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Numerical estimation of effective electromagnetic properties for design of particulate composites

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ABSTRACT

Most modern electromagnetic devices consist of dielectric and magnetic particulate composites. Predicting the effective electric permittivity and effective magnetic permeability of the envisioned composite is of great importance in validating the design for such applications. In this work, we propose a numerical method based on Yee's scheme and statistically generated representative volume element to estimate these effective electromagnetic properties for linear isotropic composites made with ellipsoidal particles. By considering particle geometry and composite microstructure precisely, it provides a more accurate tool for their design than available analytical bounds. Several numerical examples of composite microstructures are presented to demonstrate the capability of the proposed method. Comparison with analytical bounds and experimental results from literature is conducted to show validity.

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1. Introduction

Dielectric and magnetic particulate composites have become the primary choice for manufacturing electromagnetic devices [1,2] due to the potential they offer in tailoring a material with desired properties [3,4]. Dielectric insulators for capacitors [5,6] and magnetic cores for inductors [7] are two examples where interest in such composites has recently risen, driven by the requirement for higher performance to achieve further miniaturization. Particles with characteristic length ranging from *nm* to *μm* are generally sought for preparing a composite material in the *μm* to *mm* range.

Average properties obtained by homogenization, called effective properties [8], have been introduced for better characterization of the macroscopic response of such composites. For the electromagnetic (EM) applications mentioned previously, estimating the effective electric permittivity ϵ^* (in F/m) and the effective magnetic permeability μ^* (in H/m), is of prime importance to predict the behavior of the composite and assess the success of its design for a desired application. For a linear isotropic composite, these effective properties are defined as follows [9]

$$\langle \mathbf{D} \rangle_\Omega = \epsilon^* \langle \mathbf{E} \rangle_\Omega \tag{1}$$

$$\langle \mathbf{B} \rangle_\Omega = \mu^* \langle \mathbf{H} \rangle_\Omega \tag{2}$$

where Ω refers to the volume of the composite material, $\langle \mathbf{D} \rangle_\Omega$ represents the average electric flux density over Ω (in C/m^2), $\langle \mathbf{E} \rangle_\Omega$ is the average electric field intensity over Ω (in V/m), $\langle \mathbf{B} \rangle_\Omega$ gives the average magnetic flux density over Ω (in T), and $\langle \mathbf{H} \rangle_\Omega$ refers to the average magnetic field intensity over Ω (in A/m). The averaging operator $\langle \cdot \rangle_\Omega$ applies to each component of a vector field, and is defined for the i^{th} component of any vector $\mathbf{G}$ as $\langle G_i \rangle_\Omega = \frac{1}{|\Omega|}\int_\Omega G_i d\Omega$. Taking the dot product of the left and right hand sides in Eqs. (1) and (2) leads to the explicit formulation

$$\epsilon^* = \sqrt{\frac{\langle \mathbf{D} \rangle_\Omega \cdot \langle \mathbf{D} \rangle_\Omega}{\langle \mathbf{E} \rangle_\Omega \cdot \langle \mathbf{E} \rangle_\Omega}} \tag{3}$$

$$\mu^* = \sqrt{\frac{\langle \mathbf{B} \rangle_\Omega \cdot \langle \mathbf{B} \rangle_\Omega}{\langle \mathbf{H} \rangle_\Omega \cdot \langle \mathbf{H} \rangle_\Omega}} \tag{4}$$

Relative effective properties $\epsilon_r^* = \frac{\epsilon^*}{\epsilon_0}$ and $\mu_r^* = \frac{\mu^*}{\mu_0}$ are commonly used, where ϵ_0 and μ_0 are the permittivity and the permeability constants of free space, respectively. Direct evaluations of ϵ^* and μ^* using formulations 3 and 4 are not possible due to the complexities involved in evaluating the average EM fields over a composite. Several analytical formulas have been derived in the past, that provide upper and lower bounds to these effective properties values given the EM properties and volume fractions of the constituents in the composite. We can cite the widely used Wiener bounds [10] and Hashin–Shtrikman bounds [11] — the lower Hashin bound is popularly known as the Maxwell–Garnett approximation [12]. They are commonly used for first hand estimation during design, before

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conducting experimental validation. The accuracy of these bounds is however limited because they provide a range that increases significantly as the differences in the value of the properties between the constituents increase. Numerical methods were initially developed to estimate effective mechanical properties [13,14]. Extensions for effective EM properties were introduced in [9] for spherical particle-reinforced composites.

In the present study, we develop a numerical framework to estimate the effective EM properties ϵ^* and μ^* for any given linear isotropic particulate composite. Following [9,14], it consists of building a numerical sample of the composite material of interest, and applying EM field at its interface. Then, Maxwell's equations [15] are solved numerically over the sample to obtain its EM response and subsequently compute the effective EM properties. The novelty resides in the use of Yee's scheme [16], a Finite Difference Time Domain (FDTD) scheme specifically designed for Maxwell's equations. Moreover, this method is designed to handle composites with multiple phases consisting of a matrix material and multiple types of ellipsoidal particles. Illustration of such composite is presented in Fig. 1. Additionally, parallel implementation of the numerical solver is done for high computational performance, allowing material designer to conduct simulation on a single computer without requiring exceptional computational power. Precise consideration of the particles geometry in 3D allows for a more accurate estimation than the analytical bounds mentioned previously. Also, consideration of dynamic Maxwell's equations provides enough flexibility to further envision effect of external dynamic phenomena. For instance temperature rise could be significant in the applications of interest due to Joule's effect, and it has been shown to have considerable effect on the EM properties of certain thermo-sensible materials [17,18,19]. This could be taken into account by solving energy conservation equation simultaneously with Maxwell's equations, using for instance a staggered scheme for coupled physics as in [20]. Thus, this method is intended to set a basis for the multiphysics design of particulate composite intended for EM applications. A possibility that is not offered by the analytical bounds.

The organization of this paper is as follows. In Section 2, the proposed numerical method to compute the effective EM properties of particulate composites is presented. Application to model problems is realized in Section 3 to validate the method using analytical bounds and experimental results found in literature. Concluding remarks are finally drawn in Section 4. Throughout the study, we neglect thermal, stress, strain, and chemical effects. Constituents and resulting composites are assumed to be linear, isotropic, and non-dispersive. We consider the particles to be non-overlapping and having hard shell interface.

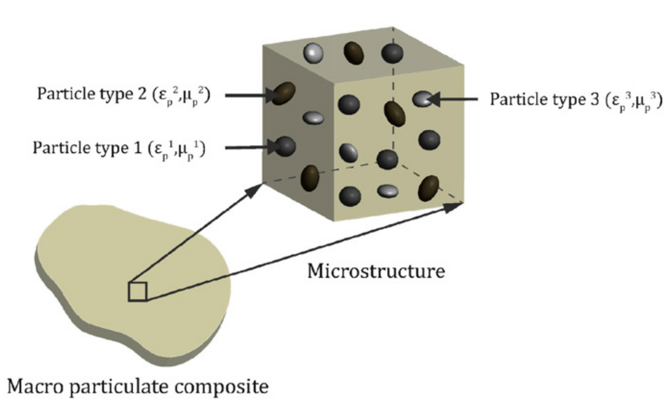

Fig. 1. Illustration of the homogenization process for a 4 phases composite made with $Q=3$ types of particles.

2. Numerical method

2.1. Representative volume element

Solving Maxwell's equations using any numerical technique would require meshing of the composite of interest. To capture the particles into the numerical scheme, and take the microstructure of the composite properly into account, a fine enough mesh would be required. Usually, a mesh size of a tenth of the characteristic length of a particle is prescribed — this is verified during application to model problems in the next section. Due to the scale difference between the overall composite size and the particle size in our problem, this would result in an enormous amount of unknowns to solve for. For instance, for a cubic composite of side $1mm$ filled with particles of diameter $1\mu m$, a mesh of $0.1\mu m$ would be adequate, resulting in 10^4 nodes in each direction and a total number of 10^{12} nodes. This would obviously be too heavy for efficient computations — a reasonable amount for computation over a single computer is 10^6 nodes in total. To overcome this problem, commonly encountered while computing effective properties numerically, the notion of a representative volume element (RVE) has been introduced [21,22]. We declare L as the characteristic length of the actual composite, l as the characteristic length of the RVE, and d as the characteristic length of the particles. A schematic of the different scales involved is shown in Fig. 2.

Basically a RVE is a cubic piece, “taken” from the actual composite material, that is small enough ($l \ll L$) so that efficient computation could be carried out and estimated properties could be considered as material point properties, but big enough to properly represent the microstructure ($l \gg d$). Additionally, the volume fraction of all constituents must be similar to the actual composite for adequate representation. Also, the particles must be randomly distributed and oriented in order to simulate randomness and isotropy of the actual composite. In this work, the simple RVE generation algorithm known as Random Sequential Adsorption (RSA) [23], is employed. Based on the specified RVE size l, the number of particle N_p^q required to satisfy the desired volume fraction v_p^q is computed for each type of particles q. Then, all particles are added to the RVE cube one by one by generating random position $(x_1^{q,r}, x_2^{q,r}, x_3^{q,r})$ for the center of gravity and random orientation $(\alpha_1^{q,r}, \alpha_2^{q,r}, \alpha_3^{q,r})$ for the principle axis of the r^{th} particle of q type. For each new particle, a check is performed to determine if overlapping occurs with any of the previously added particles using the method from [24], that basically consist of verifying if two ellipsoids share any common volume. If overlapping occurs, the position and orientation are rejected, and the process is repeated. The complete process is described in Algorithm 1, and the parameters used are illustrated in Fig. 3. We notice that this simple RVE generating algorithm limit the total volume fraction of particles to about 0.2 that is sufficient for most common composites. To incorporate studies of composites with higher particle volume fraction, advanced RVE generator algorithm could be used, as the ones described in [25]. In such algorithm, the particles are not placed randomly in the entire RVE volume but rather into restricted volume, or cell, in order to use

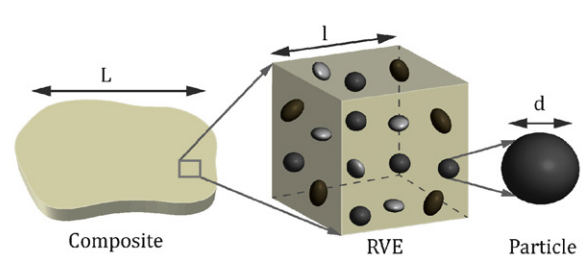

Fig. 2. Illustration of the different scales involved in RVE size estimation.

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