we define the abstract auxiliary problem mentioned above. We also explain the results from [1] concerning how to make a periodic approximation of the effective properties of random media. In section 4 we construct a class of random media and use the technique in [1] to compute effective properties of some examples from this class. Moreover, we compare these results with other methods frequently used in the literature. Finally, we give some concluding remarks in Section 5.

2. Stochastic Homogeneous Fields

Let $(\Omega, \mathcal{F}, \mu)$ be a probability space.

Definition 1. An N-dimensional dynamical system is a family of maps $T_x : \Omega \to \Omega$, $x \in \mathbf{R}^{\mathbf{N}}$, which satisfy the following conditions:

(1) The group property:

$$T_{x+y} = T_x T_y, \forall\ x, y \in \mathbf{R}^N \text{ and } T_0 = I,$$

where I is the identity map.

(2) The map T_x is measure preserving, i.e. for any $x \in \mathbf{R}^{\mathbf{N}}$ and for any μ -measurable subset $\mathcal{U} \subset \Omega$ the set $T_x \mathcal{U}$ is μ -measurable and $\mu(\mathcal{U}) = \mu(T_x \mathcal{U})$.

(3) For any measurable function f on Ω, the function $f(T_x \omega)$ defined on $\mathbf{R}^N \times \Omega$ is measurable ($\mathbf{R}^N \times \Omega$ is endowed with the measure $dx \times \mu$, dx stands for the Lebesgue measure).

A measurable function f defined on Ω is called invariant if $f(\omega) = f(T_x\omega)$ for every x in $\mathbf{R}^{\mathbf{N}}$ and a.e. ω in Ω. A dynamical system is called ergodic if any invariant function is constant a.e. in Ω.

Let $f \in L^1_{loc}(\mathbf{R}^{\mathbf{N}})$. If for any Lebesgue measurable subset $K \subset \mathbf{R}^{\mathbf{N}}$, $|K| \neq 0$, the following limit exists:

$$\lim_{\varepsilon \to 0} \frac{1}{|K|} \int_K f(\frac{x}{\varepsilon}) \, dx \tag{1}$$

and is independent of K, then the limit (1) is said to be the mean value of f and is denoted by $M(f)$. An alternative formulation is as follows: Let

$$K_t = \left\{ x \in \mathbf{R}^{\mathbf{N}} : x/t \in K, t > 0 \right\}.$$

Then, we can write

$$M(f) = \lim_{t \to \infty} \frac{1}{t^N |K|} \int_{K_t} f(x) \, dx. \tag{2}$$

If the family of functions $f(x/\varepsilon)$ is bounded in $L^\alpha_{loc}(\mathbf{R}^{\mathbf{N}})$ for some $\alpha \geq 1$ we have that

$$f(\frac{x}{\varepsilon}) \to M(f) \quad \text{weakly in } L^\alpha_{loc}(\mathbf{R}^{\mathbf{N}}).$$

The following useful theorem holds, see e.g. [3],[6] and [13]:

Theorem 1. (Birkhoff's Ergodic Theorem) *Let $f \in L^p(\Omega)$, $p \geq 1$. Then for a.e. $\omega \in \Omega$ the realization $F(x) = f(T_x\omega)$ possesses a mean value $M(F)$, in the sense that*

$$F(\frac{x}{\varepsilon}) \to M(F) \quad \text{weakly in } L^p_{loc}(\mathbf{R}^{\mathbf{N}}).$$

Moreover, the mean value $M(f(T_x\omega))$ is invariant as a function of ω and

$$\langle f \rangle := \int_\Omega f(\omega) \, d\mu = \int_\Omega M(f(T_x\omega)) \, d\mu.$$

In particular, if the system is ergodic, then

$$M(f(T_x\omega)) = \int_\Omega f(\omega) \, d\mu \quad \text{for a.e. } \omega \in \Omega.$$

We will also use the following result, see e.g. [3] or [6]:

Theorem 2. *Let Ω_0 be a measurable subset of Ω such that $\mu(\Omega_0) = 1$. Then there exists a measurable subset $\Omega_1 \subset \Omega_0$ such that $\mu(\Omega_1) = 1$ and for any $\omega \in \Omega_1$ we have $T_x\omega \in \Omega_0$ for a.e. $x \in \mathbf{R}^{\mathbf{N}}$.*

3.Homogenization of Random Operators

3.1 Main homogenization result

Let $(\Omega, \mathcal{F}, \mu)$ be a probability space and T_x $(x \in \mathbf{R}^N)$ an ergodic dynamical system on Ω. A vector field $f \in \left[L^2(\Omega)\right]^N$ is said to be potential (respectively solenoidal) if its generic realization (i.e. ω is taken from a subset of measure equal to 1) $f(T_x\omega)$ is a potential (respectively solenoidal) vector field defined on $\mathbf{R}^N$. We denote by $L^2_{\text{pot}}(\Omega)$ (respectively $L^2_{\text{sol}}(\Omega)$) the subspace of $\left[L^2(\Omega)\right]^N$ formed by potential (respectively solenoidal) vector fields. We can now define the following space of vector fields with vanishing mean value:

$$V^2_{pot}(\Omega) = \left\{ f \in L^2_{\text{pot}}(\Omega) : \int_\Omega f \, d\mu = 0 \right\}.$$

Let $A = A(\omega) = (a_{ij}(\omega))$ be a measurable matrix function such that

$$\begin{aligned}
\langle A(\omega)\xi, \xi \rangle &\geq \cdot \alpha \left|\xi\right|^2, \quad \xi \in \mathbf{R}^N, \quad \alpha > 0, \\
a_{ij}(\omega) &\leq \alpha^{-1},
\end{aligned}$$

for every $\xi \in \mathbf{R}^N$ and for $\omega \in \Omega_0$, where Ω_0 is a measurable subset of Ω such that $\mu(\Omega_0) = 1$. By Theorem 2 there exists a measurable subset $\Omega_1 \subset \Omega_0$ such that $\mu(\Omega_1) = 1$ and $T_x\omega \in \Omega_0$ for $\omega \in \Omega_1$ and for a.e. $x \in \mathbf{R}^N$. This implies that for $\omega \in \Omega_1$ the realizations $A(x, \omega) := A(T_x\omega)$ have the following properties: $A(\cdot, \omega)$ is measurable and

$$\begin{aligned}
\langle A(x, \omega)\xi, \xi \rangle &\geq \alpha \left|\xi\right|^2, \quad \xi \in \mathbf{R}^N, \quad \alpha > 0 \\
a_{ij}(x, \omega) &\leq \alpha^{-1},
\end{aligned}$$

for every $\xi \in \mathbf{R}^N$ and a.e. $x \in \mathbf{R}^N$.

Let (ε) be a sequence of positive numbers converging to 0 and Q an open bounded subset of $\mathbf{R}^N$. Given $f \in W^{-1,2}(Q)$ let us consider the following Dirichlet boundary value problem:

$$\begin{cases}
-\text{div}(A(\frac{x}{\varepsilon}, \omega)Du_\varepsilon) = f \text{ on } Q, \\
\\
u_\varepsilon \in W^{1,2}_0(Q).
\end{cases} \tag{3}$$

By the Lax-Milgram lemma there exists a unique solution $u_\varepsilon \in W^{1,2}_0(Q)$ for each ε.

We have the following homogenization result:

Theorem 3. *Let (u_ε) be the solutions of (3). Then for a.e. $\omega \in \Omega$ we have that*

$$u_\varepsilon \quad \to \quad u \quad \text{weakly in } W_0^{1,2}(Q),$$

$$A(x/\varepsilon, \omega)Du_\varepsilon \quad \to \quad A_{\text{hom}}Du \quad \text{weakly in } \left[L^2(Q)\right]^N,$$

where u is the unique solution of the homogenized equation

$$\begin{cases} -\text{div}(A_{\text{hom}}Du) = f \quad \text{on } Q, \\[2mm] u \in W_0^{1,2}(Q). \end{cases}$$

The operator $A_{\text{hom}} : \mathbf{R}^N \to \mathbf{R}^N$ is defined for every $\eta \in \mathbf{R}^N$ by

$$A_{\text{hom}}\eta = \int_\Omega A(\omega)(\eta + v_\eta(\omega)) \, d\mu,$$

where v_η is the solution of the auxiliary problem: Find $v_\eta \in V_{\text{pot}}^2(\Omega)$ such that

$$A(\omega)(\eta + v_\eta(\omega)) \in L_{\text{sol}}^2(\Omega).$$

For a proof of this fact see e.g. [6], [12], [13] and [14]. We also refer to the articles [4] and [5] concerning related results in stochastic homogenization.

3.2. Periodic approximation of A_{hom}

Let the matrix $A(x, \omega)$ be restricted to the cube $Y_\delta = [0, \delta]^N$ and then extended by periodicity to $\mathbf{R}^N$. We denote the extension $A_{\delta,\text{per}}(x, \omega)$. Then for each ω we have a family of equations

$$\begin{cases} -\text{div}(A_{\delta,\text{per}}(\frac{x}{\varepsilon}, \omega)Du_\varepsilon) = f \text{ on } Q, \\[2mm] u_\varepsilon \in W_0^{1,2}(Q), \end{cases} \tag{4}$$

with periodic coefficients. Thus (4) can be homogenized in the standard way. The so defined homogenized matrix $A_{\delta,\text{hom}}$ is given by

$$A_{\delta,\text{hom}}\eta = \frac{1}{|Y_\delta|} \int_{Y_\delta} A(y, \omega) (\eta + D\omega_\eta(y)) \, dy, \tag{5}$$

where v_η is the solution of

$$-\text{div}(A(y, \omega)(\eta + D\omega_\eta(y)) = 0 \quad \text{on } Y_\delta, \quad D\omega_\eta \in W_{\text{per}}^{1,2}(Y_\delta).$$

For more information concerning periodic homogenization, see e.g. [6] and [13]. Recently it was proved in [1] that

$$A_{\delta,\text{hom}} \to A_{\text{hom}} \quad \text{as } \delta \to \infty,$$

that is, $a_{ij}^{\delta,\text{hom}} \to a_{ij}^{\text{hom}}$ as $\delta \to \infty$, $i,j = 1,\dots,N$.

This remarkable fact makes it possible to relate stochastic homogenization to periodic homogenization. For example we show in this paper that it is important for the numerical analysis of different applications.

4. A Class of Random Media

In this section we construct a class of matrices $A(x,\omega)$ which admit homogenization as described in section 3. Moreover, we use the technique of periodic approximation to compute effective properties of some examples from this class of random composite media. We also compare these results with other methods frequently used in the literature.
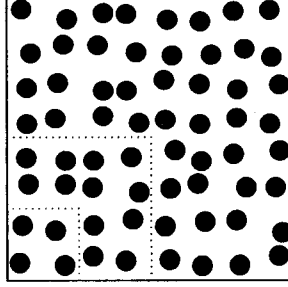

Figure 1: Y_8 for one realization of randomly distributed circles. Indicated are also Y_4 and Y_2.

4.1 Construction

We will now via an example (randomly distributed circles) show how to construct a family of stochastic heterogeneous media described by random fields.

Let each point $(m,n) \in \mathbf{Z}^2$ be the centre of a circle of radius ρ, where $0 \le \rho < 1/2$. In this way we have split $\mathbf{R}^2$ into two sets, namely points inside the circles and points outside the circles. We assume that $\mathbf{R}^2$ consists of two different isotropic materials, material 1 in the circles and the rest of material 2, with conductivities a_1 and a_2, respectively.

We proceed by randomly moving each circle a distance r_x in the x-direction and a distance r_y in the y-direction, where $0 \le r_x, r_y \le 1/2 - \rho$. On the set $S_{mn} = (0,1/2 - \rho) \times (0,1/2 - \rho)$, $((m,n) \in \mathbf{Z}^2)$ we define the measure $\lambda_S = 1/(1/2 - \rho)^2 \, dx dy$. Let $\Gamma = \prod_{(m,n)\in\mathbf{Z}^2} S_{mn}$ and λ_Γ be the product measure on Γ. Γ can now be identified with the set of functions

Γ^*, where

$$\Gamma^* = \{\gamma : \gamma = 1 \text{ on each moved circle and } \gamma = 2 \text{ otherwise}\}.$$

To the set Γ^* we now add all the functions which are obtained by a shift. In this way we obtain a new set Ω of functions, namely

$$\Omega = \{\omega : \omega(t) = \gamma(t + \eta), \gamma \in \Gamma^*, \eta \in \mathbf{R}^2\}.$$

The set Ω is naturally associated with $\Gamma \times \mathbf{R}^2/\mathbf{Z}^2$ and we can define a measure μ on Ω as $\mu = \lambda_\Gamma \times dx$, where dx stands for the Lebesgue measure. By construction Ω is translationally invariant, i.e. contains all functions of the form $\omega(\cdot + x)$. We introduce the dynamical system $T_x : \Omega \to \Omega$ defined as

$$(T_x\omega)(t) = \omega(t + x).$$

Let the function $a : \Omega \to \mathbf{R}$ be defined as

$$a(\omega) = \begin{cases} a_1 \text{ if } \omega(0) = 1, \\ \\ a_2 \text{ if } \omega(0) = 2. \end{cases}$$

We define the random field $A(x,\omega) = a(x,\omega)I$ in terms of realizations of the function a in the following way:

$$A(x,\omega) = a(T_x\omega)I = \begin{cases} a_1 I \text{ if } \omega(x) = 1, \\ \\ a_2 I \text{ if } \omega(x) = 2. \end{cases}$$

To sum up, we have now constructed a random field which may be used to model certain 2-phase composite materials with circular inclusions. Moreover, it is clear that the dynamical system is ergodic (see e.g. the book [3], page 180).

This example can in an obvious way be generalized to cover a whole class of random media. For instance, assume that we instead would like to construct a composite consisting of ellipses that are randomly rotated between the angles α and β. Then $\Gamma = \prod_{(m,n)\in\mathbf{Z}^2} S_{mn}$, where $S_{mn} = (\alpha, \beta)$. Moreover, λ_Γ is then the product measure of the normalized Lebesgue measure on the interval (α, β) (see our second example below).

4.2 Numerical analysis

We will here use the technique of periodic approximation (see Section 3.2) to compute effective properties of the examples described above. We will also compare these results with other methods frequently used in the

literature. Contrary to the method of periodic approximation there is no indication on how the other methods are related to the rigorous method of stochastic homogenization. For more information concerning the computation of effective properties of random materials we refer to the book [15].
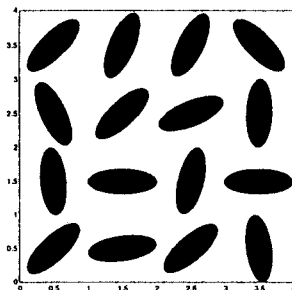

Figure 2: Y_4 for one realization of randomly rotated ellipses.

Remark 1. We want to emphasize that all the computations are done by finite element methods because they are simple to use and offer satisfyingly good accuracy. There are however several different methods more suitable to computations of this kind if high accuracy is of importance. We refer to the articles [7],[8],[9],[10] and [11].

4.2.1 Randomly distributed circles

Let us consider a stochastic two-phase composite in $\mathbf{R}^2$ generated as described in section 4.1 with circles of radii $\rho = 0.3$. Moreover, $a_1 = 1000$ (thermal conductivity in the circles) and $a_2 = 1$ (thermal conductivity outside the circles). In Figure 1 we see Y_8 (defined in Section 3) for one realization.

To be able to apply the numerical homogenization method described in section 3.2 we fix a realization. In Figure 3 we have used solid lines to indicate $A_{\delta,\mathrm{hom}}$ (defined in (5)) for three different realizations and for $\delta = 1, \ldots, 12$.

There is also another frequently used method for computing effective properties of random composite media, see e.g. [2]. The method is as follows: Assume that we have a cell of periodicity (e.g. Y_4) in which we randomly distribute 16 circles according to the rule described in Section 4.1 (we remark that the precise definition of randomly is unclear in many papers). Then we use the standard periodic homogenization to compute the effective properties. We repeat this procedure N times and compute

the average. This average is used as a numerical value of the effective properties. We used $N = 400$ and Y_8 to calculate the effective properties in this way (we repeated the procedure for Y_6, Y_4 and Y_2, obtaining the same effective conductivity as for Y_8 within an accuracy of three decimals). The result is plotted as a dashed line in Figure 3.
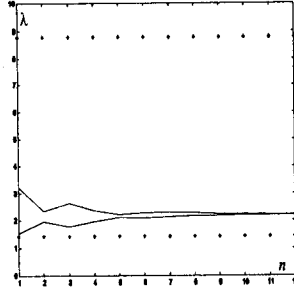

Figure 3: Numerical results for randomly distributed circles. λ denotes the effective conductivity and n is the number of cells.

We emphasize that the computation based on the rigorous theory of stochastic homogenization uses one single realization while the straight line is based on a mean value for 400 realizations. From Figure 3 we can see that in our example the two methods seem to give the same result. However, the theoretical reason for this is unclear.

4.2.2 Randomly rotated ellipses

Let us now consider another composite structure in $\mathbf{R}^2$ within the class described in section 4.1. Indeed, the composite is made up of randomly rotated ellipses with centers in $(m, n) \in \mathbf{Z}^2$ having an eccentricity e of 0.93 and the same volume fraction of inclusions as in the example in the previous subsection. The corresponding set S_{mn} is in this case $(0, 2\pi)$. In Figure 2 we see Y_4 for one realization.

Let us now compute the effective properties according to the method based on stochastic homogenization when $a_1 = 1000$ (thermal conductivity in the ellipses) and $a_2 = 1$ (thermal conductivity outside the ellipses). In Figure 4 we have plotted these results. The two curves correspond to the effective conductivities in the x_1- and x_2-directions, respectively, for subcells Y_δ, $1 \leq \delta \leq 12$, of one fixed realization. As expected they seem to converge to the same value. We have also marked the conductivity in the x_1-direction by *-lines for the two extreme situations (upper and lower bounds) where all ellipses are directed either horizontally or vertically. It can be interesting to note that the "stochastic" distribution is closer to the
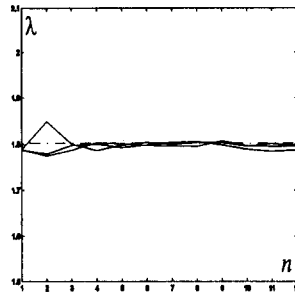
lower bound.

Figure 4: Numerical results for randomly distributed ellipses. λ denotes the effective conductivity and n is the number of cells.

Next, we use the second numerical method for computing effective properties. The calculations are based on 400 realizations and Y_8 as the cell of periodicity. Moreover, $a_1 = 10$ (thermal conductivity in the ellipses) and $a_2 = 1$ (thermal conductivity outside the ellipses). The 400 values obtained by periodic homogenization are plotted in Figure 5 together with the famous G-closure, containing all possible pairs of eigenvalues (see e.g. page 194 in [6].

5. Concluding Remarks

Most papers on stochastic homogenization either deal with theoretical aspects or with questions regarding computational issues. The main contribution of this paper is that we have tried to connect these two directions.

We started by giving some basic definitions of stochastic fields. Then we presented the main ideas and results on how to homogenize random media. As shown in Section 3, the effective properties of a random medium are expressed in terms of a solution of an auxiliary problem. Unfortunately this auxiliary problem is stated in an abstract probability space making it impossible to numerically compute the effective properties. However, it was recently shown in [1] that it is possible to find a converging sequence of periodic approximations that easily can be computed.

In many papers dealing with the computation of effective properties of random composites, the main method used is such: Take a periodic unit cell with thousands of inclusions. Then displace every inclusion a small amount so that it will not cause an overlap with other inclusions. Repeat this procedure until an equilibrium is achieved. Compute the effective properties of this unit cell using standard periodic homogenization. Now

iterate this full procedure many times and finally take the average of all effective values obtained. This average is then used as an approximation of the effective properties of a random medium. Though this method seems to work well and is intuitively correct, it is not very rigid from the stochastic homogenization standpoint.
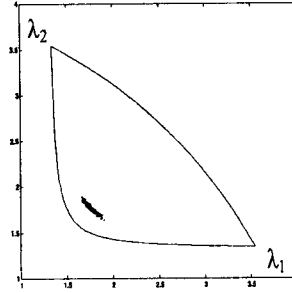

Figure 5: Distribution of the conductivities for 400 different realizations of Y_8. λ_i denotes the effective conductivity in the x_i direction.

In this paper we have compared the recent method described in [1] with the method of iterations mentioned above. We applied both methods to two different examples of random media and noticed that they seem to give same results. However, as we have pointed out before, the theoretical reason for this is unclear since only the first method is based on a rigorous mathematical foundation. We also point out that in many works concerning the estimation of effective properties of random media, the precise description of randomness is often diffuse or not indicated. By this article, we hope that the questions and issues described above will be paid more attention in forthcoming papers.

As a final remark we want to mention that when one considers elastic properties of composite materials the results of this paper are still valid. In particular, it is straightforward to generalize the results concerning periodic approximation in [1] to the vector-valued (elasticity) case.

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