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Influence of the inclusions distribution on the effective properties of heterogeneous media

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Abstract

In this paper we investigate the effective conductivity of composite materials by means of the homogenization method. We concentrate on composites with circular or elliptic cylindrical inclusions. In particular, we are interested in the effect of the distribution of the cylinders in the continuous material on the effective properties. We compare rectangular and hexagonal distributions with random distributions for different volume fractions of the inclusions. We also study the effect of the number of inclusions in each periodic cell for the random structure as well as shape influence of the elliptical inclusions.
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1. Introduction

Composite materials are becoming increasingly popular in many branches of engineering. A common feature for these materials is that the locally heterogeneous material behaves like a homogeneous medium when the characteristic size of the inclusions is much smaller than the size of the whole specimen. In this situation the behavior of the composite can be described by the so called effective properties which are obtained by some type of averaging. One method to obtain effective properties is by using the homogenization method, developed in the study of partial differential equations with rapidly varying coefficients. For a detailed exposition on the subject of homogenization, we refer to Refs. [1–3].

A common assumption in the homogenization method is to assume that the inclusions are periodically distributed in the material. However, this assumption might often not be in accordance with the situation in real-world composites, where the inclusions in most cases are randomly distributed. We will in this paper compare the effect of the geometries and the distributions of the inclusions on the effective conductivity of some composites.

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2. The homogenization method

In this section we give some basic results from the theory of homogenization. Let Ω be a open bounded subset of $\mathbf{R}^n$, Y the unit cube in $\mathbf{R}^n$ and $\langle\cdot,\cdot\rangle$ the Euclidean inner product. Let us define $A^h(x) = A(x/\varepsilon_h)$, where the conductivity matrix $A(x) = (a_{ij}(x))$ satisfies $a_{ij} = a_{ji}$, $a_{ij} \in L^\infty(\Omega)$ and is Y-periodic for every $i,j = 1,\ldots,n$. Consider the weakly formulated stationary heat conduction problem

$$\begin{cases} \int_\Omega \langle A^h(x)\nabla u_h, \nabla\phi\rangle \mathrm{d}x = \int_\Omega f\phi \,\mathrm{d}x, & \forall\phi \in H_0^{1,2}(\Omega), \\ u_h \in H_0^{1,2}(\Omega), \end{cases} \tag{2.1}$$

where $f \in L^2(\Omega)$ is the internal heat source and (ε_h) is a sequence of positive real numbers converging to zero. Since ε_h is a measure of the size of the periodicity of the material, we may expect the inhomogeneity to vanish in the limit. The homogenization method deals with questions regarding whether the sequence of solutions (u_h) converge in some sense to an element u_0 and in that case, whether u_0 then is the solution of a homogeneous problem, that is, the solution of a problem with a constant conductivity matrix B. The answers to these questions are contained in Theorem 2.1.

Theorem 2.1. *Consider problem (2.1). Then*

$u_h \rightharpoonup u_0$ weakly in $H_0^{1,2}(\Omega)$,

and

$A^h(x)\nabla u_h \rightharpoonup B\nabla u_0$ weakly in $(L^2(\Omega))^n$,

where u_0 is the unique solution of the homogenized problem

$$\begin{cases} \int_\Omega \langle B\nabla u_0, \nabla\phi\rangle \mathrm{d}x = \int_\Omega f\phi \,\mathrm{d}x, & \forall \phi \in H_0^{1,2}(\Omega), \\ u_0 \in H_0^{1,2}(\Omega). \end{cases}$$

The constant matrix B is given by the expression

$$Be_k = \frac{1}{|Y|}\int_Y A(x)(e_k + \nabla w_k)\mathrm{d}x,$$

where w_k is the unique solution of the cell problem

$$\begin{cases} \int_Y \langle A(x)(e_k + \nabla w_k), \nabla\phi\rangle \mathrm{d}x = 0, & \forall \phi \in H_\square^{1,2}(Y), \\ w_k \in H_\square^{1,2}(Y). \end{cases}$$

Here e_k denotes the kth unit vector and $H_\square^{1,2}(Y)$ is the subset of $H^{1,2}(Y)$ of Y-periodic functions u with mean value zero. A proof of this theorem can be found in Ref. [1].

Let us now concentrate on problems in $\mathbf{R}^2$. We write the effective conductivity matrix B as

$$B = \begin{bmatrix} b_1 & b_{12} \\ b_{12} & b_2 \end{bmatrix}.$$

3. Numerical computation of *B*

Suppose that the matrix $A(x) = a(x)I$ possesses a symmetry of the kind

$$a(x_1, x_2) = a(-x_1, x_2) \quad \text{or} \quad a(x_1, x_2) = a(x_1, -x_2),$$

for every $x = (x_1, x_2)$, which is the case when we have hexagonal or rectangular distribution. Then it is possible to prove that $b_{12} = 0$ and that b_k can be found by either of the minimization problems

$$b_k = \frac{1}{|Y|}\min_{v\in H_{\mathrm{per}}^{1,2}(Y)}\left\{\int_Y a(x)|e_k + \nabla v|^2 \mathrm{d}x\right\},$$

$$\frac{1}{b_k} = \frac{1}{|Y|}\min_{v\in H_{\mathrm{per}}^{1,2}(Y)}\left\{\int_Y \frac{1}{a(x)}|e_l + \nabla v|^2 \mathrm{d}x\right\},$$

where e_l is orthogonal to e_k and $H_{\mathrm{per}}^{1,2}(Y)$ is the space of Y-periodic functions belonging to the Sobolev space $H^{1,2}(Y)$. We refer to Refs. [3,4] and for these facts.

The exact value of b_k is unknown for most cases. However, we can obtain upper and lower numerical estimates of b_k. Indeed, if V is any finite-element subspace of $H_{\mathrm{per}}^{1,2}(Y)$ and b_k^+ and b_k^- are the values defined by

$$b_k^+ = \frac{1}{|Y|}\min_{v\in V}\left\{\int_Y a(x)|e_k + \nabla v|^2 \mathrm{d}x\right\},$$

$$\frac{1}{b_k^-} = \frac{1}{|Y|}\min_{v\in V}\left\{\int_Y \frac{1}{a(x)}|e_l + \nabla v|^2 \mathrm{d}x\right\},$$

then it is obvious that

$$b_k^- \le b_k \le b_k^+.$$

One can get the values of b_k^+ and b_k^- by simple computations with standard FEM software. We will use the approximation

$$\bar{b}_k = \frac{b_k^- + b_k^+}{2},$$

for b_k with a maximal error of

$$\varepsilon_k = \frac{b_k^+ - b_k^-}{2}.$$

4. Bounds on the effective properties

If $a(x)$ only takes the values a_1 and a_2, $0 < a_1 < a_2$, with volume fractions ν_1 and $\nu_2 = 1 - \nu_1$, respectively, then the following well known inequalities hold (see Ref. [3])

$$\frac{1}{a_2 - \lambda_1} + \frac{1}{a_2 - \lambda_2} \le \frac{2}{\nu_1(a_2 - a_1)} - \frac{\nu_2}{\nu_1 a_2}, \tag{4.1}$$

$$\frac{1}{\lambda_1 - a_1} + \frac{1}{\lambda_2 - a_1} \le \frac{2}{\nu_2(a_2 - a_1)} + \frac{\nu_1}{\nu_2 a_1}, \tag{4.2}$$

(the generalized Hashin–Shtrikman bounds), where λ_i are the eigenvalues of the homogenized matrix B. The set of pairs (λ_1, λ_2) satisfying both Eqs. (4.1) and (4.2) gives us all possible effective properties that can be obtained for given a_1, a_2 and ν_1 (Fig. 1). One usually refers to structures which

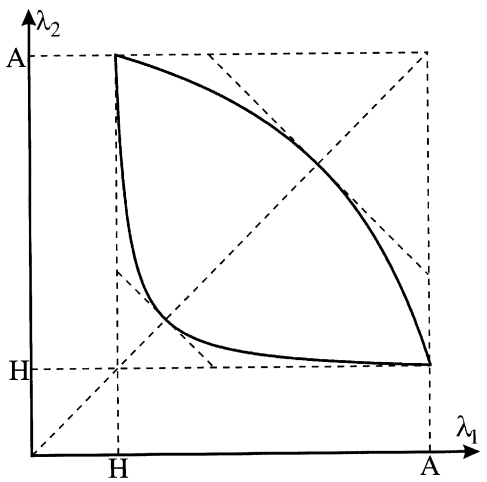


Fig. 1. The so called G-closure, the set of all possible effective conductivities.

realize equality in Eqs. (4.1) or (4.2) as upper optimal and lower optimal structures.

5. Numerical results

We will in this section give some numerical examples of the geometric influence of the inclusions on the effective conductivity of some composite materials. In particular, we will concentrate on the difference between random and periodic dispersions of disks in a continuous matrix material. The problem of obtaining accurate numerical solutions of the corresponding PDE in the case where we have a large number of close-to-touching inclusions have been studied for instance in Refs. [5–13]. In this paper, we use the MATLAB toolbox FEMLAB to compute the effective properties. In general, the finite element method is not the best method to solve these equations, but it is reasonably good for the number of inclusions we use in this paper.

For a given number of inclusions in one periodic cell, we generate a series of different realizations where the inclusions are randomly dispersed. On an overall basis, each realization yields a periodic material, but as the number of inclusions in each periodic cell goes to infinity, the material will become totally random. By taking the mean values and standard deviations of the effective conductivities for at least 200 different realizations, we get an approximation of the effective conductivity for the random material.

Each quasi-random realization are generated by a Monte Carlo procedure of Metropolis type, see Refs. [14–16]. This is done by first placing every inclusion in a rectangular or hexagonal array. Each disk is then given a small tentative displacement in a random direction. The move is accepted or rejected whether or not the move will cause the disk to overlap a neighboring disk. One iteration step consists of trying to move each disk once. The length of the displacement is chosen such that the ratio of acceptance is 30–50%. This process is repeated several times until an equilibrium state is obtained (Fig. 2). We use up to 8000 iteration steps for the realizations with high volume fractions of inclusions to get a good random material. See Ref. [17] for a discussion on the number of simulations required.

5.1. How many inclusions do we need to get a satisfactory random composite?

We start with an example to determine the number of inclusions required to get a fairly good value of the effective conductivity of a random material. This question have been discussed in Ref. [6]. We investigate this by considering a quasi-random composite with 4, 16, 64 and 144 inclusions in each periodic cell. For this analysis, we assume that $a_1 = 1$, $a_2 = 10$ with a corresponding volume fraction of $\nu_2 = 0.5$, where we refer to the inclusions as material 2. Note that another set of conductivities can mean that fewer or more inclusions are required to get a satisfactory value of the effective conductivity. We present the results in Table 1. The first column shows the number of inclusions in each periodic cell, the second column shows the mean value and the standard deviation of the effective conductivity and the third column shows the mean value and the standard deviation of b_{12}/b_1, a measure of the anisotropy of the composite. Actually, b_{12}/b_1 is the quotient between the flux in the x_2-direction and the flux in the x_1-direction when a temperature difference of one is applied in the x_1-direction. In the random limit, the material is perfectly isotropic and the quotient should be zero.

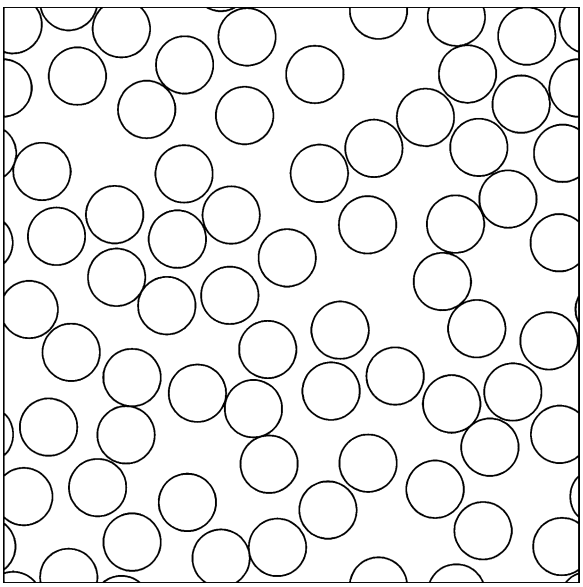


Fig. 2. One realization of a quasi-random periodic cell with 64 circular inclusions of a total volume fraction of 0.5.

By comparing with the effective conductivity ($\bar{b} = 2.546 \pm 0.009$), for this composite given in Ref. [6], we draw the conclusion that for this particular composite 64 inclusions are enough. However, we see that even 16 inclusions give a satisfactory value of the effective conductivity for our analysis. We note that the standard deviations of the effective conductivity and the measure of anisotropy decrease more or less like the square root of the number of inclusions, which is in agreement with what we expect from a Monte Carlo process.

Table 1

Incl.	$\bar{b} \pm$ SD	Anisotropy
4	2.476 ± 0.093	−0.001 ± 0.019
16	2.543 ± 0.076	0.001 ± 0.017
64	2.546 ± 0.036	0.000 ± 0.009
144	2.546 ± 0.023	−0.001 ± 0.005

Table 2

ν_2	Hex.	Rect.	$\bar{b} \pm$ SD	Anisotropy
0.1	1.1782	1.1782	1.182 ± 0.006	0.000 ± 0.004
0.2	1.3913	1.3915	1.410 ± 0.018	−0.000 ± 0.008
0.3	1.6506	1.6520	1.697 ± 0.034	0.001 ± 0.014
0.4	1.9733	1.9806	2.068 ± 0.054	−0.002 ± 0.018
0.5	2.3864	2.4155	2.543 ± 0.076	0.001 ± 0.017
0.6	2.9375	3.0372	3.170 ± 0.098	−0.000 ± 0.018
0.7	3.7190	4.0617	3.945 ± 0.086	0.001 ± 0.010
0.8	4.9488	–	5.153 ± 0.062	0.000 ± 0.005

5.2. The effective conductivity with respect to volume fraction

In this example, we compare random distribution with hexagonal and rectangular distributions of the inclusions for different volume fractions. We consider a composite with $a_1 = 1$ and $a_2 = 10$, where we refer to the inclusions as material 2. We present the results in Table 2. The first column shows the volume fraction of the inclusions, the second column shows the effective conductivity for hexagonal distribution, the third column shows the effective conductivity for rectangular distribution and the fourth and fifth columns show the effective properties of the random distribution with 16 inclusions. The results from Table 2 are plotted in Fig. 3 together with the lower Hashin–Shtrikman bound.

We note that hexagonal distribution gives the lowest effective conductivity, near the lower Hashin–Shtrikman bound, followed by rectangular distribution (except for high volume fractions) whereas random distribution gives the highest effective conductivity. This is due to the fact that individual inclusions are farthest apart in hexagonal packing, compared to a random composite where we get percolation effects when the inclusions are close-to-touching. However,

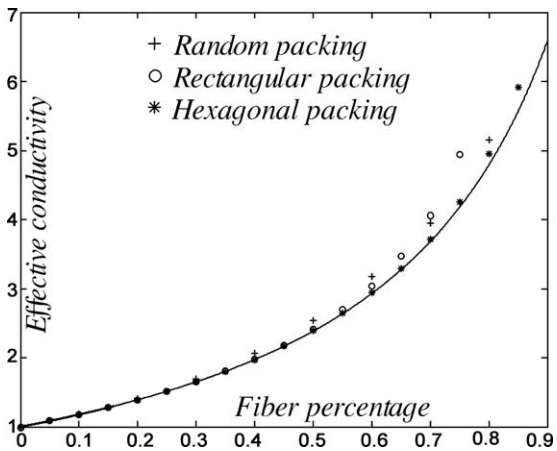


Fig. 3. Effective conductivities of hexagonally, rectangularly and randomly distributed inclusions compared with the lower Hashin–Shtrikman bound.

Table 3

a_1	a_2	Hex.	Rect.	$\bar{b} \pm$ SD	Anisotropy
1	10	2.3864	2.4155	2.543 ± 0.076	0.001 ± 0.017
1	100	2.9266	2.9948	3.407 ± 0.236	−0.000 ± 0.033
1	1000	2.9967	3.0714	3.555 ± 0.275	0.002 ± 0.037
10	1	4.1903	4.1400	3.936 ± 0.126	0.001 ± 0.018
100	1	34.170	33.392	29.57 ± 1.77	0.002 ± 0.035
1000	1	333.70	325.59	281.5 ± 22.4	−0.001 ± 0.042

for high volume fractions we see that rectangular distribution gives the highest effective conductivity. In this case, we get a higher percolation effect in the rectangular material since the inclusions in the rectangular array are more close-to-touching in an average sense than the inclusions in the random material. This effect does not occur in the hexagonal material since the hexagonal packing is optimal.

5.3. The effect of the constituents individual conductivities

This example demonstrates the effect of the individual conductivities of the constituents. We consider a composite with a volume fraction of $\nu_2 = 0.5$. The results are presented in Table 3. The first and second columns show the conductivities of the continuous material and the inclusions, respectively. The third column shows the effective conductivity for hexagonal distribution, the fourth column shows the effective conductivity for rectangular distribution and the fifth and sixth columns show the effective properties of the random distribution with 16 inclusions.

We observe that the relative differences between the effective conductivities of the random material and the periodic materials increase as the ratio between a_1 and a_2 increases/decreases. For instance, the effective conductivity for the random material is 6.6% higher for $a_2/a_1 = 10$ and 18.6% higher for $a_2/a_1 = 1000$ than for the corresponding hexagonal material.

5.4. Effective conductivities of elliptic inclusions

We compare the effective properties in the two major directions of horizontally aligned elliptical inclusions with different ratios *a*/*b* between the major and minor axes. We

Table 4a

a/*b*	Hex.	Rect.	$\bar{b}_1 \pm$ SD
1.0	2.386	2.416	2.543 ± 0.076
1.2	2.475	2.449	2.658 ± 0.080
1.5	2.584	2.494	2.814 ± 0.083
2.0	2.721	2.557	3.042 ± 0.085
3.0	2.893	2.650	3.452 ± 0.150
5.0	3.066	2.757	3.982 ± 0.155
10.0	3.225	2.864	4.606 ± 0.155

Table 4b

a/b	Hex.	Rect.	$\bar{b}_2 \pm$ SD
1.0	2.386	2.416	2.543 ± 0.076
1.2	2.310	2.386	2.451 ± 0.066
1.5	2.244	2.354	2.348 ± 0.064
2.0	2.188	2.320	2.244 ± 0.058
3.0	2.144	2.286	2.141 ± 0.060
5.0	2.118	2.263	2.054 ± 0.047
10.0	2.104	2.249	1.974 ± 0.039

consider a composite with $a_1 = 1$, $a_2 = 10$ and with a volume fraction of $\nu_2 = 0.5$, where we refer to the inclusions as material 2. In Table 4a we tabulate the effective conductivities in the direction of the major axis and in Table 4b we tabulate the effective conductivities in the direction of the minor axis. The first column show the quotient *a/b* between the major and minor axes whereas columns 2–4 show the effective properties for hexagonal, rectangular and random distribution with 16 inclusions.

The values in the above tables are plotted together with the G-closure in Fig. 4. We note that random distribution of ellipses is much more effective than periodic distribution to get to the extreme points of the G-closure.

5.5. Randomly rotated elliptic inclusions

As a final example, we consider composites containing 16 randomly rotated elliptic inclusions with different ratios *a/b* between the major and minor axes (Fig. 5). We consider a composite with $a_1 = 1$, $a_2 = 10$ and with a volume fraction of $\nu_2 = 0.5$, where we refer to the inclusions as material 2. The first column in Table 5 shows the quotient *a/b* between the major and minor axes whereas the second and the third columns show the effective properties for random distribution.

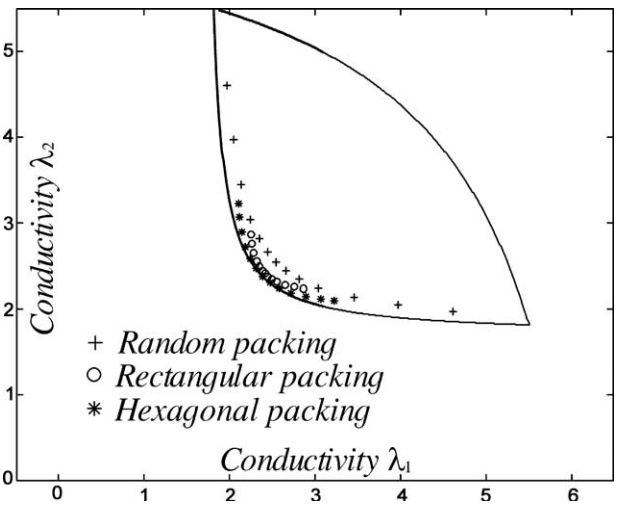


Fig. 4. Effective conductivities for composites with hexagonally, rectangularly and randomly distributed elliptic inclusions plotted together with the G-closure.

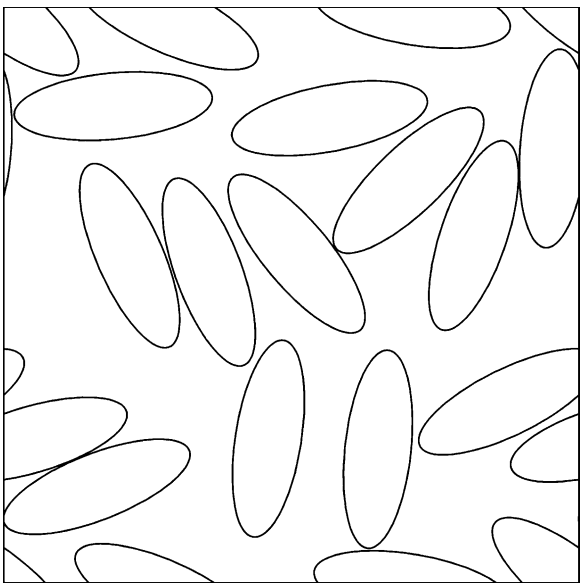


Fig. 5. One realization of a quasi-random periodic cell consisting of 16 rotated elliptic inclusions with $a/b = 3$ and volume fraction 0.5.

Table 5

a/b	$\bar{b} \pm$ SD	Anisotropy
1.0	2.543 ± 0.076	0.001 ± 0.017
1.5	2.574 ± 0.080	0.003 ± 0.022
2.0	2.649 ± 0.105	−0.003 ± 0.027
3.0	2.778 ± 0.184	−0.003 ± 0.044
4.0	2.882 ± 0.213	−0.008 ± 0.064

We note that the effective conductivity increases as the ratio *a/b* increases. This is due to the fact that the heat flux easier can find long paths of highly conducting material in both directions for structures with large ratios of *a/b*.

6. Discussion

We have compared the effective properties for composites with periodic and random inclusions. In general, when the inclusions have higher conductivity than the continuous phase, the effective conductivity is significantly higher for random distributions than for periodic distributions. Hence in the modelling of conductivity problems of physical composites, the periodicity assumption in homogenization might render values of the effective properties that are different from the actual conductivity of the composite. We expect the same phenomenon to appear in the elasticity case and plan to extend this analysis to problems in plane elasticity as well as to problems of three-dimensional character.

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