ON THE EFFECTIVE BEHAVIOR OF 3D POROUS CONDUCTIVE MATERIALS

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RESUMEN
Para estimar la conductividad efectiva de un material isotrópico poroso periódico lineal tridimensional por medio del Método de Homogeneización Asintótica, es necesario resolver los llamados problemas locales. Dado que el camino analítico directo usual resulta ser muy complejo, se adoptó una estrategia de elementos finitos. La conductividad efectiva estimada es comparada con finas cotas lineales disponibles que prueban su consistencia. Finalmente, por medio de un ejemplo ilustrativo, esta aproximación es aplicada al mejoramiento de cotas variacionales para compuestos no lineales, que resulta ser muy significativa para poros casi en percolación.

ABSTRACT
In order to estimate the effective conductivity of a 3D linear periodic porous isotropic composite via the Asymptotic Homogenization Method, it is required the so-called local problems to be solved. As the common direct analytical approach turns out to be quite complicated, a finite-element strategy is adopted. The estimated effective conductivity is compared to available fine linear bounds, proving to be consistent. Finally, by means of an illustrative example, this approximation is applied to the improvement of variational bounds for nonlinear porous composites, resulting to be remarkable for quasi-percolating pores.

INTRODUCTION

Derivation of the effective behavior of heterogeneous media starting on the geometrical and physical properties of the constituents has become a main subject in present-time research, which is confirmed by the increasing number of applications concerning reinforced composite materials [1, 2]. Such global behavior is described by means of the effective properties and, in this direction, two different approaches have arisen: asymptotic and variational procedures of homogenization [3, 4, 5], which, in fact, complement each other. The first of these approaches commonly yields closed-form approximations, while the second one results in bounds.

The first part of this paper deals with the application of the Asymptotic Homogenization Method (AHM) [3] in order to estimate the effective conductivity of a linear porous isotropic composite consisting in periodically distributed spherical voids in a solid isotropic matrix. Such estimation relies on the solution of the so-called local problems, for which, in this case, the Finite Element Method (FEM) [6] was employed. The AHM-FEM approximation is compared to available fine bounds [7], which proves the consistency of our prediction.

The second part of this paper is devoted to illustrate the application of the AHM-FEM result to the estimation of the effective behavior of nonlinear composites by means of an example. In this case, the application consists in improving some available nonlinear variational bounds [8].

STATEMENT OF THE AHM PROBLEM

It is our interest to study the effective conductivity $\hat{\varepsilon}$ of a linear periodic isotropic composite obtained by replicating a cell Q consisting in a solid isotropic cubic matrix containing a centered empty spherical inclusion. Without loss of generality, it can be assumed that Q has unit volume and is centered at the origin of an Oy_1, y_2, y_3 Cartesian coordinate system. It is convenient to denote the solid matrix and void inclusion phases by Q_M and Q_I, respectively, so $Q = Q_M \cup Q_I$.

It is well known that the differential equations which govern this problem have rapidly oscillating coefficients, so a direct analytical or numerical treatment is practically impossible. A successful alternative is to apply the AHM, from which a system of homogenized equations with smooth coefficients is obtained. Such averaged system, of which the

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coefficients are the effective ones, models a homogeneous medium equivalent to the original one in the sense that they behave equally.

In order to obtain the mentioned effective coefficients, the so-called local problems, which come also as partial results from the application of the AHM, have to be solved. In this case, taking into account the symmetry of the cell [3], the local problem is stated in the first octant Q^+ of Q, as

$$\frac{\partial}{\partial y_i}\left(\varepsilon_{ij}(y)\frac{\partial M_k(y)}{\partial y_i}\right)=0,\ y\in Q_M^+ \quad (1)$$

$$M_k(y)=\frac{1}{2},\ y\in\partial Q_M^+\cap\left\{y_1=\frac{1}{2}\right\}$$

$$M_k(y)=0,\ y\in\partial Q_M^+\cap\{y_1=0\} \quad (2)$$

$$\left(\varepsilon_{ij}(y)\frac{\partial M_k(y)}{\partial y_i}\right)n_i=0,$$

$$y\in\partial Q_I^+\cup\left[\bigcup_{i=2}^{3}\left(\partial Q_M^+\cap\{y_i=0\}\right)\right]\cup\left[\bigcup_{i=2}^{3}\left(\partial Q_M^+\cap\left\{y_i=\frac{1}{2}\right\}\right)\right]$$

where $M_k(y) = N_k(y) + y_k$. The solutions $N_k(y)$ are 1-periodic functions in variable y. On the other hand, the AHM leads directly to the strong formulation of the local problems, so the effective conductivity tensor is given by

$$\hat{\varepsilon}_{ik}=\int_Q\left(\varepsilon_{ik}(y)+\varepsilon_{ij}(y)\frac{\partial N_k(y)}{\partial y_i}\right)dy \quad (3)$$

Due to the global isotropic behavior of the composite, it is sufficient to obtain

$$\hat{\varepsilon}=2^3\int_{Q^+}\varepsilon(y)\frac{\partial M_1(y)}{\partial y_1}dy \quad (4)$$

as $\hat{\varepsilon}_{ij}=\hat{\varepsilon}\delta_{ij}$ and $\varepsilon_{ij}(y)=\varepsilon(y)\delta_{ij}$ with $\varepsilon(y)=\varepsilon_M(\varepsilon(y)=0)$ for $y\in Q_M(y\in Q_I)$.The formulation of the problem given above is consistent with the required formulation for the FEM simulation in the next section.

FEM simulation

FEM calculations were performed using 10-node tetrahedrons to construct the mesh of the geometrical model Q_M^+. The amount of needed elements varies with the inclusion concentration c_I, for instance for $c_I = 0.17$, a mesh with 966 elements was fine enough to represent accurately the geometry and to obtain accurate results, however, in order to avoid distorted elements for large c_I, a finer mesh was employed: the model for $c_I = 0.47$, was meshed using 10507 elements, as it is shown in Figure 1.

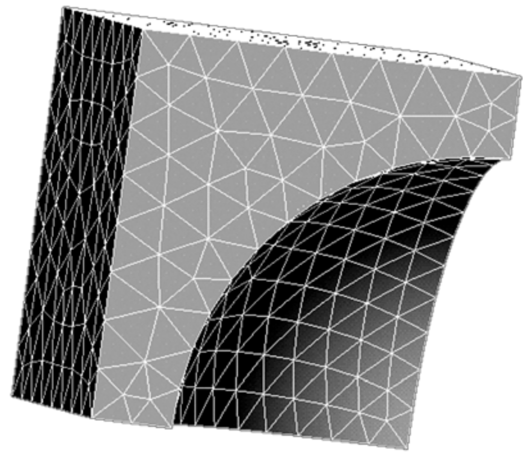

Figure 1. Mesh of Q^+ for $c_I = 0.47$.

For control purposes, the AHM-FEM results were compared to specialization of the linear bounds by Bruno [4] for the normalized effective conductivity $m = \frac{\hat{\varepsilon}}{\varepsilon_M}$ to our case, that is, m(0) the effective conductivity of a matrix with unit conductivity containing void inclusions ($\varepsilon_I = 0$). Such comparison is shown in Figure 2 against c_I up to the percolation limit. The curves are labeled as follows: A subscript U or L indicates whether the curve is an upper or lower bound; a superscript B or H stands for “Bruno” or “Homogenization”. It can be seen that the AHM-FEM estimate of m is closer to the upper bound, while significantly improves over the lower bound.

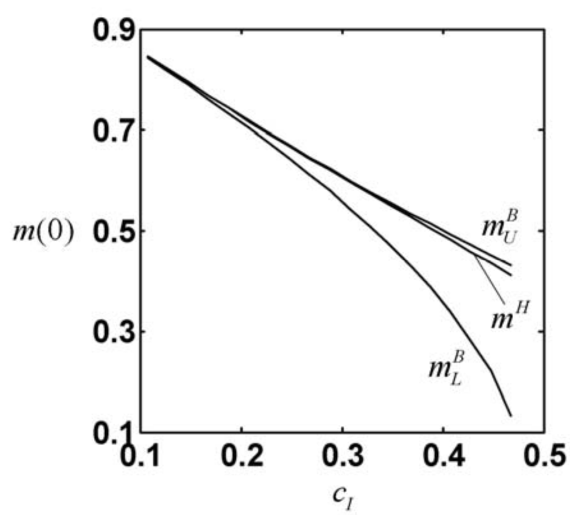

Figure 2. Plots of bounds and AHM-FEM estimate for the normalized effective conductivity.

Application to nonlinear composites

This section is devoted to the presentation of how the previously shown results are applied to a specific matter: the estimation of the effective behavior of nonlinear composites which is formally stated by means of the minimum energy principle as

$$\hat{W}(\bar{E}) = \inf_{E \in S(\bar{E})} \int_Q W(E, y) dy \quad (5)$$

where $S(\bar{E})$ is the set of self-equilibrated electric field with mean value $\bar{E}$, and

$$W(E, y) = W_M(E) f_M(y) + W_I(E) f_I(y) \quad (6)$$

is the constitutive potential describing the behavior of each phase. Here, the f's are the characteristic functions of the phases. Consider, for motivation purposes, a material showing the microgeometry studied in the preceding sections, in which the matrix behaves according to the law [8, 9]

$$V_M(E) \equiv W_N(E) = \tfrac{1}{2}\, \varepsilon_N |E|^2 + \tfrac{1}{4}\, \gamma |E|^4, \; \gamma > 0 \quad (7)$$

while $W_I \equiv 0$ as the inclusions are empty. The elementary upper and lower bounds are given by

$$\left\{ \overline{W^*} \right\}^* (\bar{E}) \le \hat{W}(\bar{E}) \le \overline{W}(\bar{E}) \quad (8)$$

where the overbar and the asterisk stand for averaging and Legendre-transforming processes, respectively. It can be shown that in the case of porous materials the elementary lower bound is $\left\{ \overline{W^*} \right\}^* \equiv 0$. As the matrix is nonlinear, the best bound available is a lower one requiring the use of a linear comparison composite with the same micro-geometry as the nonlinear material. The matrix of such comparison material is described by the potential

$$W_0(E) = \tfrac{1}{2}\, \varepsilon_0 |E|^2 \quad (9)$$

while in this case the inclusions are voids. With this consideration, the lower bound reads

$$W_L(\bar{E}) = \tfrac{1}{2} \hat{\varepsilon}_0 \left| \bar{E} \right|^2 + c_M \min_E (W_M - W_0)(E) \quad (10)$$

where $\hat{\varepsilon}_0$ is the effective conductivity of the linear comparison composite depending on the conductivity ε_0 of the matrix. Note that an estimate or lower bound for $\hat{\varepsilon}_0$ is required to be available. For the particular nonlinear law consider here, the bound specializes to

$$\hat{W}_L(\bar{E}) = \tfrac{1}{2} \hat{\varepsilon}_0 \left| \bar{E} \right|^2 - \tfrac{1}{2} c_M \frac{(\varepsilon_N - \varepsilon_0)^2}{\gamma} \quad (11)$$

Now, this bound can be maximized with respect to ε_0, that is, choosing the comparison material which provides the best bound $\hat{W}_L$. Consider now a linear homogeneous medium with potential W_{LN} characterized by the same conductivity ε_N as the matrix of the nonlinear composite. Then, normalization and optimization of $\hat{W}_L$ yields

$$\frac{\hat{W}_L}{W_{LN}}(\bar{E}) = m(0) \left(\frac{m(0)}{2c_M} \frac{\gamma \left| \bar{E} \right|^2}{\varepsilon_N} + 1 \right) \quad (12)$$

where $m(0) = \dfrac{\hat{\varepsilon}_0}{\varepsilon_0}$. From the normalization of the elementary upper bound

$$\frac{\overline{W}}{W_{LN}}(\bar{E}) = c_M \left(1 + \tfrac{1}{2} \frac{\gamma \left| \bar{E} \right|^2}{\varepsilon_N} \right) \quad (13)$$

In Figure 3, plots of the normalized elementary upper bound and the lower bound by Ponte Castaneda are presented for $c_I = 0.47$ near percolation against a parameter involving all the information about the nonlinear behavior. The curves are labeled as follows: a subscript U or L indicates whether it is an upper or a lower bound; a superscript E stands for an elementary bound; while a superscript B or H specifies the method used for the normalized effective conductivity m(0), that is, the lower bound by Bruno (1991) or the homogenization AHM-FEM procedure presented in the previous section. Note that, for c_I near percolation, the improvement provided by using the AHM-FEM method is remarkable.

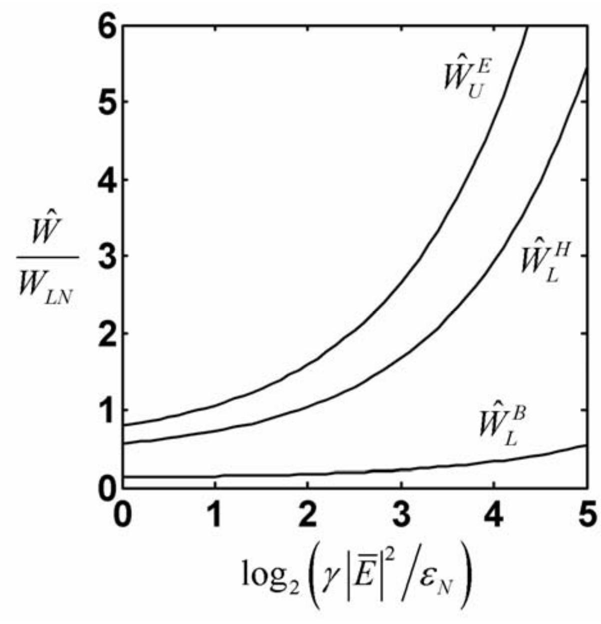

Figure 3. Plots of normalized bounds for $c_I = 0.47$.

CONCLUDING REMARKS

In this paper, the effective conductivity of a linear porous composite was obtained by means of the AHM. The local problems were solved using a FEM strategy. A comparison of the AHM-FEM results with available bounds is carried out, yielding in consistency and improvement of accuracy of the estimation for large concentrations of the empty inclusion. Finally, an application to a particular nonlinear case has revealed that remarkable improvement is obtained for concentrations near percolation.

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