Improved bounds for the effective energy of nonlinear 3D conducting composites

A. León-Mecías[a], J. Bravo-Castillero[a], A. Mesejo-Chiong[a], L.D. Pérez-Fernández[b], and F.J. Sabina[c,*]
[a]*Facultad de Matemática y Computación, Universidad de La Habana, San Lázaro y L, Habana 4, CP-10400, Cuba.*
[b]*Instituto de Cibernética, Matemática y Física, Calle 15 e/t C y D, Vedado 10400, Habana 4, Cuba.*
[c]*Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México, Apartado Postal 20–726, Delegación de Alvaro Obregón, 01000 México D.F., México.*

Recibido el 6 de abril de 2006; aceptado el 26 de abril de 2007

Recent variational inequalities of Talbot are used to improve the lower and upper bounds for the effective energy of nonlinear 3-D two-phase conducting composites. The effective conductivity of the linear isotropic two-phase periodic conducting composite used as comparison material in the inequalities is computed through an asymptotic homogenization model by finite element analysis of the local problem on the three-dimensional cubic unit cell with one spherical inclusion. A brief mathematical description of the numerical method is included. Numerical calculations of the effective conducting linear property are compared with Bruno's bounds. It shows that the numerical solution for the limit cases of superconducting and empty inclusions improves the bounds when the inclusion volume fraction is greater than about 0.4. It is natural to expect an improvement in the whole volume fraction of Talbot's bounds for nonlinear conducting composites when the numerical calculation is used instead of bounds for the linear comparison problem, as is the case here.

Keywords: Variational bounds; effective properties; conducting composites; asymptotic homogenization method; finite element method.

Las cotas inferior y superior para la energía efectiva de un compuesto conductor no lineal, tridimensional bifásico son mejoradas usando desigualdades variacionales de Talbot. La conductividad efectiva del compuesto de comparación periódico, bifásico, lineal, usado en las desigualdades, se obtiene resolviendo los problemas locales que aparecen al aplicar el método de homogeneización asintótica, mediante un análisis de elemento finito, tomando como celda unitaria un cubo con una inclusión esférica. Los métodos numéricos empleados se describen brevemente. Los resultados numéricos para la propiedad efectiva del compuesto de comparación se comparan con las cotas de Bruno. Se observa que una de las cotas está muy cerca de la solución numérica, para los casos límites de inclusión superconductora y vacía, y cuando la fracción volumétrica de la inclusion es mayor que 0.4, ésta se aleja. Es natural entonces esperar una mejora, en todo el rango de fracciones volumétricas de las cotas de Talbot para compuestos conductores no lineales, cuando se usan los cálculos numéricos, en lugar de las cotas para el compuesto de comparación lineal, como es aquí el caso.

Descriptores: Cotas variacionales; propiedades efectivas; compuestos conductores; método de homogeneización asintótica; método de elemento finito.

PACS: 02.70.Dc; 46.15.Cc; 66.70.+f

1. Introduction

The derivation of the average behaviour of a heterogeneous medium based on knowledge of its components is a very important topic because of the increasing use of reinforced composite materials in many applications (see, for instance, the recent review given in Refs. 14 and 28). This work considers the determination of tighter bounds for the effective energy of a nonlinear conducting composite material.

The general problem related to the calculation of global properties (or effective coefficients) has been the object of study by many researchers, for random media or for media distributed in a particular way and for linear and nonlinear composites. In Ref. 11 the best possible bounds on the effective conductivity were found for linear isotropic two-phase composites with perfect contact at the interface, providing only volume fraction information of the phases. In Refs. 29 and 25, these variational principles were generalized and developed to nonlinear problems. In Ref. 19, a method is introduced to estimate bounds for the effective properties of a nonlinear composite using information of the effective properties of a linear comparison composite with the same microstructure. In Ref. 9, very good approximations for global energy of nonlinear conducting composites were obtained by combining the variational principles of Ref. 19, using the prediction of Ref. 25 for the comparison material. Improved new bounds for nonlinear dielectric composites were derived in Ref. 26 and applied to two-phase matrix inclusion composites by combining their variational inequalities with the bounds derived in Ref. 4.

The goal of the present work is to obtain better lower and upper bound approximations of the effective energy for a nonlinear two-phase conducting composite. Variational inequalities reported in Ref. 26 combined with the results from the effective properties of linear conducting composites are used. The Asymptotic Homogenization Method (AHM) based on two-scale asymptotic expansions [2, 3, 15, 23], and the Finite Element Method (FEM) [12, 30], are used to calculate the effective conductivity of a two-phase 3-D composite material having a periodic structure consisting of a sphere immersed in a cube. This kind of medium requires special treatment because of the rapid variation of its materials properties.

The AHM is a rigorous mathematical technique for modeling the global behaviour of these types of heterogeneous media (see, for instance, Refs. 7 and 17). By means of this method, the system of partial differential equations with rapidly oscillating coefficients, governing the medium occupied by the composite, is transformed into another one without this variation. The coefficients in the new problem are the effective coefficients, and their determination depend on the solution of the so-called problems on the cell or local problems. The solution of the local problems have been the subject of many scientific works. Exact solutions for one-dimensional homogenization problems (laminate composite) can be seen in Refs. 5, 8, and 18. Analytical solutions for some particular two-dimensional homogenization problems such as unidirectional fibrous reinforced composite can be found in the recent papers [6, 10, 16, 20–22]. These exact solutions are useful as a control guide to numerical methods applied to problems involving a more complicated geometrical microstructure. In the above mentioned works, one can find a great variety of references related to the topic of analytical and numerical applications to 1-D and 2-D homogenization problems. Examples from 3-D homogenization problems for linear and nonlinear composites include for instance the methods proposed in Refs. 27 and 28, and in the recent works [13, 24].

The structure of the article is as follows: Sec. 2 gives improved variational bounds for the effective energy density properties of a nonlinear conducting composite are stated. Section 3 describes the formal procedure of the AHM for obtaining the homogenized equation and the local problem which allows us to derive the effective coefficient for a periodic two-phase 3D isotropic conducting medium. Some comments related to the mathematical justification of this method are included. Section 4 offers a brief mathematical description of the numerical method employed and summarizes some aspects related to its computational implementation. Numerical examples to illustrate the efficiency and importance of the calculations are also shown in this section. Finally, Sec. 5 is devoted to some concluding remarks.

2. Improved bounds for the effective energy of nonlinear conducting composites

Following the variational procedure given by Talbot in Ref. 26, which incorporates microstructural information, improved bounds for the effective energy density properties of a nonlinear conducting composite will be obtained.

In order to derive variational bounds in composites, a basic problem is to bound the density of the effective energy of the composite, W^{eff}, defined by

$$W^{eff}\left(\overline{E}\right) = \inf_{E\in K} \int_R W\left(E,x\right)dx, \tag{1}$$

where

$$K = \{E : E \text{ is R-periodic}, E = -\nabla\Psi, \int_R E\left(x\right)dx = \overline{E}\},$$

$E = -\nabla\Psi$ is the electric field, Ψ is the electric potential, x is the Cartesian coordinate of the point.

Consider an isotropic composite with n isotropic phases, and assume that the composite is periodic. For this type of a composite, the local energy density function is given by

$$W\left(E,x\right) = \sum_{r=1}^{n} W_r\left(E\right) f_r\left(x\right),$$

where W_r and f_r are the energy and characteristic functions of the domain occupied by the r-phase, respectively.

A comparison material with energy function $\widehat{W}$ will be introduced. This comparison material has the same microgeometry as the nonlinear one. We shall deal with the particular problem of bounding the effective energy density of a two-phase 3-D conducting composite, for two cases, consisting of the following:

$a)$ One isotropic linear phase, the inclusion, with energy function

$$W_L\left(E\right) = \frac{1}{2}\kappa_L\left|E\right|^2,$$

and a nonlinear one, the matrix, with energy function

$$W_N\left(E\right) = \frac{1}{2}\kappa_N\left|E\right|^2 + \frac{1}{4}\gamma\left|E\right|^4,$$

where κ_L, κ_N and γ are constants.

For the comparison material, the energy functions are

$$\widehat{W}_I = W_L \quad \text{and}$$

$$\widehat{W}_M = \frac{1}{2}\kappa_0\left|E\right|^2,$$

where the subindices I, M refer to inclusion and matrix, respectively; by formula (3.9), page 3622 in Ref. 26, the lower bound for the normalized effective energy density can be derived as

$$\frac{W^{eff}}{W_L}\left(\overline{E}\right) \geq \frac{\kappa_0}{\kappa_L} m\left(\frac{\kappa_L}{\kappa_0}\right) + p_2\left(\frac{\kappa_N}{\kappa_L} - \frac{\kappa_0}{\kappa_L}\right)^2 / \frac{\gamma\left|\overline{E}\right|^2}{2\kappa_L}, \tag{2}$$

where κ_0 is a free parameter, p_2 is the matrix volume fraction, $\overline{E}$ is the mean value of E and $m\left(\kappa_L/\kappa_0\right)$ is the effective conductivity of a matrix with unitary conductivity and inclusion with conductivity κ_L/κ_0. Any lower bound for the effective property $m\left(\kappa_L/\kappa_0\right)$ can be substituted in (2) and the best bound follows by maximizing the right-hand side with respect to κ_0. In Figs. 1 and 2, the normalized effective energy W^{eff}/W_L is plotted against the parameter $\log_2\left(S_1\right)$

$$\left(S_1 = \left(\frac{\gamma\left|\overline{E}\right|^2}{2\kappa_L}\right)\right)$$

for $\kappa_N/\kappa_L = 2$ and for values of the volume fraction $p_1 = 0.1715$ and $p_1 = 0.470597$, respectively. In both figures we compare Talbot's lower bound (labelled Talbot 99 LB) replacing $m(\kappa_L/\kappa_0)$ with the bound of Bruno and the lower bound obtained using the FEM approximation for the effective property (labelled FEM LB). We note that a much improved lower bound of the effective energy near percolation is obtained.

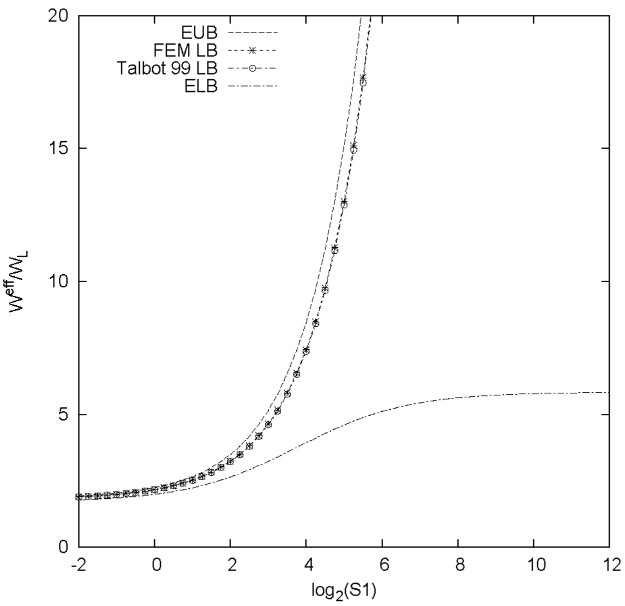

FIGURE 1. Bounds for linear inclusions in a nonlinear matrix with fixed volume fraction $p_1 = 0.1715$. The curves are labelled: EUB and ELB are the simple upper and lower bounds obtained in Ref. 26 by substituting constant trial fields into Eq. (1) or in its dual; Talbot 99 LB and FEM LB, are the lower bounds obtained substituting the effective property into Eq. (2) with the lower bound of Bruno and the FEM approximation, respectively.

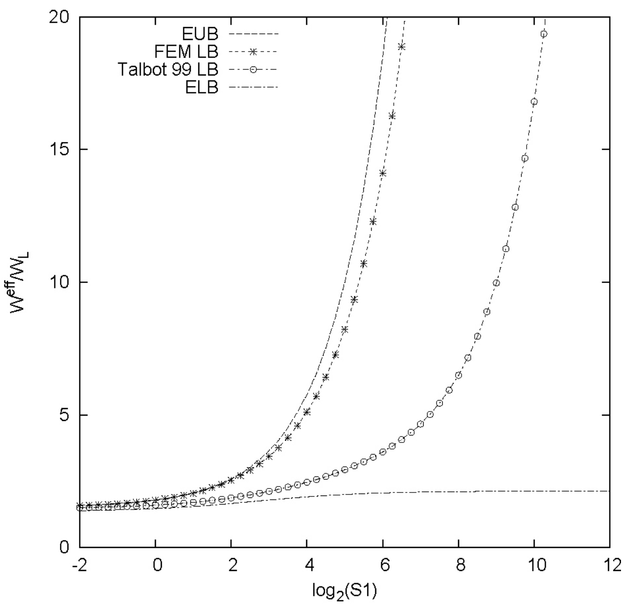

FIGURE 2. As Fig. 1 except that $p_1 = 0.470597$.

$b)$ A linear matrix containing nonlinear inclusion

In this case the problem considered is that of improving Talbot's upper bound Talbot in Ref. 26 by taking

$$\widehat{W_I} = \frac{1}{2}\kappa_0 \left|E\right|^2, \qquad \widehat{W_M} = W_L.$$

From the formula (3.8), page 3622 in Ref. 26, it is possible to obtain the following optimized upper bound for the effective energy density normalized by the linear phase energy:

$$\frac{W^{eff}}{W_L}\left(\overline{E}\right) \leq m\left(\infty\right) - \frac{\left(m\left(\infty\right)-1\right)^2\left(F^2-2F\right)}{p_1\left(\frac{\kappa_N}{\kappa_L}-1\right)+m\left(\infty\right)-1} + \frac{p_1\left(m\left(\infty\right)-1\right)^4 F^4}{2\left(p_1\left(\frac{\kappa_N}{\kappa_L}-1\right)+m\left(\infty\right)-1\right)^4}\frac{\gamma\left|\overline{E}\right|^2}{\kappa_L}, \tag{3}$$

where F is the real solution of

$$\frac{\gamma\left|\overline{E}\right|^2}{\kappa_L}\frac{p_1\left(m\left(\infty\right)-1\right)^2}{\left(p_1\left(\frac{\kappa_N}{\kappa_L}-1\right)+m\left(\infty\right)-1\right)^3}F^3 + F = 1.$$

Here $m(\infty)$ is always an upper bound for the effective conductivity constant $m(z)$ of the comparison material (a matrix with conductivity constant equal to unity containing inclusion with conductivity equal to z, in this case $z = 10^5$). In Fig. 3, the normalized effective energy W^{eff}/W_L against the parameter $\log_2(S_1)$ is plotted for $\kappa_N/\kappa_L = 2$ and for volume fraction $p_1 = 0.470597$. We compare Talbot's upper bound, replacing $m(\infty)$ with Bruno's linear bound and the effective prediction obtained by the FEM. There is also an improvement here on the effective energy upper bound, near percolation, as a nonlinear conducting composite is observed.

3. Effective conductivity coefficients and local problems for a periodic medium, as derived from the AHM

The composite material under study is assumed to have a periodic structure (certainly an idealization except for man-made regular composites), which means a structure with slowly changing geometric characteristics with a period ε (known as the *scaling parameter*). The periodic distributions consist of repetitions of a unit cell made of a conducting spherical inclusion Y_I (dark color) and a conducting matrix Y_M (light color), as shown in Fig. 4. The inclusion is at the center of the cube with radius R (≤ 0.5). Each phase of the medium is homogeneous and isotropic. The structure has period εY and occupies a region $\Omega_\varepsilon \subset \mathbb{R}^3$. The above assumptions lead to the following family of boundary value problems indexed by the scaling parameter, in the heterogeneous body ε:

$$\frac{\partial}{\partial x_i}\left(\kappa_{ik}^{\varepsilon}(x)\frac{\partial \Psi^{\varepsilon}(x)}{\partial x_k}\right)=0, \tag{4}$$

$$\Psi^{\varepsilon}(x)\big|_{\Gamma_1^{\varepsilon}}=0, \tag{5}$$

$$\kappa_{ik}^{\varepsilon}(x)\frac{\partial \Psi^{\varepsilon}(x)}{\partial x_k}n_i\bigg|_{\Gamma_2^{\varepsilon}}=g. \tag{6}$$

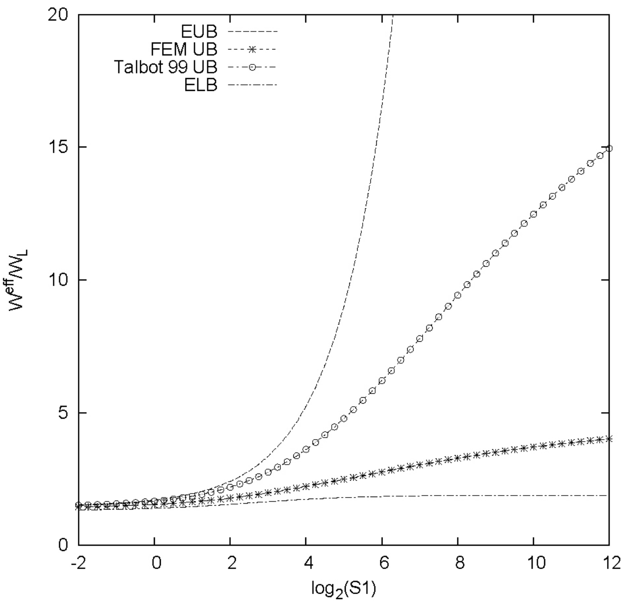

FIGURE 3. Bounds for nonlinear inclusions in a linear matrix with fixed volume fraction $p_1 = 0.470597$. The curves are labelled as in Fig. 1 with UB the upper bound obtained from Eq. (3).

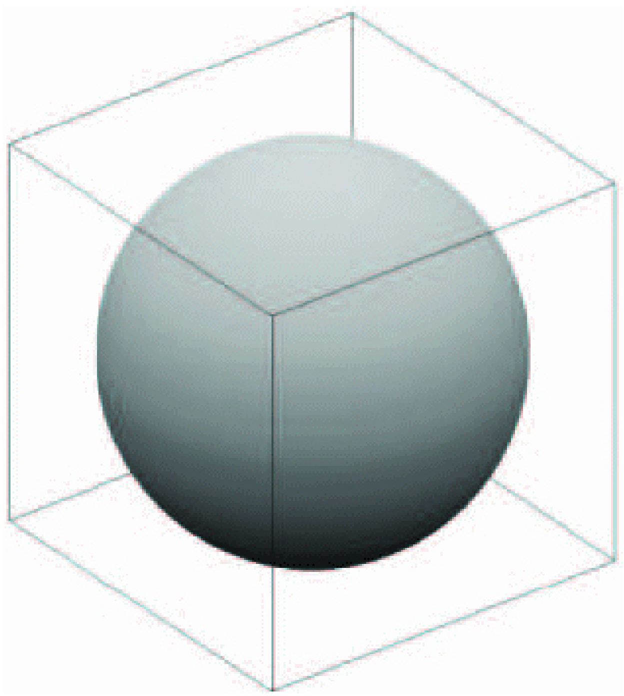

FIGURE 4. Periodic unit cell, a spherical inclusion immersed in a cube.

The coefficients are periodically oscillating and physical fields depend on $x = (x_i) \in \Omega_\varepsilon$. Here $\kappa = (\kappa_{ij})$ stands for the conductivity second rank tensor (although it should be noticed that the system of equations for the magnetic permeability and dielectric permittivity coefficients are analogous), Ψ for the electric potential field. The summation convention over repeated Latin indices running from 1 to 3 is understood. The boundary $\partial\Omega_\varepsilon$ is $\Gamma_1^{\varepsilon}\bigcup\Gamma_2^{\varepsilon}$. Perfect contact conditions at the interphase are considered.

Two different scales will be introduced, one denoted by x in the domain Ω_ε at which the heterogeneities are invisible, and the other a microscopic one denoted by $y = x/\varepsilon$. Dependence on x (*global variable*) describes macro-effects, while dependence on y (*local variable*) describes micro-effects. For a fixed $\varepsilon > 0$, we have the following expression for the coefficients of the conductivity isotropic tensor:

$$\begin{aligned}\kappa_{ik}^{\varepsilon}(x) &= \kappa_{ik}\left(\frac{x}{\varepsilon}\right)\\ &= \kappa_I\delta_{ik}I_I(y)+\kappa_M\delta_{ik}I_M(y).\end{aligned}$$

These are piecewise constant functions in x and Y–periodic functions in y. Here $I_I(y)$ and $I_M(y)$ are the characteristic functions of inclusion and matrix respectively. Further, we assume that $\kappa_{ik}(y) \in L^{\infty}(\Omega)$ positive definite, that is $\kappa_{ik}(y)\xi_i\xi_k \geq \alpha\xi_i\xi_i$, for some $\alpha > 0$.

Due to the rapid oscillation of $\kappa_{ik}^{\varepsilon}(x)$, an efficient direct numerical treatment of (4)-(6) is impossible. One task in this work is to find the effective coefficients $\kappa_{ik}^{h}(x)$ by using the well-known method of two-scale asymptotic homogenization [2,3] and the FEM [30].

3.1. Asymptotic Homogenization

The basic idea of the two-scale asymptotic homogenization method is to embed the specific problem in question in a family of problems parametrized by the scale parameter $\varepsilon > 0$. By letting the microscale tend to zero, homogenized differential equations are obtained.

To derive the limit problem in a formal way (see for instance Ref. 2) one starts from the ansatz that the unknown function $\Psi^{\varepsilon}(x)$ possesses an asymptotic expansion with respect to ε of the form

$$\Psi^{\varepsilon}(x)=\Psi_0(x,y)+\varepsilon\Psi_1(x,y)+\varepsilon^2\Psi_2(x,y)+..., \tag{7}$$

where $\Psi_0(x,y), \Psi_1(x,y), ...$ are Y periodic functions in y. By substituting (7) in (4)-(6), following the chain rule for $\Psi = \Psi(x,y)$

$$\frac{\partial\Psi}{\partial x}=\left(\frac{\partial\Psi}{\partial x}+\varepsilon^{-1}\frac{\partial\Psi}{\partial y}\right)\bigg|_{y=\frac{x}{\epsilon}}$$

and comparing the terms associated with the same powers of ε, we find from the terms of order ε^{-2}, by considering x and y as independent variables, that the function $\Psi_0(x,y)$

does not depend on y. For the factor corresponding to ε^{-1}, we get

$$\frac{\partial}{\partial y_i}\left(\kappa_{ij}(y)\frac{\partial \Psi_1(x,y)}{\partial y_j}\right) = -\frac{\partial}{\partial y_i}\left(\kappa_{ij}(y)\right)\frac{\partial \Psi_0(x)}{\partial x_j},$$

and the expressions for the functions $\Psi_1(x,y)$ can be written as follows:

$$\Psi_1(x,y) = N_k(y)\frac{\partial \Psi_0(x)}{\partial x_k},$$

where $N_k(y)$ are the unique Y-periodic solutions, up to a constant in $H^1(Y)$ of the local problem defined by Eqs. (12)-(15), below.

Finally, for terms of order zero, the homogenized problem can be obtained as following:

$$\frac{\partial}{\partial x_i}\left(\kappa_{ik}^h\frac{\partial \Psi^0(x)}{\partial x_k}\right) = 0, \tag{8}$$

$$\Psi^0(x)\big|_{\Gamma_1^0} = 0, \tag{9}$$

$$\kappa_{ik}^h(x)\frac{\partial \Psi^0(x)}{\partial x_k}n_i\bigg|_{\Gamma_2^0} = g, \tag{10}$$

whose solution $\Psi^0(x)$ is the limit of the family of solutions $\Psi^\varepsilon(x)$ of the original one when $\varepsilon \to 0$. Convergence results can be seen, for instance, in Refs. 1, 2 and 15. The effective conductivity tensor κ_{ik}^h is given by the formula

$$\kappa_{ik}^h = \frac{1}{|Y|}\int_Y\left(\kappa_{ik}(y) + \kappa_{ij}(y)\frac{\partial N_k(y)}{\partial y_j}\right)dy, \tag{11}$$

where the real-valued and Y–periodic functions $N_k(y)$ are solutions of the local problems

$$\frac{\partial}{\partial y_i}\left(\kappa_{ij}(y)\frac{\partial N_k(y)}{\partial y_j}\right) = -\frac{\partial}{\partial y_i}\kappa_{ik}(y), \tag{12}$$

with periodicity conditions

$$N_k(y)\big|_{y_r=0} = N_k(y)\big|_{y_r=1} \tag{13}$$

$$\left.\frac{\partial N_k(y)}{\partial y_r}\right|_{y_r=0} = \left.\frac{\partial N_k(y)}{\partial y_r}\right|_{y_r=1} \tag{14}$$

and perfect contact conditions at the interface between the inclusion and the matrix:

$$\|N_k(y)\| = 0, \tag{15}$$

$$\left\|\left(\kappa_{ij}(y)\frac{\partial N_k(y)}{\partial y_j} + \kappa_{ik}(y)\right)n_i\right\| = 0, \tag{16}$$

where n is the outward unit normal to the sphere, and the double bar notation denotes the jump across the interface.

The solutions to (12)-(14), $N_k(y)$, for $k = 1,2,3$, are 1-periodic in y, and are found up to an arbitrary constant. The choice of the constant is fixed by the condition $\langle N_k(y)\rangle = 0$,

$$\langle N_k(y)\rangle = \frac{1}{|Y|}\int_Y N_k(y)dy$$

(see for instance page 106 in Ref. 2). This local problems come also as partial results from the application of the AHM.

In fact the two-scale asymptotic method leads directly to the strong formulation of the local problems. Consequently, the material functions involved must be more regular, at least of class $C^1(Y)$. However, the weak (variational) form of (12)-(14) can be used, c.f. Ref. 8.

4. Numerical computation of the effective coefficients

In order to compute the coefficient (11) we have to solve (12)-(14). Due to numerical reasons, instead of solving Eqs. (12), we will employ the equivalent ones

$$\frac{\partial}{\partial y_i}\left(\kappa_{ij}(y)\frac{\partial M_k}{\partial y_j}\right) = 0 \tag{17}$$

where $M_k = N_k(y) + y_k$.

To solve (17) by the FEM with professional software, it is convenient to transform the periodicity conditions into boundary conditions.

Following [2], taking into account the symmetry of the cell and considering the cube

$$Q = \left\{-\frac{1}{2} \le y_1, y_2, y_3 \le \frac{1}{2}\right\}$$

as the periodicity domain, we find that instead of seeking for a Y- periodic solution of (12)-(14), we shall look for a solution $M_k(y)$ that is periodic in all the $y_q, (q \ne k)$ such that

$$\frac{\partial}{\partial y_i}\left(\kappa_{ij}(y)\frac{\partial}{\partial y_j}M_k(y)\right) = 0, \tag{18}$$

$$M_k(y)\big|_{y_k=d} = d, \tag{19}$$

$$\kappa_{ij}(y)\frac{\partial}{\partial y_j}M_h(y)\bigg|_{y_i=d} = 0, \tag{20}$$

where $d = 0$, $d = 0.5$, $i \ne k$ and perfect interface conditions.

Then we get the following expression for the effective coefficient:

$$\kappa^h = \kappa_{11}^h = 2^3\int_Q \kappa_{11}(y)\frac{\partial M_1(y)}{\partial y_1}dQ. \tag{21}$$

In this case, due to the isotropic global behaviour of the composite

$$\kappa_{11}^h = \kappa_{22}^h = \kappa_{33}^h,$$

and similarly to (21)

$$\kappa_{\alpha\alpha}^h = 2^3\int_Q \kappa_{\alpha\alpha}(y)\frac{\partial M_\alpha(y)}{\partial y_\alpha}dQ \tag{22}$$

(there is no summation over α)

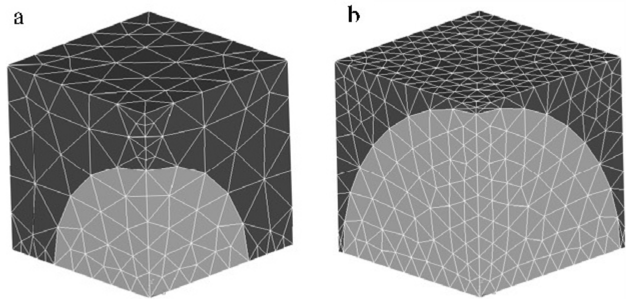

FIGURE 5. Mesh scheme for two volume fractions a) $p_1 = 0.1715$ and b) $p_1 = 0.470597$.

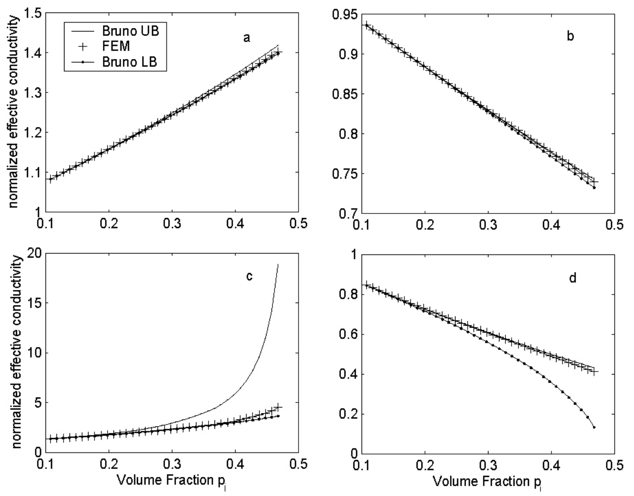

FIGURE 6. Comparison of the FEM results with Bruno's bounds for the normalized effective conductivity against inclusion volume fraction for a conducting sphere in a conducting matrix, a) $\kappa_I/\kappa_M = 2$, b) $\kappa_I/\kappa_M = 0.5$, c) $\kappa_I/\kappa_M \to \infty$ and c) $\kappa_I/\kappa_M = 0$.

to get the effective conductivity coefficient we must solve (18)-(20).

The finite element calculations were made using ANSYS and by incorporating some necessary auxiliary programs. Periodic boundary conditions were replaced by boundary conditions, as mentioned above in Ref. 2. The model volume ($1/8$ of the cubic unit cell Y with an spherical inclusion) were meshed using 10-node tetrahedron thermal solid elements (Solid 87). The number of elements needed varies with the inclusion volume fraction p_1, for instance for $p_1 = 0.1715$ (see Fig. 5a); a mesh with 900 elements and 1737 nodes was fine enough to represent accurately the geometry and to obtain accurate results. However, in order to avoid (or to reduce to a minimum) distorted elements for a large volume fraction of the sphere, a finer mesh was employed; for instance, the model for $p_1 = 0.470597$ (see Fig. 5b) was meshed using 3834 elements with 6574 nodes. To check the accuracy of the standard meshes, the mesh was refined in some cases, and the differences in the effective conductivities constants computed with the standard; the refined meshes were below 0.0008%.

4.1. Numerical examples

Three different sets of material properties for a two-phase conducting composite were considered here, a conducting sphere in a conducting matrix, for $\kappa_I/\kappa_M = 2$ and $\kappa_I/\kappa_M = 0.5$ based on data taken from Ref. 17, a superconducting and a void spherical inclusion in a conducting matrix. It is of interest to compare the results calculated using the FEM with classical upper and lower bounds, for instance the bounds from Bruno [4] of normalized material and engineering constants as a function of the inclusion volumetric fraction p_1 up to the percolation limit. It is shown in Fig. 6 that the effective conductivity of the simulated composite lies between the predictions of Bruno's bounds, showing a better approximation for a small volume fraction than for larger one. Note that for the cases concerning superconducting and empty inclusion, Figs. 6c and d, the upper and lower bounds, respectively, differ from the numerical solution when $p_1 \geq 0.3$. Thus it is natural to hope that the FEM solution would give better results for the approximation of the effective energy of the nonlinear conducting composite than using Bruno's bounds. The choice of the volume fractions in our calculations is dictated by the choice of Bruno's q parameter, which is regularly spaced and already tabulated.

5. Concluding remarks

Using the variational inequalities of Talbot which appeared in Ref. 26, improved lower and upper bounds of the effective energy near percolation for a nonlinear conducting composite are obtained using a FEM solution of a linear comparison medium. These results should prove useful in making better predictions for the effective energy for nonlinear composites for all volume fractions and parameter

$$S_1 = \left(\frac{\gamma \left| \overline{E} \right|^2}{2\kappa_L} \right),$$

which is a measure of the nonlinearity. The effective conductivity for the linear composite material taken as comparison material were accurately computed by the application of the FEM in solving the local problems (coming from the AHM) with the corresponding boundary conditions equivalent to the original periodic conditions. The FEM calculations were made using ANSYS, observing that for large volume fraction of the spherical inclusion, the amount of elements needed to obtain reasonable results was larger than for a small one. The numerical computed effective conductivity was compared with Bruno's bounds [4], and that provided an improvement in the limit cases $\kappa_I/\kappa_M = \infty$ and $\kappa_I/\kappa_M = 0$, particularly when $p_1 \geq 0.3$, which produced an improvement of Talbot's bounds for the effective energy for the nonlinear conducting composite when the FEM approximation are used.

Acknowledgements

The authors are grateful to professor Harald Berger from Otto von Guericke University for useful comments during his visit to Havana University and to Lino E. Borroto from ICIMAF, Cuban Academy of Science, who taught us the first steps using ANSYS. Suggestions and recommendations of members of the Group of Solids Mechanics (R. Rodríguez Ramos and R. Guinovart Díaz) from Havana University, were also very important in this work. The provisions of the Projects PNCB CITMA No. 9/2004 and PAPIIT, DGAPA, UNAM IN101705 are also acknowledged. We wish to express out thanks to the Department of Mathematics and Mechanics of the IIMAS-UNAM and in particular to Ana Pérez Arteaga and Ramiro Chávez for computational support. AL is very grateful for the grant of a scholarship from Red de Macro-Universidades de América Latina y el Caribe. JB recognizes the support of a scholarship from Foundation CIMAC. The authors gratefully acknowledge the Referee's recommendations.

∗ Corresponding author: Telephone: + (52) 55 56223544, Fax: + (52) 55 56223564, e-mail: fjs@mym.iimas.unam.mx

1. G. Allaire, *SIAM J Math Anal* **23** (1992) 1482.
2. N. Bakhvalov and G. Panasenko, *Homogenisation: Averaging Processes in Periodic Media. Mathematics and Applications* (Dordrecht: Kluwer Academic Publishers, 1989).
3. A. Bensoussan, J.L. Lions, and G. Papanicolaou, *Asymptotic Analysis for periodic Structures* (Amsterdam: North-Holland, 1978).
4. O.P. Bruno, *Proc. R. Soc. Lond. A* **433** (1991) 353.
5. J.B. Castillero, J.A. Otero, R.R. Ramos, and A. Bourgeat, *Int. J. Sol. Struct.* **35** (1998) 527.
6. J. Bravo-Castillero, R. Guinovart-Díaz, F.J. Sabina, and R. Rodríguez-Ramos, *Mech. Mater.* **33** (2001) 237.
7. Z. Fang, W. Sun, and J.T. Tzeng, *J. of Composite Materials* **38** (2004) 1371.
8. A. Galka, J.J. Telega, and R. Wojnar, *Comp. Assisted Mech. Eng. Sci.* **3** (1996) 133.
9. L. Gibiansky and S. Torquato, *J. Appl. Phys.* **84** (1998) 301.
10. R. Guinovart-Díaz, J. Bravo-Castillero, R. Rodríguez-Ramos, and F.J. Sabina, *J. Mech. Phys. Solids* **49** (2001) 1445.
11. Z. Hashin and S. Shtrikman, *J. Appl. Phys.* **33** (1962) 3125.
12. P. Knabner and L. Angermann, *Numerik partieller Differentialgleichungen* (Berlin Heidelberg: Springer, 2000).
13. J. Llorca, M. Elices, and Y. Termona, *Acta mater.* **48** (2000) 4589.
14. G.W. Milton, *The Theory of Composites* (Cambridge University Press 2002).
15. O.A. Oleinik, A.S. Schmaev, and G.A. Yosifian, *Mathematical problems in elasticity and homogenization* (Amsterdam: North Holland Publishing Company, 1992).
16. J.A. Otero, J. Bravo-Castillero, R. Guinovart-Díaz, R. Rodríguez-Ramos, and G.A. Maugin, *Arch. Mech.* **55** (2003) 357.
17. F. Périn, *European Journal of Mechanics A/Solids* **23** (2004) 139.
18. B.E. Pobedrya, *Mechanics of composites Materials* (Moscow:Moscow University Press, Russian 1984).
19. P. Ponte Castañeda, *Phil. Trans. R. Soc. Lond. A* **340** (1992) 531.
20. R. Rodríguez-Ramos, F.J. Sabina, R. Guinovart-Díaz, and J. Bravo-Castillero, *Mech. Mater.* **33** (2001) 223.
21. F.J. Sabina, R. Rodríguez-Ramos, J. Bravo-Castillero, and R. Guinovart-Díaz, *J. Mech. Phys. Solids* **49** (2001) 1463.
22. F.J. Sabina, J. Bravo-Castillero, R. Guinovart-Díaz, R. Rodríguez-Ramos, and O.C. Valdiviezo-Mijangos, *International Journal of Solids and Structures* **39** (2002) 483.
23. E. Sánchez-Palencia, *Non Homogeneous Media and Vibration Theory. Lecture Notes in Physics* (Berlin: Springer Verlag, 1980).
24. J. Segurado and J. Llorca, *J. Mech. Phys. Solids* **50** (2002) 2107.
25. D.R.S. Talbot and J.R. Willis, *IMA J. Appl. Math.* **35** (1985) 39.
26. D.R.S. Talbot, *Proc. R. Soc. Lond. A* **455** (1999) 3617.
27. S. Torquato, *J. Appl. Phys.* **58** (1985) 3790.
28. S. Torquato, *Random Heterogeneous Materials. Microstructure and Macroscopic Properties* (Springer, 2002).
29. J.R. Willis, *J. Appl. Mech.* **50** (1983) 1202.
30. O.C. Zienkiewicz, *The Finite Element Method in Engineering Science* (McGraw-Hill Publishing Company, 1977).