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Duality, inverse problems and nonlinear problems in solid mechanics

Microstructurally-based homogenization of electromagnetic properties of periodic media

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Abstract

A general method for homogenization of the electromagnetic properties of a heterogeneous periodic medium is developed, based on its microstructure. This method is inspired by micromechanics (Nemat-Nasser and Hori, 1999). Contrary to other conventional techniques, commonly used in electromagnetism to calculate the overall properties of composites, this microstructurally-based method does not require an explicit numerical solution of the Maxwell equations. We define the macroscopic field quantities as volume averages of the spatially variable fields, taken over a representative volume element (RVE), consisting of a unit cell of the periodic medium (Hill, 1963; Willis, 1981; Hashin, 1983; Nemat-Nasser, 1986). The boundary conditions are based on the Bloch representation of wave propagation in the heterogeneous media. Instead of explicitly solving the Maxwell equations, these equations are directly used in the averaging scheme. This distinguishes our method from others, where usually a known point-wise solution is used to obtain the average field quantities. The resulting constitutive relations therefore may be used to directly estimate the response of any heterogeneous periodic assembly of material constituents of given geometry and properties. ***To cite this article: A.V. Amirkhizi, S. Nemat-Nasser, C. R. Mecanique 336 (2008).***

Résumé

Homogénéisation des propriétés électromagnétiques des milieux périodiques fondée sur une base microstructurelle. On développe une méthode générale d'homogénéisation des propriétés électromagnétiques des milieux périodiques hétérogènes fondée sur une base microstructurelle. Cette méthode est inspirée de la micromécanique (Nemat-Nasser and Hori, 1999). Contrairement à d'autres techniques conventionnelles, couramment utilisées en électromagnétisme pour calculer les propriétés globales des composites, cette méthode à base microstructurelle ne nécessite pas de solution numérique explicite des équations de Maxwell. Nous définissons les champs macroscopiques comme des moyennes volumiques des champs spatialement variables sur un volume représentatif élémentaire (VRE), qui consiste en une cellule de base du milieu périodique (Hill, 1963 ; Willis, 1981 ; Hashin, 1983 ; Nemat-Nasser, 1986). Les conditions aux limites reposent sur la représentation de Bloch de la propagation d'ondes dans le milieu hétérogène. Au lieu de résoudre explicitement les équations de Maxwell, ces équations sont directement utilisées dans l'opération de moyenne. Ceci distingue notre méthode d'autres qui utilisent généralement une solution connue point par point pour obtenir les champs moyens. Les équations constitutives résultantes peuvent par conséquent être utilisées pour estimer directement la réponse d'un assemblage périodique hétérogène de constituants matériels de géométrie et de propriétés données. ***Pour citer cet article : A.V. Amirkhizi, S. Nemat-Nasser, C. R. Mecanique 336 (2008).***

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1. Introduction and motivation

Modeling the mechanical behavior of heterogeneous solids is, by its nature, a complicated problem. It is usually difficult to solve analytically the field equations for static or dynamic problems of heterogeneous media. In certain cases, one can reduce the problem to a homogeneous one without losing important physical effects in the solution. This is possible when the length scale associated with the heterogeneity of the medium is small enough compared with the other length scales of the problem, including the dimensions of the body, the minimum length of the spatial variation of the loading, and other problem-specific lengths. For example, for the case of periodic solids and structures, the size of the periodic unit cell is the heterogeneity length scale; see Fig. 1. If this is small enough compared to the macroscopic size of the body or structure, i.e., if the length scales can be separated, then the heterogeneous material can be replaced with a macroscopically equivalent homogeneous one. Such equivalent materials are introduced for elasto-plastic problems in a rational way, using micromechanics methods; for comprehensive discussions of these methods, see Mura [1] and Nemat-Nasser and Hori [2]. Extension of such techniques to other physical phenomena such as piezoelectricity is already a broad field of research (Dunn and Taya [3]; Benveniste [4]; Dvorak and Benveniste [5]; Chen [6]). We seek to use this same rational principle in electromagnetism. Most notably, Willis [7] has formulated the variational principles and integral equations for electromagnetic waves in heterogeneous media.

There are several established methods of calculating the overall material properties in electromagnetism; see for example Bensoussan et al. [12], Sihvola [13], and Milton [14]. Robinson [15] has demonstrated the difficulties involved in the derivation of the macroscopic Maxwell equations from those involving microscopic fundamental fields, **E** and **B**, the electric field and the magnetic induction, respectively. The averaging method required in the definition of the fields **D** and **H**, the electric displacement and the magnetic field, respectively, based on the atomistic considerations, is critically examined by Robinson. We suggest that similar care is necessary in examining the electromagnetic homogenization schemes.

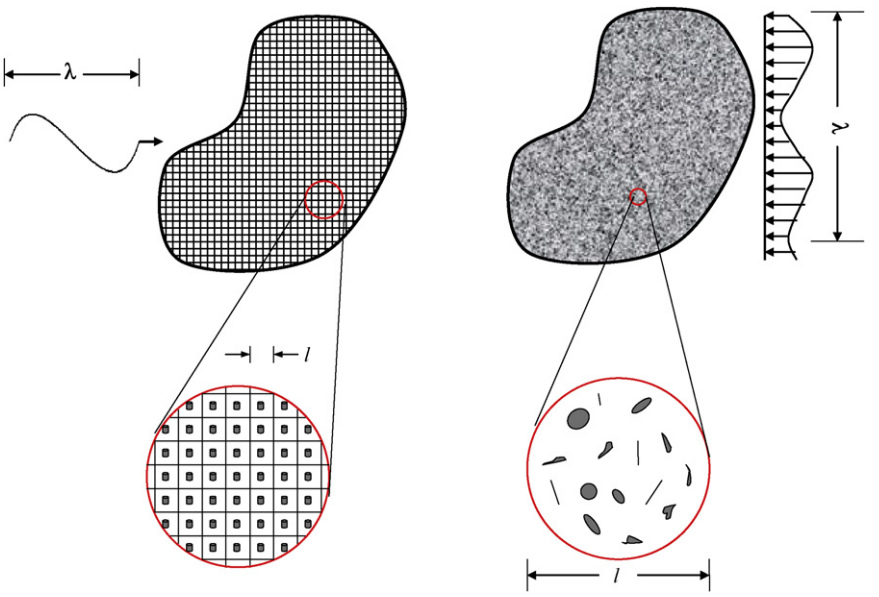

Fig. 1. Homogenization. The largest heterogeneity length scale, l, should be small enough compared to the smallest length scale, λ, that is of physical importance. For a periodic medium (left) l is the unit cell size while in a random medium (right) it should be the smallest size of a sphere which at any position is a statistical representative of the entire body, i.e., a representative volume element (RVE) (for further details, see [8–11]. λ depends on all attributes of a problem. For wave propagation problems (left), it is the smallest wavelength of interest. For a general loading (right), it may be defined as the smallest wavelength in the spatial Fourier expansion of the imposed excitation.

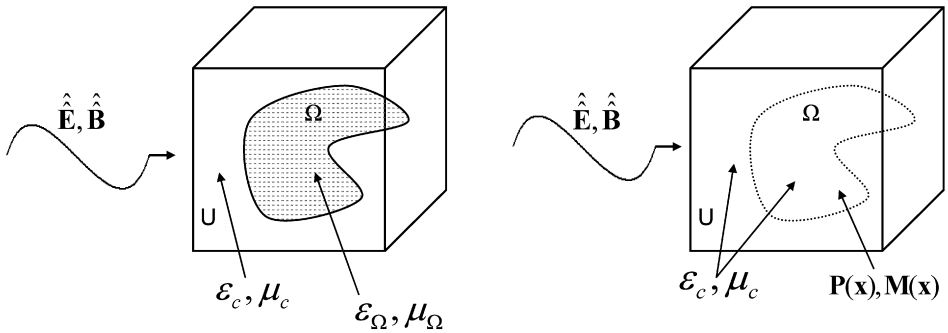

Fig. 2. A two-phase heterogeneous unit cell (left) and its equivalent homogeneous unit cell with the imposed polarization fields **P** and **M** (right).

Pendry [16,17] has developed a method for the calculation of equivalent homogeneous material properties using line and surface integrals of the field quantities. The application of this method to chiral media is given elsewhere (Amirkhizi and Nemat-Nasser, [18]). Smith and Pendry [19] have also used this approach to estimate the bi-anisotropy parameters of the split-ring resonator (SRR) medium. To apply this method to specific problems, one needs to obtain point-wise solutions of the Maxwell equations and evaluate the appropriate averaging integrals. This has the disadvantage that for any desired direction of wave propagation, a new numerical solution must be obtained. Here we develop a method based on the direct volume average of the electromagnetic fields, and where applicable, we give the full 3-dimensional tensorial expressions of the overall material properties for any direction of wave propagation and given frequency, provided that the wavelength is within the effective medium limit.

2. Description of the method for simple media

The microstructurally-based method relies on the assumption that only volume averages of the field variables are measurable as macroscopic physical quantities. The solution to the Maxwell equations is then expressed as the sum of the volume average and a local perturbation:

$$\mathbf{F} = \mathbf{F}^0 + \mathbf{F}^p \tag{1}$$

Here **F** is any of the electromagnetic fields **E**, **B**, **D**, or **H**. We seek to derive a set of equations that includes only the macroscopic quantities, using the Maxwell equations that contain both the average and the perturbation fields. The coefficients of this new set of equations are the overall material properties. These material properties are uniform in space. Here we present an outline of this method. However, its application to an arbitrary geometry requires lengthy numerical calculations.

First we replace the heterogeneous unit cell with a homogenized cell. Then in the replacement medium we include externally-imposed polarization fields such that point-wise the fields **F** coincide with the ones in the heterogeneous cell; see Fig. 2.

Next we expand the fields in a spatial Fourier series. Here we consider the problem of propagation of a single frequency wave in a periodic medium. We start with the Bloch form of the fields:

$$\hat{\hat{\mathbf{F}}}(\mathbf{x}, t) = \mathrm{Re}\{\hat{\mathbf{F}}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\omega t}\} = \mathrm{Re}\{\mathbf{F}(\mathbf{x})\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}-\omega t)}\} \tag{2}$$

Here $\hat{\hat{\mathbf{F}}}(\mathbf{x}, t)$ represents any of the electromagnetic fields as functions of time and space. The Bloch representation (2) separates the harmonic time dependence $\mathrm{e}^{-\mathrm{i}\omega t}$ and the macroscopic plane wave factor $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}-\omega t)}$ from the microscopic fields in the unit cell. It is the phasor form of a monochromatic wave traveling in the **k** direction. For a fixed frequency, the Maxwell equations in the absence of external charge and current densities can be written as:

$$\nabla \cdot \hat{\mathbf{D}} = \mathbf{0} \tag{3}$$

$$\nabla \cdot \hat{\mathbf{B}} = \mathbf{0} \tag{4}$$

$$\nabla \times \hat{\mathbf{E}} - \mathrm{i}\omega\hat{\mathbf{B}} = \mathbf{0} \tag{5}$$

$$\nabla \times \hat{\mathbf{H}} + \mathrm{i}\omega\hat{\mathbf{D}} = \mathbf{0} \tag{6}$$

Now, as explained before, we replace the heterogeneous unit cell with a homogeneous one having uniform $\boldsymbol{\varepsilon}_C(\omega)$ and $\boldsymbol{\mu}_C(\omega)$ material properties. *We will drop the frequency dependence from now on with the understanding that the problem is being solved for a given single frequency.* In order to reproduce the actual electromagnetic fields in the homogenized unit cell, the polarization fields $\mathbf{P}(\mathbf{x})$ and $\mathbf{M}(\mathbf{x})$ are introduced everywhere the material properties differ from the selected uniform values (Nemat-Nasser and Amirkhizi [26]):

$$\mathbf{D}(\mathbf{x}) = \varepsilon_C \mathbf{E}(\mathbf{x}) + \mathbf{P}(\mathbf{x}) \tag{7}$$

$$\mathbf{H}(\mathbf{x}) = \mu_C^{-1} \mathbf{B}(\mathbf{x}) - \mathbf{M}(\mathbf{x}) \tag{8}$$

For simplicity, and without loss of generality, we have assumed that the uniform (reference) material properties $\boldsymbol{\varepsilon}_C(\omega) = \varepsilon_C(\omega)\mathbf{1}$ and $\boldsymbol{\mu}_C(\omega) = \mu_C(\omega)\mathbf{1}$ are isotropic tensors; this assumption is not necessary and one may improve the resulting estimates by choosing the reference uniform properties such that they reflect the expected final values. Where the material properties are equal to the selected uniform values, the polarization fields vanish. The wave equations for the fields $\mathbf{E}$ and $\mathbf{B}$ can now be re-written as follows:

$$\nabla \to \nabla + \mathrm{i}\mathbf{k} \tag{9}$$

$$(\nabla + \mathrm{i}\mathbf{k}) \times \big((\nabla + \mathrm{i}\mathbf{k}) \times \mathbf{E}\big) - \omega^2 \mu_C \varepsilon_C \mathbf{E} = \omega^2 \mu_C \mathbf{P} + \mathrm{i}\omega \mu_C (\nabla + \mathrm{i}\mathbf{k}) \times \mathbf{M} \tag{10}$$

$$(\nabla + \mathrm{i}\mathbf{k}) \times \big((\nabla + \mathrm{i}\mathbf{k}) \times \mathbf{B}\big) - \omega^2 \mu_C \varepsilon_C \mathbf{B} = -\mathrm{i}\omega \mu_C (\nabla + \mathrm{i}\mathbf{k}) \times \mathbf{P} + \mu_C (\nabla + \mathrm{i}\mathbf{k}) \times \big((\nabla + \mathrm{i}\mathbf{k}) \times \mathbf{M}\big) \tag{11}$$

Note that the fields in these equations would be uniform in space if it were not for the presence of the imposed polarization fields. Based on the Bloch decomposition (2), the fields in these equations are periodic and can be expanded as spatial Fourier series over the unit cell:

$$\mathbf{F}(\mathbf{x}) = \mathbf{F}^0 + \mathbf{F}^p = \langle \mathbf{F} \rangle_U + \sum_{\boldsymbol{\xi} \neq \mathbf{0}} \mathbf{F}(\boldsymbol{\xi}) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{x}} \tag{12}$$

$$\langle \mathbf{F} \rangle_U = \frac{1}{U} \int_U \mathbf{F}(\mathbf{x}) \, \mathrm{d}V_x \tag{13}$$

$$\mathbf{F}(\boldsymbol{\xi}) = \frac{1}{U} \int_U \mathbf{F}(\mathbf{x}) \mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{x}} \, \mathrm{d}V_x \tag{14}$$

$$U = 8 a_1 a_2 a_3 \tag{15}$$

$$\boldsymbol{\xi} = \frac{n_1 \pi}{a_1} \mathbf{e_1} + \frac{n_2 \pi}{a_2} \mathbf{e}_2 + \frac{n_3 \pi}{a_3} \mathbf{e}_3; \quad n_i \text{ integers} \tag{16}$$

The quantities $\mathbf{F}^0 = \langle \mathbf{F} \rangle_U$ denote the average fields taken over the unit cell and appear in the macroscopic description of the medium. The remainder, $\mathbf{F}^p = \sum_{\boldsymbol{\xi} \neq \mathbf{0}} \mathbf{F}(\boldsymbol{\xi}) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{x}}$, represents the local perturbation from the average values. In these equations, U is the volume and a_i are half the length of the edges of the unit cell. Solving the wave equations (10), (11) we have:

$$\mathbf{E}(\boldsymbol{\xi}) = \frac{1}{\boldsymbol{\zeta}\cdot\boldsymbol{\zeta} - k_0^2} \left(\omega^2 \mu_C \left(\mathbf{1} - \frac{1}{k_0^2} \boldsymbol{\zeta} \otimes \boldsymbol{\zeta} \right) \cdot \mathbf{P}(\boldsymbol{\xi}) - \omega \mu_C \boldsymbol{\zeta} \times \mathbf{M}(\boldsymbol{\xi}) \right) \tag{17}$$

$$\mathbf{B}(\boldsymbol{\xi}) = \frac{1}{\boldsymbol{\zeta}\cdot\boldsymbol{\zeta} - k_0^2} \left(\omega \mu_C \boldsymbol{\zeta} \times \mathbf{P}(\boldsymbol{\xi}) + \mu_C \boldsymbol{\zeta} \cdot \boldsymbol{\zeta} \left(\mathbf{1} - \frac{1}{\boldsymbol{\zeta}\cdot\boldsymbol{\zeta}} \boldsymbol{\zeta} \otimes \boldsymbol{\zeta} \right) \cdot \mathbf{M}(\boldsymbol{\xi}) \right) \tag{18}$$

$$\boldsymbol{\zeta} = \boldsymbol{\xi} + \mathbf{k} \tag{19}$$

$$k_0^2 = \omega^2 \mu_C \varepsilon_C \tag{20}$$

Therefore the perturbation fields can be written as sums of certain integrals of the polarization fields over the unit cell. The coefficient matrices $\boldsymbol{K}$, $\boldsymbol{L}$, $\boldsymbol{M}$, and $\boldsymbol{L}$ are calculated in Eqs. (17), (18):

$$\mathbf{E}^p(\mathbf{x}) = \sum_{\boldsymbol{\xi} \neq \mathbf{0}} \left(\boldsymbol{K}(\boldsymbol{\xi}) \cdot \frac{1}{U} \int_U \mathbf{P}(\mathbf{y}) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{y})} \, \mathrm{d}V_y + \boldsymbol{L}(\boldsymbol{\xi}) \cdot \frac{1}{U} \int_U \mathbf{M}(\mathbf{y}) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{y})} \, \mathrm{d}V_y \right) \tag{21}$$

$$\mathbf{B}^p(\mathbf{x}) = \sum_{\boldsymbol{\xi} \neq \mathbf{0}} \left(\boldsymbol{M}(\boldsymbol{\xi}) \cdot \frac{1}{U} \int_U \mathbf{P}(\mathbf{y}) \, \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{y})} \, \mathrm{d}V_y + \boldsymbol{N}(\boldsymbol{\xi}) \cdot \frac{1}{U} \int_U \mathbf{M}(\mathbf{y}) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{y})} \, \mathrm{d}V_y \right) \tag{22}$$

To make the homogeneous unit cell equivalent with the original heterogeneous unit cell, the polarization fields must satisfy the following *consistency conditions*:

$$\boldsymbol{\varepsilon}(\mathbf{x})\cdot(\mathbf{E}^0+\mathbf{E}^p)=\varepsilon_C(\mathbf{E}^0+\mathbf{E}^p)+\mathbf{P}(\mathbf{x}) \tag{23}$$

$$\boldsymbol{\mu}^{-1}(\mathbf{x})\cdot(\mathbf{B}^0+\mathbf{B}^p)=\mu_C^{-1}(\mathbf{B}^0+\mathbf{B}^p)-\mathbf{M}(\mathbf{x}) \tag{24}$$

Now by substituting the perturbation fields with their expression based on the polarization fields from Eqs. (21), (22), we reach two coupled integral equations in series form. To obtain a general point-wise representation of the original heterogeneous medium, these equations must be solved for the polarizations in terms of the average fields. This gives the polarization fields that can fully replace the heterogeneity of the medium in any physical problem. However, our primary objective is to find the average fields and the point-wise solution is not necessary for this purpose.

Let us assume that the unit cell can be divided into a series of sub-regions, Ω_α, each with some uniform material properties. One can average the perturbation fields over any such region and arrive at,

$$\langle\mathbf{E}^p\rangle_{\Omega_\alpha}=\frac{1}{\Omega_\alpha}\int\limits_{\Omega_\alpha}\mathbf{E}^p(\mathbf{x})\,\mathrm{d}V_x=\sum_{\boldsymbol{\xi}\neq\mathbf{0}}g_\alpha(\boldsymbol{\xi})\left(\boldsymbol{K}(\boldsymbol{\xi})\cdot\frac{1}{U}\int\limits_U\mathbf{P}(\mathbf{y})\mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{y}}\,\mathrm{d}V_y+\boldsymbol{L}(\boldsymbol{\xi})\cdot\frac{1}{U}\int\limits_U\mathbf{M}(\mathbf{y})\mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{y}}\,\mathrm{d}V_y\right) \tag{25}$$

$$\langle\mathbf{B}^p\rangle_{\Omega_\alpha}=\sum_{\boldsymbol{\xi}\neq\mathbf{0}}g_\alpha(\boldsymbol{\xi})\left(\boldsymbol{M}(\boldsymbol{\xi})\cdot\frac{1}{U}\int\limits_U\mathbf{P}(\mathbf{y})\mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{y}}\,\mathrm{d}V_y+\boldsymbol{N}(\boldsymbol{\xi})\cdot\frac{1}{U}\int\limits_U\mathbf{M}(\mathbf{y})\mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{y}}\,\mathrm{d}V_y\right) \tag{26}$$

$$g_\alpha(\boldsymbol{\xi})=\frac{1}{\Omega_\alpha}\int\limits_{\Omega_\alpha}\mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{x}}\,\mathrm{d}V_x \tag{27}$$

Note that the function g defined in the integral form (27) is only a geometrical quantity.

Our discussion up to this point involved exact equations. Here we introduce an approximation. We assume that the integrals in (25), (26) can be estimated by the following sum:

$$\frac{1}{U}\int\limits_U\mathbf{F}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\mathbf{y}}\,\mathrm{d}V_y\approx\sum_\beta f_\beta g_\beta(-\boldsymbol{\xi})\mathbf{F}_\beta \tag{28}$$

$$f_\beta=\frac{\Omega_\beta}{U} \tag{29}$$

$$\mathbf{F}_\beta=\langle\mathbf{F}\rangle_{\Omega_\beta} \tag{30}$$

Here $\mathbf{F}$ represents either of the polarization fields $\mathbf{P}$ or $\mathbf{M}$. Therefore, Eqs. (25), (26) can be approximated by the linear equations,

$$\mathbf{E}_\alpha^p=\sum_\beta(\mathbf{R}_{\alpha\beta}\cdot\mathbf{P}_\beta+\mathbf{S}_{\alpha\beta}\cdot\mathbf{M}_\beta) \tag{31}$$

$$\mathbf{B}_\alpha^p=\sum_\beta(\mathbf{T}_{\alpha\beta}\cdot\mathbf{P}_\beta+\mathbf{U}_{\alpha\beta}\cdot\mathbf{M}_\beta) \tag{32}$$

Now we average the consistency conditions (23), (24) over each sub-region. The result is a set of linear equations for the average polarization fields in each sub-region in terms of the average fields $\mathbf{F}^0$,

$$\sum_\beta\big(\big((\boldsymbol{\varepsilon}_\alpha-\varepsilon_C\mathbf{1})\cdot\mathbf{R}_{\alpha\beta}-\delta_{\alpha\beta}\mathbf{1}\big)\cdot\mathbf{P}_\beta+(\boldsymbol{\varepsilon}_\alpha-\varepsilon_C\mathbf{1})\cdot\mathbf{S}_{\alpha\beta}\cdot\mathbf{M}_\beta\big)=-(\boldsymbol{\varepsilon}_\alpha-\varepsilon_C\mathbf{1})\cdot\mathbf{E}^0 \tag{33}$$

$$\sum_\beta\big(\big(\boldsymbol{\mu}_\alpha^{-1}-\mu_C^{-1}\mathbf{1}\big)\cdot\mathbf{T}_{\alpha\beta}\cdot\mathbf{P}_\beta+\big((\boldsymbol{\mu}_\alpha^{-1}-\mu_C^{-1}\mathbf{1})\cdot\mathbf{U}_{\alpha\beta}-\delta_{\alpha\beta}\mathbf{1}\big)\cdot\mathbf{M}_\beta\big)=-(\boldsymbol{\mu}_\alpha^{-1}-\mu_C^{-1}\mathbf{1})\cdot\mathbf{B}^0 \tag{34}$$

Here the coefficient tensors are given by:

$$\mathbf{R}_{\alpha\beta} = \sum_{\boldsymbol{\xi}\neq\mathbf{0}} g_\alpha(\boldsymbol{\xi}) f_\beta g_\beta(-\boldsymbol{\xi}) \boldsymbol{K}(\boldsymbol{\xi}) \tag{35}$$

$$\mathbf{S}_{\alpha\beta} = \sum_{\boldsymbol{\xi}\neq\mathbf{0}} g_\alpha(\boldsymbol{\xi}) f_\beta g_\beta(-\boldsymbol{\xi}) \boldsymbol{L}(\boldsymbol{\xi}) \tag{36}$$

$$\mathbf{T}_{\alpha\beta} = \sum_{\boldsymbol{\xi}\neq\mathbf{0}} g_\alpha(\boldsymbol{\xi}) f_\beta g_\beta(-\boldsymbol{\xi}) \boldsymbol{M}(\boldsymbol{\xi}) \tag{37}$$

$$\mathbf{U}_{\alpha\beta} = \sum_{\boldsymbol{\xi}\neq\mathbf{0}} g_\alpha(\boldsymbol{\xi}) f_\beta g_\beta(-\boldsymbol{\xi}) \boldsymbol{N}(\boldsymbol{\xi}) \tag{38}$$

Each of the above equations is repeated for all α regions. They can be solved collectively to give $\mathbf{P}_\beta$ and $\mathbf{M}_\beta$. It must be noted here that this approximation can be made as accurate as desired by dividing the unit cell into a sufficient number of subregions. Of course, as the number of subregions increases, the approximate solution approaches to the exact solution of the problem. From the solutions of (33), (34) for $\mathbf{P}_\beta$ and $\mathbf{M}_\beta$ one calculates the average polarization fields over the unit cell:

$$\mathbf{P}^0 = \sum_\alpha f_\alpha \mathbf{P}_\alpha = \boldsymbol{\chi}^{\mathrm{PE}} \cdot \mathbf{E}^0 + \boldsymbol{\chi}^{\mathrm{PB}} \cdot \mathbf{B}^0 \tag{39}$$

$$\mathbf{M}^0 = \sum_\alpha f_\alpha \mathbf{M}_\alpha = \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 + \boldsymbol{\chi}^{\mathrm{MB}} \cdot \mathbf{B}^0 \tag{40}$$

The coefficient tensors in these equations are calculated by solving (33), (34). Now we are able to write down the equivalent material properties as follows:

$$\mathbf{D}^0 = \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{E}^0 = \varepsilon_C \mathbf{E}^0 + \mathbf{P}^0 = \varepsilon_C \mathbf{E}^0 + \boldsymbol{\chi}^{\mathrm{PE}} \cdot \mathbf{E}^0 + \boldsymbol{\chi}^{\mathrm{PB}} \cdot \mathbf{B}^0 \tag{41}$$

$$\mathbf{H}^0 = \bar{\boldsymbol{\mu}}^{-1} \cdot \mathbf{B}^0 = \mu_C^{-1} \mathbf{B}^0 - \mathbf{M}^0 = \mu_C^{-1} \mathbf{B}^0 - \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 - \boldsymbol{\chi}^{\mathrm{MB}} \cdot \mathbf{B}^0 \tag{42}$$

Using the relations

$$\mathbf{B}^0 = \frac{\mathbf{k}}{\omega} \times \mathbf{E}^{\mathbf{0}} \tag{43}$$

$$\mathbf{D}^0 = -\frac{\mathbf{k}}{\omega} \times \mathbf{H}^0 \tag{44}$$

the overall material properties, for simple (non-chiral) media, can be written as,

$$\bar{\boldsymbol{\varepsilon}} = \varepsilon_C \mathbf{1} + \boldsymbol{\chi}^{\mathrm{PE}} - \frac{1}{\omega} \boldsymbol{\chi}^{\mathrm{PB}} \cdot (\mathbf{e} \cdot \mathbf{k}) \tag{45}$$

$$\bar{\boldsymbol{\mu}}^{-1} = \left(\mathbf{1} + \frac{1}{\omega} \boldsymbol{\chi}^{\mathrm{ME}} \cdot \bar{\boldsymbol{\varepsilon}}^{-1} \cdot (\mathbf{e} \cdot \mathbf{k}) \right)^{-1} \cdot (\mu_C^{-1} \mathbf{1} - \boldsymbol{\chi}^{\mathrm{MB}}) \tag{46}$$

Here $\mathbf{e}$ is the permutation symbol used to replace the cross product of $\mathbf{k}$ with a matrix representation. It must be emphasized that all of the above calculations are for a single macroscopic sinusoidal wave with frequency ω and wave vector $\mathbf{k}$. We did not impose any condition relating these two quantities. This condition which is the macroscopic dispersion relation can now be found by substituting the two overall material properties (45), (46) into the macroscopic wave equation,

$$\mathbf{k} \times \bar{\boldsymbol{\mu}}^{-1} \cdot \left(\frac{1}{\omega} \mathbf{k} \times \mathbf{E}^0 \right) + \omega \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{E}^0 = \mathbf{0} \tag{47}$$

In order for this equation to have non-trivial solutions, the determinant of the coefficient matrix must vanish,

$$\mathrm{Det} \left| \omega^2 \bar{\boldsymbol{\varepsilon}} + (\mathbf{e} \cdot \mathbf{k}) \cdot \left(\bar{\boldsymbol{\mu}}^{-1} \cdot (\mathbf{e} \cdot \mathbf{k}) \right) \right| = 0 \tag{48}$$

Eq. (48) involves 4 parameters: the frequency and the components of the wave vector. Given any 3, one can solve for the other. For example one can find the frequency for any given wave vector, or one can calculate the wave number for a given frequency and direction. After the dispersion relation is established, the overall material properties for any direction of propagation are found from (45), (46). This completes the description of the method.

3. Examples

For all non-magnetic materials, Eqs. (45), (46) simplify to,

$$\bar{\boldsymbol{\mu}} = \mu_0 \mathbf{1} \tag{49}$$

$$\bar{\boldsymbol{\varepsilon}} = \varepsilon_C \mathbf{1} + \boldsymbol{\chi}^{\mathrm{PE}} \tag{50}$$

For general geometries the infinite sums (35)–(38) have to be truncated to a finite number of terms. The series are symbolically evaluated using Mathematica (Wolfram, [20]). To illustrate the method, we have solved 2 simple cases of two-phase media and have compared our results with *static estimates* (2 bounds, an approximate random model, and the Maxwell Garnett rule for the case of spheres) as well as with the simulation results using the code Ansoft-HFSS (Ansoft, [21]). The static lower and upper bounds, respectively, are (Nemat-Nasser and Hori, [2]):

$$\bar{\varepsilon} = \frac{1}{\frac{f}{\varepsilon_\Omega} + \frac{1-f}{\varepsilon_C}} \tag{51}$$

$$\bar{\varepsilon} = f\varepsilon_\Omega + (1-f)\varepsilon_C \tag{52}$$

The static random model estimate is (Nemat-Nasser et al., [22]):

$$\bar{\varepsilon} = \frac{(\varepsilon_C + \varepsilon_\Omega) - f(\varepsilon_C - \varepsilon_\Omega)}{(\varepsilon_C + \varepsilon_\Omega) + f(\varepsilon_C - \varepsilon_\Omega)} \tag{53}$$

The selected geometries are shown in Fig. 3. For both cases the dielectric constant of the matrix was chosen to be 1 and that of the inclusion was 101 to amplify the effects. The volume fraction for the infinite cylinders and the spheres were $9\pi/64$ and $9\pi/128$, respectively. The ratio of the effective wavelength (macroscopic, through the homogenized material) to the length of the unit cell is 5π for the values reported here. The results from Mathematica calculation are frequency-dependent, as expected. This is most notable for the cylindrical geometry.

For the infinite cylinders the static upper bound, lower bound, and random model give dielectric constants of 45.18, 1.78, and 2.53, respectively. The simulation (dynamic) predicts 48.11 and 2.55 for the electric field polarized parallel and normal to the axis of cylinders, respectively. Our method gives 48.105 and 2.555, respectively. Note the close agreement between the simulation and the present method. Also note that the value of the dielectric constant when the electric field is polarized parallel to the axis of cylinders exceeds the static upper bound. This is due to the fact that the upper bound is only applicable to infinite wavelength (static). In fact, when the limit of the wavelength is taken to infinity (or equivalently, when the frequency is taken to zero) the value of the dielectric constant calculated from our method converges to the static upper bound. Therefore our method estimates the dielectric constant successfully for both the limiting value ($f = 0$, compared to the static upper bound) and a typical non-zero frequency dependent case (compared to the simulation results). The method predicts correct overall dispersive results from non-dispersive

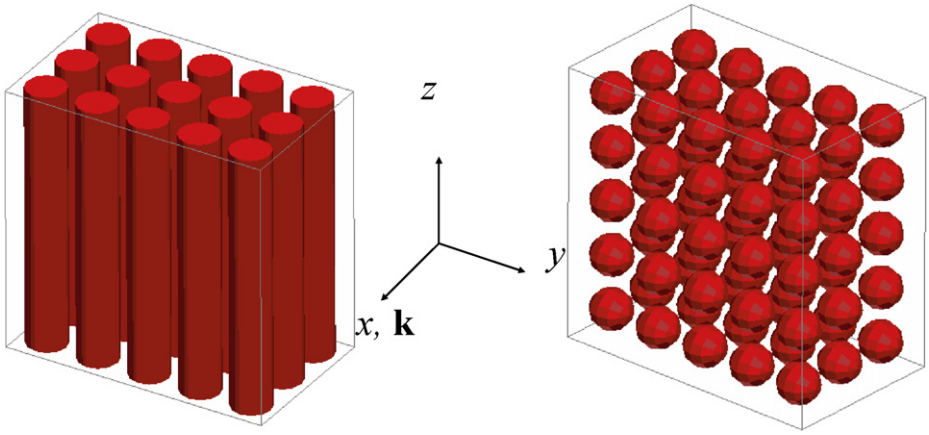

Fig. 3. Examples for the microstructurally-based homogenization method: left: 2D square array of infinite cylinders; right: 3D cubic array of spheres.

local material properties as expected from analytical solutions and simulations. The numerical results, however, are reported here for a single frequency component corresponding to $\lambda/2a = 5\pi$.

For the case of spheres, the static upper bound, lower bound, and random model give dielectric constant values of 23.09, 1.28, and 1.55, respectively. The simulation predicts 1.78 and our method calculates 1.834. The Maxwell Garnett rule for spherical inclusions and isotropic material (Maxwell Garnett, [23])

$$\bar{\varepsilon} = \varepsilon_C \left(1 + 3f \frac{\varepsilon_\Omega - \varepsilon_C}{\varepsilon_\Omega + 2\varepsilon_C - f(\varepsilon_\Omega - \varepsilon_C)} \right) \tag{54}$$

gives 1.821. The close agreement between the simulation and our method compared with the other models is satisfactory.

4. Magnetic moment due to electric current distribution

The present method gives good results for dielectric materials. However, application to conductors and/or magnetic materials requires further consideration. The application to the cases where magnetic permeability is heterogeneous does not seem to pose any significant problem and it is, in fact, included in this work. The main issue is incorporating the magnetic effect of the oscillating electric field in the conductors into the formulation. The issue here is that introducing complex properties for the conductors can modify the overall magnetic properties, but the proposed microstructurally-based formalism does not introduce any such effect. Eq. (49), (50) in their current form do not show any magnetic perturbations due to non-magnetic conductors. Furthermore, in a lossy or conductive heterogeneous medium, the dispersion equation (48) will involve complex-valued solutions for the wave vector $\mathbf{k}$. These complications and others introduce certain challenges that have to be addressed.

The overall magnetic response is modified when there are circular or solenoidal electrical currents. However, in the present formulation such current densities are canceled out upon averaging. It is necessary to include such current distribution directly in the formulation. We are currently working on this problem and the generalized formulation along with results will be presented elsewhere.

Here, however, we consider the following heuristic approach. The magnetic polarization of a current distribution is usually defined by (Jackson, [24]):

$$\mathbf{M} = \frac{1}{2} \int_U \mathbf{x} \times \mathbf{J}(\mathbf{x}) \, \mathrm{d}V_x. \tag{55}$$

We start by assuming that there are no magnetic materials in the unit cell, i.e., $\mu(\mathbf{x}) = \mu_0 \mathbf{1}$. Then, Eqs. (17), (18) reduce to,

$$\mathbf{E}(\boldsymbol{\xi}) = \frac{\omega^2 \mu_0}{\boldsymbol{\zeta} \cdot \boldsymbol{\zeta} - k_0^2} \left(\mathbf{1} - \frac{1}{k_0^2} \boldsymbol{\zeta} \otimes \boldsymbol{\zeta} \right) \cdot \mathbf{P}(\boldsymbol{\xi}) \tag{56}$$

$$\mathbf{B}(\boldsymbol{\xi}) = \frac{\boldsymbol{\zeta}}{\omega} \times \mathbf{E}(\boldsymbol{\xi}) \tag{57}$$

All the resulting equations are also simplified, yielding

$$\mathbf{R}_{\alpha\beta} = \sum_{\boldsymbol{\xi} \neq \mathbf{0}} g_\alpha(\boldsymbol{\xi}) f_\beta g_\beta(-\boldsymbol{\xi}) \boldsymbol{K}(\boldsymbol{\xi}) \tag{58}$$

$$\sum_\beta \big((\boldsymbol{\varepsilon}_\alpha - \varepsilon_C \mathbf{1}) \cdot \mathbf{R}_{\alpha\beta} - \delta_{\alpha\beta} \mathbf{1} \big) \cdot \mathbf{P}_\beta = -(\boldsymbol{\varepsilon}_\alpha - \varepsilon_C \mathbf{1}) \cdot \mathbf{E}^0 \tag{59}$$

$$\mathbf{P}^0 = \sum_\alpha f_\alpha \mathbf{P}_\alpha = \boldsymbol{\chi}^{\mathrm{PE}} \cdot \mathbf{E}^0 \tag{60}$$

Now we define the overall magnetic moment of the unit cell using ($f = \sum_\alpha f_\alpha$)

$$\mathbf{J}_\beta^{\mathrm{sol.}} = \frac{\partial (\mathbf{P}_\beta - \mathbf{P}_0 / f)}{\partial t} = -\mathrm{i}\omega (\mathbf{P}_\beta - \mathbf{P}_0 / f) \tag{61}$$

$$\mathbf{M}^0 = \frac{1}{2U} \int_U \mathbf{x} \times \mathbf{J}^{\mathrm{sol.}}(\mathbf{x}) \, \mathrm{d}V_x \approx \frac{-\mathrm{i}\omega}{2} \sum_\beta f_\beta \mathbf{x}_\beta \times (\mathbf{P}_\beta - \mathbf{P}_0 / f) \tag{62}$$

Here $\mathbf{x}_\beta$ is the position vector of the center of mass of region β, measured from the center of the unit cell. Using the solutions of the system of Eqs. (59), Eq. (62) is rewritten as,

$$\mathbf{M}^0 = \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 \tag{63}$$

Note that $\boldsymbol{\chi}^{\mathrm{PE}}$ and $\boldsymbol{\chi}^{\mathrm{ME}}$ are functions of both independent variables, $\mathbf{k}$ and ω. Their relation gives the dispersion equation that is found by considering the wave equation,

$$\mathbf{D}^0 = \varepsilon_C \mathbf{E}^0 + \boldsymbol{\chi}^{\mathrm{PE}} \cdot \mathbf{E}^0 = -\frac{\mathbf{k}}{\omega} \times \mathbf{H}^0 \tag{64}$$

$$\mathbf{H}^0 = \frac{1}{\mu_0}\mathbf{B}^0 - \mathbf{M}^0 = \frac{\mathbf{k}}{\mu_0 \omega} \times \mathbf{E}^0 - \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 \tag{65}$$

$$(\varepsilon_C \mathbf{1} + \boldsymbol{\chi}^{\mathrm{PE}}) \cdot \mathbf{E}^0 + \frac{\mathbf{k}}{\mu_0 \omega} \times \frac{\mathbf{k}}{\omega} \times \mathbf{E}^0 - \frac{\mathbf{k}}{\omega} \times \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 = \mathbf{0} \tag{66}$$

Eq. (66) can be written in matrix form in terms of $\mathbf{E}^0$

$$\mathbf{A}(\mathbf{k}, \omega) \cdot \mathbf{E}^0 = \mathbf{0} \tag{67}$$

In order for (67) to have nontrivial solutions, the determinant of the coefficient matrix must vanish. The resulting expression is solved for the complex-valued $\mathbf{k}$, given the frequency and the direction of $\mathbf{k}$. For each solution, the eigenvector solutions for $\mathbf{E}^0$ give the principal polarization. The other field quantities are then calculated from Eqs. (64), (65).

The overall material properties are

$$\mathbf{D}^0 = (\varepsilon_C \mathbf{1} + \boldsymbol{\chi}^{\mathrm{PE}}) \cdot \mathbf{E}^0 \tag{68}$$

$$\mathbf{H}^0 = \mu_0^{-1} \mathbf{B}^0 - \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0 \tag{69}$$

Or, equivalently,

$$\mathbf{B}^0 = \mu_0 (\mathbf{H}^0 + \boldsymbol{\chi}^{\mathrm{ME}} \cdot \mathbf{E}^0). \tag{70}$$

Since from this formulation all the field vector quantities can be directly expressed in terms of only one field quantity, say $\mathbf{E}^0$, the representation in Eqs. (68)–(70) is not unique. Ideally we would like to express this in a more familiar form, such as (Lindell et al., [25])

$$\mathbf{D} = \bar{\boldsymbol{\varepsilon}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{E} + \bar{\boldsymbol{\xi}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{H} \tag{71}$$

$$\mathbf{B} = \bar{\boldsymbol{\zeta}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{E} + \bar{\boldsymbol{\mu}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{H} \tag{72}$$

Here $\bar{\boldsymbol{\xi}}$ and $\bar{\boldsymbol{\zeta}}$ are dyadic tensor quantities distinct from the previously used vector quantities. Also $\hat{\mathbf{k}}$ is the unit vector in the propagation direction. The symmetry of the unit cell is now quite important. For example if it is known that the structure is not chiral or bi-anisotropic, then the overall material properties can be written as

$$\bar{\boldsymbol{\varepsilon}} = \varepsilon_C \mathbf{1} + \boldsymbol{\chi}^{\mathrm{PE}}(\omega, \hat{\mathbf{k}}) \tag{73}$$

$$\bar{\boldsymbol{\mu}} = \mu_0 \left(\mathbf{1} + \boldsymbol{\chi}^{\mathrm{ME}}(\omega, \hat{\mathbf{k}}) \cdot \bar{\varepsilon}^{-1} \cdot \frac{\mathbf{e} \cdot \mathbf{k}}{\omega} \right) \tag{74}$$

As before $\mathbf{e} \cdot \mathbf{k} = e_{lmn} k_m \mathbf{e}_l \otimes \mathbf{e}_n$ is used to replace the cross product.

If the unit cell does not possess the mirror-image symmetry, then the composite may demonstrate chiral behavior. However, since the permittivity and permeability tensors must remain invariant under spatial reflection (Lindell et al., [25]), one may homogenize the mirror image unit cell and calculate the corresponding polarization fields, $\mathbf{P}^{0r}$ and $\mathbf{M}^{0r}$, as well as the associated $\mathbf{D}^{0r}$ and $\mathbf{B}^{0r}$. The chirality tensors, and the permittivity and permeability tensors are now obtained from the difference and sum of these solutions, as follows:

$$\mathbf{D}^0 + \mathbf{D}^{0r} = 2\bar{\boldsymbol{\varepsilon}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{E}^0 \tag{75}$$

$$\mathbf{D}^0 - \mathbf{D}^{0r} = 2\bar{\boldsymbol{\xi}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{H}^0 \tag{76}$$

$$\mathbf{B}^0 + \mathbf{B}^{0r} = 2\bar{\boldsymbol{\mu}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{H}^0 \tag{77}$$

$$\mathbf{B}^0 - \mathbf{B}^{0r} = 2\bar{\boldsymbol{\zeta}}(\omega, \hat{\mathbf{k}}) \cdot \mathbf{E}^0 \tag{78}$$

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