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# Approximation of the effective moduli of particulate composite with the fixed grid finite element method



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#### ABSTRACT

The fixed grid finite element method is introduced to approximate the effective moduli of particulate composite. The difficulty of domain discretization induced by the inclusions is avoided in the fixed grid finite element method, as the discretization is independent of the inclusions. The elastic properties of every finite element are approximated by a weighted function, and the volume fractions of the constituents in the element are taken as the weights. A simple scheme is proposed to approximate the volume fractions in every element. The validities of the fixed grid finite element method are verified, by comparing the effective moduli obtained from the fixed grid finite element method with those obtained from finite element method. The anisotropy of particulate composite is discussed with the fixed grid finite element, and the applicability of the fixed grid finite element method for composite with multiple irregular inclusions is illustrated.

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### 1. Introduction

Particulate composite like the polymer matrix composite, metal matrix composite, and ceramic composite has vast application. Particulate composite is reinforced with regular or irregular particle inclusions, which have different phases from the matrix. Two-phase composite can be categorized into three kinds in terms of the inclusion-to-matrix modulus ratio [\[1\]:](#page--1-0) (1) composites with high inclusion-to-matrix modulus ratio larger than 20; (2) composites with low inclusion-to-matrix modulus ratio ranging from 1 to 5; and (3) composite with inclusion-to-matrix modulus ratio smaller than 1.0. Particulate composite has the advantage of blending the properties of individual materials [\[2\].](#page--1-0) However, the determination of the effective moduli of particulate composite is a challenging issue as the coexistence of multiple phases in it. Great efforts have been made in the past few decades to predict the effective moduli of particulate composite with a variety of analytical and numerical methods.

Based on the pioneering work by Eshelby [\[3\]](#page--1-0) on the elastic stress field of a composite with a single inclusion when it is subjected to far-field stresses, some analytical solutions are proposed to calculate the effective moduli of particulate composite. The analytical methods single out themselves by considering the interaction between the inclusions with their unique ways, while the dilute solution is an exception as it ignores the interaction between the inclusions [\[4\].](#page--1-0) In the self-consistent method (SC) [\[5,6\],](#page--1-0) the interaction between the inclusions is considered by assuming that inclusions are inserted into the equivalent medium rather than the matrix. In the direct derivative method (IDD) [\[7\]](#page--1-0) and the Mori–Tanaka method (MT) [\[8,9\],](#page--1-0) the original far-field traction applied on the surface of the composite is replaced with a new one to consider the interaction between the inclusions. The differential method [\[10\]](#page--1-0) assumes that inclusion is gradually inserted into the medium with known equivalent elastic modulus. The generalized selfconsistent method (GSC) [\[11\]](#page--1-0) assumes that the inclusion and the matrix are bounded by the infinite equivalent medium to consider the interactions between the inclusions. There are some disadvantages for the analytical methods. Generally, these analytical methods require the explicit solution of eigen strain [\[3\]](#page--1-0) for inclusions, which can be achieved only for some regular inclusions. In addition, most of the analytical methods have limited ability to study the anisotropy of particulate composite.

The finite element method  $[12-23]$ , as well as the boundary element method [\[24-27\]](#page--1-0), is an important alternative tool to calculate the effective moduli of particulate composite. The challenging problem for finite element method is mesh generation, especially when the representative volume element (RVE) is 3D and the inclusions in it are irregular and multi-shaped. This is due to the requirement of fitted mesh, which means that the interface between the phases in the RVE should be perfectly represented by the boundaries of the elements. A variety of measures have been

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tried to deal with the problem. These measures include the application of digital image technique where each pixel and voxel represents a 2-D and 3-D finite element, respectively [\[12,19,28\],](#page--1-0) unified application of state-of-art software packages [\[16,21\]](#page--1-0), and the combination of extended finite element techniques with level set method [\[15,20\]](#page--1-0). However, mesh generation for particulate composite with arbitrary inclusion shapes is still not an easy task [\[15\],](#page--1-0) as the requirement of the fitted mesh is too strict. Recently, an iterative finite element method [\[29\]](#page--1-0) is proposed to approximate the effective moduli of particulate composite. Although the method avoids the difficulty of domain discretization, it is only applicable to the case with the inclusion-to-matrix modulus ratio lower than 2.

The fundamental character of particulate composite is that it is multi-phased. In recent years, the technique of fixed grid finite element method (FGFEM) [\[30\]](#page--1-0) has been successfully applied to tackle multi-phased problems. The applications include fluid– structure interaction [\[31\],](#page--1-0) phase transformation [\[32\]](#page--1-0), heat conduction [\[33\],](#page--1-0) and unconfined seepage [\[34,35\]](#page--1-0). Garcia extends the method into elasticity problems [\[36\],](#page--1-0) followed by the application for shape optimization [\[37\]](#page--1-0), and the dynamic analysis of structures with holes [\[38,39\].](#page--1-0)

In this paper, a numerical scheme based on FGFEM is introduced to approximate the effective moduli of particulate composite. The difficulty of domain discretization is avoided in FGFEM, as RVE is discretized with finite elements independently and the inclusions are not involved in the discretization. Unlike the iterative finite element method [\[29\]](#page--1-0), this method can be applied to composite with much high inclusion-to-matrix modulus ratio. The rest of this paper is organized as follows. In Section 2, the theoretical basis to calculate the effective moduli of particulate composite is introduced for self-completeness. In Section 3, the concept of FGFEM, as well as the proposed numerical scheme, is introduced. The verification and some application of FGFEM along with some discussion are supplied in [Section 4.](#page--1-0) Some conclusions are made in [Section 5.](#page--1-0)

#### 2. Theoretical basis

Set the RVE of a particulate composite as shown in Fig. 1 applied with a traction  $\sigma^0 \cdot \mathbf{n}$  on its surface, of which  $\mathbf{n}$  is the unit outward normal on the surface. With the assumption of no bound slip on the constituent interface in the RVE, the strain energy of the RVE is

$$
U = \frac{1}{2} \sigma_{ij}^0 \overline{C}_{ijmn} \sigma_{mn}^0 V \tag{1}
$$

of which  $U$  is the strain energy,  $\sigma_{ij}^0$  is a component of  $\pmb{\sigma}^0,$   $\overline{\mathsf{C}}_{ijmn}$  is a component of the effective compliance stiffness tensor of the RVE, and V is the volume of the RVE. The summation convention is used for repeated indices in this section.



Alternatively, we have

$$
U = \frac{1}{2} \int_{V} \sigma_{ij} \varepsilon_{ij} dv
$$
 (2)

where  $\sigma_{ii}$  is a component of the stress tensor in the RVE, and  $\varepsilon_{ii}$  is a component of the strain. Due to the symmetry of  $\varepsilon_{ii}$  and  $\sigma_{ii}$ , Eq. (2) is recast into

$$
U = \frac{1}{2} \int_{V} (\sigma_{ij} u_i)_j dv - \frac{1}{2} \int_{V} \sigma_{ij} u_i dv
$$
 (3)

where  $u_i$  is a displacement component.

According to the equilibrium condition, i.e.,  $\sigma_{ii,i} = 0$ , and the divergence theorem, Eq. (3) is simplified into

$$
U = \frac{1}{2} \int_{s} \sigma_{ij} n_{j} u_{i} ds \tag{4}
$$

where s is the surface area of RVE. Obviously,  $\sigma_{ij}n_j$  equals  $\sigma_{ij}^0n_j$  on the RVE surface. Therefore, Eq. (4) is rewritten into

$$
U = \frac{1}{2} \sigma_{ij}^0 \int_s n_j u_i ds \tag{5}
$$

Based on the divergence theorem, Eq. (5) is rewritten into

$$
U = \frac{1}{2} \sigma_{ij}^0 \int_V \varepsilon_{ij} dV = \frac{1}{2} \sigma_{ij}^0 \bar{\varepsilon}_{ij} V \tag{6}
$$

where  $\overline{\varepsilon}_{ij}$  is the average strain in RVE.

It is seen in Eqs. (1) and (6) that the essence of determining  $\overline{C}_{ijmn}$  is to determine the relationship between  $\overline{\epsilon}_{ij}$  and  $\sigma_{mn}^0$ . By setting  $\overline{\epsilon}_{ij} = C_{ijmn} \sigma_{mn}^0$ , we have

$$
\overline{C}_{ijmn} = (C'_{ijmn} + C'_{mnij})/2
$$
\n(7)

Therefore, the effective compliance moduli of the composite can be determined based on the relationship between the applied traction and the average strain in the composite. Similarly, a displacement field can be applied on the RVE surface to determine the effective stiffness moduli of the composite.

## 3. Fixed grid finite element method (FGFEM)

In FGFEM, the analysis domain of interest is enclosed by a smallest bounding box as shown in Fig. 2. Unlike the traditional finite element method that discretizes the analysis domain regularly or irregularly for fitted mesh, FGFEM discretizes the bounding box with regular finite elements resulting in non-fitted mesh. Therefore, the elements in the bounding box as shown in Fig. 2 are classified into three types  $[36]$ : (a) the inside elements which are completely enclosed by the physical domain; (b) the outside elements which completely lay out of the physical domain, and (c) the boundary elements which cover the boundary of the physical domain.

For a particulate composite, its RVE coincides with the bounding box, and it also has three type of elements: (a) the inclusion elements which have a single inclusion phase; (b) the matrix elements which only have matrix phase; and (c) the hybrid elements which have at least two phases.



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