An Introduction to Micromechanics

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Abstract

This article provides a brief introduction to micromechanics using linear elastic materials as an example. The fundamental micromechanics concepts including homogenization and dehomogenization, representative volume element (RVE), unit cell, average stress and strain theories, effective stiffness and compliance, Hill-Mandel macrohomogeneity condition. This chapter also describes the detailed derivations of the rules of mixtures, and three full field micromechanics theories including finite element analysis of a representative volume element (RVE analysis), mathematical homogenization theory (MHT), and mechanics of structure genome (MSG). Theoretical connections among the three full field micromechanics theories are clearly shown. Particularly, it is shown that RVE analysis, MHT and MSG are governed by the same set of equations for 3D RVEs with periodic boundary conditions. RVE analysis and MSG can also handle aperiodic or partially periodic materials for which MHT is not applicable. MSG has the unique capability to obtain the complete set of 3D properties and local fields for heterogeneous materials featuring 1D or 2D heterogeneities.

1 Introduction

Composites by nature are anisotropic and heterogeneous while most conventional materials such as metals can be safely assumed to be isotropic and homogeneous. Anisotropy can be dealt with using coordinate transformation by transforming the material properties measured in the material coordinate into those expressed in the problem coordinates. In principle, heterogeneity can be handled by direct numerical simulation (DNS) of the composite structure containing all the microstructural details using the finite element analysis (FEA). But this requires an extremely fine scale finite element mesh with enormous numbers of degrees of freedom (DOFs). For example, using the finite element analysis to analyze epoxy/caborn fiber reinforced composites capturing the fiber details, we need the element size to be smaller than the diameter of the carbon fiber, usually a few microns. With this type of discretization, we need to have dozens of millions DOFs in our FEA model to analyze even a very tiny 1 mm^3 material block. For most realistic composite

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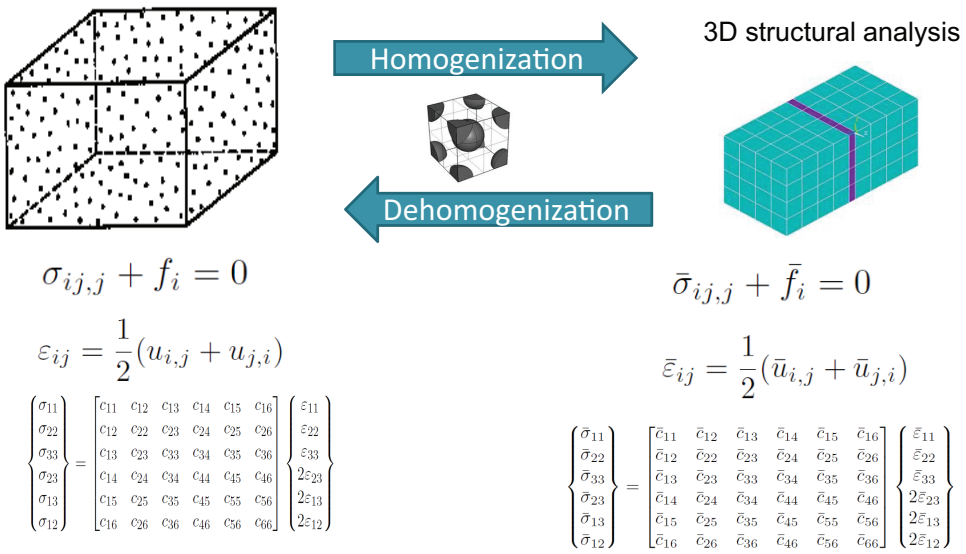

Figure 1: Basic idea of micromechanics

structures in engineering, trillions of DOFs are needed. Most engineers will not have access to computing hardware and software which can handle such a huge finite element model. In another hand, it is often an unnecessary waste of engineers' time and computing resources to use DNS for composite structures capturing fiber details. With properly constructed models, we can replace composites with an effective homogeneous material to achieve almost the same accuracy as DNS at a cost many orders of magnitude less, except at the places having significant changes in geometry, load conditions, material properties, or close to the boundaries. The saving of engineers' time and computing resources can be used for exploring more advanced designs and technological innovations. The concept to replace the original heterogeneous materials with homogeneous material which are imaginary, yet equivalent in some sense, is called homogenization. This concept is fundamental in engineering design and analysis because we usually characterize a material, composites or not, in terms of continuous field and neglect the underlying atomic structure of the material. For example, temperature is defined as a measurement of the average kinetic energy of the molecules in an object or system. Such a homogenization can be achieved using experiments or atomistic simulations. Particularly for composites, we deal with heterogeneities at the size of micron and larger and assume the constituents of composites can be adequately described as continuum with the constitutive models of constituents simpler than the constitutive models we need to use to model the composite.

The basic idea of micromechanics is to replace the original heterogeneous material with an imaginary homogenous material so that the analysis of the original structure made of heterogeneous materials can be simplified (Fig. 1). The first aim of micromechanics is to theoretically predict the effective macroscopic properties of heterogeneous materials in terms of microstructure. Here microstructure contain geometry and constitutive relations of constituents. This step is also commonly called homogenization, and many early models were developed solely for this purpose [1, 2, 3, 4, 5, 6, 7]. Homogenization can be used either for virtual material characterization, i.e., simulating the overall material response

under simple loading conditions, or constitutive modeling, where the complete set of effective material properties must be deduced and used as inputs for the structural analysis to predict the macroscopic behavior. The material properties obtained are usually properties for three-dimensional (3D) structural analysis. The second aim of micromechanics is to predict the microscopic fields such as displacement, stress and strain fields within the microstructure from the macroscopic behavior. This step is also commonly called localization or dehomogenization and is very critical for assessment of the strength and failure of heterogeneous materials. Dehomogenization is usually more demanding than homogenization as the local fields are very sensitive to the microstructural details. To achieve the above two aims, micromechanics has to assume that the constitutive models and material properties of the constituents are known. However, it is often difficult to measure the constituent properties but it is relatively easier to measure the composite properties. To this end, micromechanics can be used to back calculate the constituent properties from composite properties through an inverse analysis, so-called reverse engineering, the solution of which is usually not unique and the analysis can be casted as an optimization problem.

Many modeling techniques have been introduced to provide either rigorous bounds, such as the rules of mixtures [8], Hashin-Shtrikman bounds [9], third-order bounds [3], higher-order bounds [10], or approximate predictions including mean field approaches such as dilute method, Mori-Tanaka method, self-consistent method, generalized self-consistent method, or full field approaches such as the method of cells [11, 12] and its variants [13, 14, 15], mathematical homogenization theories (MHT) [16, 17, 18, 19], finite element approaches using conventional stress analysis of RVE [20, 21], Voronoi cell finite element method [22], and mechanics of structure genome (MSG) [23].

2 Microstructure, Representative Volume Element, and Unit Cell

We purposely neglected the microstructure of composites in our macroscopic structural analyses for efficiency. However, we need to capture the effects of microstructure on effective properties and local fields using micromechanics models. Although we can observe the physical microstructure of a material, its complexity may prevent its use in micromechanics modeling. Hence, the microstructures we use in micromechanics may or may not correspond to what we can observe in reality. This presents a direct contrast with other mechanics subject such as structural mechanics, which we usually have a well defined domain with easily recognizable boundaries to work with. The reason being that the heterogeneous material is essentially represented as a point in our macroscopic structural analysis, the size of that material point is irrelevant and it could contain one or many fundamental building blocks of the material, if such fundamental building blocks can be identified. However, we do need a microstructure to infer how the effective material properties of the heterogeneous material relate with the geometry and properties of its constituents. The fundamental requirement of a microstructure for micromechanics model is being representative of the material of which the macroscopic structure can be considered as made of.

It is the very first step of micromechanics to come up with the right microstructure. The choice of microstructure is not only related with the real material but also depends on the micromechanics model the analyst chooses to use. For example, if rules of mixtures are used, then the microstructure can be simply described using volume fractions of constituents. This is actually the simplest microstructure. As a general rule, the complexity, usually also the representativeness, of the microstructure increases with the increased complexity of micromechanics models.

Generally speaking, there are four ways to obtain a microstructure for the purpose of micromechanics modeling. First, one can idealize the observed microstructural features of the material using simple geometric models such as composite cylinders assembly, square or hexagonal pack microstructure for continuously fiber reinforced composites (CFRC), etc. Second, one can reconstruct a microstructure based on the statistical information such as correlation functions obtained from the corresponding real microstructure [10]. The one-point correlation function actually corresponds to the volume fraction of the constituent. The third approach is to reconstruct the microstructure using image data obtained using techniques such as using X-ray microtomography. Computer software tools like Simpleware can be used for this purpose. This approach has the potential to come up with the most realistic representation of the microstructure, although it usually end up with a huge finite element model for the micromechanics analysis. The four approach is to predict the microstructure from simulating the manufacturing process. With increased fidelity and predictive capability of manufacturing simulation software, this approach can obtain more and more realistic microstructures needed for micromechanics modeling.

The predictability of any micromechanics model greatly depends on whether we can accurately account for the material behavior of individual constituents and their geometry and topology. To this end, we need to first identify a microscopic domain representative of the heterogeneous material, usually called the representative volume element (RVE) in micromechanics taxonomy. RVE was originally defined as a material volume entirely typical of the whole mixture on average and contains a sufficient number of inclusions for the apparent overall properties to be effectively independent of the boundary conditions [24]. Although this definition is theoretically sound on the ergodic principle, it creates a paradox. On one hand, RVE must include a sufficient number of heterogeneities for the effective properties independent of boundary conditions, while on the other hand, it must be small enough to be justified as a material point for the macroscopic structural analysis. To resolve this dilemma, other definitions of RVE have been proposed [25, 26, 27, 6]. Most definitions are a posteriori as they mainly focus on minimizing the statistical scatter of effective properties, which are known only after one has chosen the RVE and performed the micromechanical analysis. In addition to different assumptions inherently implied by different RVE definitions, micromechanics models, particularly the earlier analytical models, also commonly make assumptions regarding geometry shape and topology of the RVE and its constituents, such as the composite spheres model, the composite cylinder model, and the three-phase model [1]. Although different mathematically oriented definitions are given for an RVE in the literature [2], we give a practice-oriented definition for an RVE as any block of material the analyst wants to use for the micromechanical analysis to find the effective properties to replace it with an equivalent homogeneous material. This liberal definition is intended for maximizing the freedom in choosing the RVE. It can be justi-

fied from the view point of material characterization using physical experiments. When experimentalists want to find properties of a material, they cut representative pieces of the material according to their own judgment and do the testing to get the properties and associated statistics.

The term unit cell (UC) is also used extensively and sometimes interchangeably with RVE in the literature. UC refers to the fundamental building block of the material. Its use is more frequently associated with materials featuring periodic heterogeneities and UC can be clearly defined as a repeating unit cell for these materials. Fundamentally speaking, by assuming the existence of RVE, we actually implicitly assume that homogeneous material we used in the macroscopic structural analysis contains many such RVEs. In other words, we implicitly assume that the material features periodic heterogeneities, at least locally in the neighborhood of the material particle we used the effective properties computed from the RVE. In principle, if the material microstructure changes significantly, we might need to have different RVEs at different locations of the composite structure. But not matter what, at each location of the composite structure, the material are implicitly assumed to contain many same RVEs at the same location. Otherwise, micromechanics is not applicable. Therefore, it is not right to say that one micromechanics method can handle aperiodic materials yet another one cannot. Micromechanics fundamentally assumes the material is at least locally periodic where RVE or UC is defined. Another point worthy to point out is that the choice of RVE and UC is not unique, even for periodic materials. For example as shown in Figure 2, one can chose six different UCs to represent the microstructure of a CFRC. In fact, there are infinite many choices of the UC as long as this material can be assembled by composing many such UCs, neglecting the partial cells at the boundary. As we are modeling the same CFRC material, a good micromechanics theory should compute the same effective properties. It is analogous to solve the same problem using different coordinate systems. Unfortunately this is not the case for most micromechanics theories. Most micromechanics theories can only deal with UCs with straight edges normal to each other (UC1, UC2, UC3 in Fig. 2). And even for these three choices, some micromechanics theories might compute different effective properties.

To facilitate mathematical formulation, we describe the macroscopic structure using a global coordinate system x_i. As the size of RVE is much smaller than the size of the macroscopic structure, we introduce a local coordinate system $y_i = x_i/\delta$ to describe the RVE, with δ being a small parameter. This basically enables a zoom-in view of the RVE at the size similar as the macroscopic structure.

3 Volume Average

As the RVE is effectively considered as a material point in the macroscopic analysis, we need to come up with a single value to represent the RVE in the macroscopic analysis. For this purpose, it is natural to compute the volume average of quantities of interest over the RVE such that

$$\bar{f} = \langle f \rangle \equiv \frac{1}{V} \int_V f \mathrm{d}V \tag{1}$$

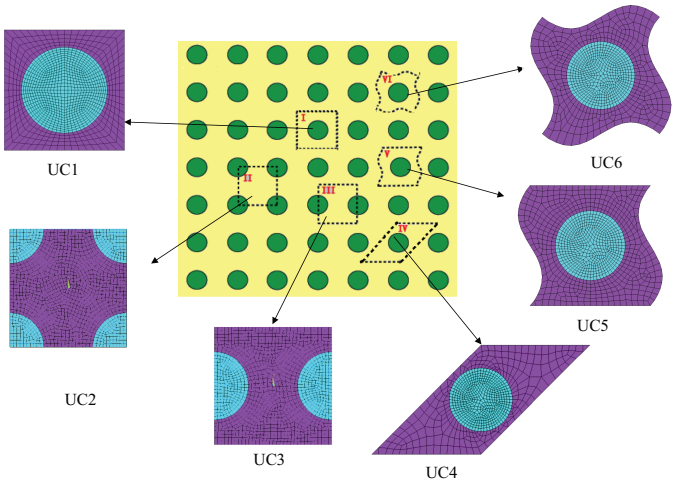

Figure 2: Six UC choices for CFRC

where V is the volume of RVE and the angle brackets denote the volume average. Note f could be a scalar, vector, or tensor and is in general a pointwise varying function within the RVE while $\bar{f}$ is the corresponding effective quantity.

Using the conservation of mass, the effective density can be computed as

$$\bar{\rho} = \langle \rho \rangle \tag{2}$$

3.1 Average Stress Theorem

If a heterogenous body, in static equilibrium, is subjected only to tractions along the boundary which is generated by a constant stress tensor $\bar{\sigma}_{ij}$ along the boundary. That is, the applied traction vector is $t_i^0 = \bar{\sigma}_{ij} n_j$ with n_j as the outward normal of the boundary. Then, the average of the stress field inside the body is equal to $\bar{\sigma}_{ij}$.

In general the stress field, σ_{ij}, is not constant within the body, as the body is heterogeneous. Because the body is only subjected to tractions (no body force), the stress field should satisfy the equilibrium equation

$$\sigma_{ij,j} = 0 \tag{3}$$

with comma denoting partial derivative with respect to the local coordinate system y_j. We have

$$\sigma_{ij} = \sigma_{ik}\delta_{jk} = \sigma_{ik}\frac{\partial y_j}{\partial x_k} = (\sigma_{ik}y_j)_{,k} - \sigma_{ik,k}y_j = (\sigma_{ik}y_j)_{,k} \tag{4}$$

Then we can deduce the following:

$$\begin{aligned} \langle \sigma_{ij} \rangle &= \frac{1}{V}\int_V \sigma_{ij}\mathrm{d}V = \frac{1}{V}\int_V (\sigma_{ik}y_j)_{,k}\mathrm{d}V = \frac{1}{V}\oint_{\partial V} \sigma_{ik}y_j n_k \mathrm{d}S \\ &= \frac{\bar{\sigma}_{ik}}{V}\oint_{\partial V} y_j n_k \mathrm{d}S = \frac{\bar{\sigma}_{ik}}{V}\int_V y_{j,k}\mathrm{d}V = \bar{\sigma}_{ij} \end{aligned} \tag{5}$$

where S denotes the bounding surface of the volume. This is a fundamental result in micromechanics called *Average Stress Theorem*. What this theorem tells us is that when

a heterogeneous body is subjected to the traction boundary condition generated by a constant stress tensor $\bar{\sigma}_{ij}$, the stress averaged over the entire body is the same as $\bar{\sigma}_{ij}$, regardless the complexity of the stress field within the body.

Eq. (5) also implies that the average stress of an RVE can be computed by the tractions t_i^0 along the boundary such that

$$\bar{\sigma}_{ij} = \langle \sigma_{ij} \rangle = \frac{1}{V} \oint_{\partial V} \sigma_{ik} y_j n_k \mathrm{d}S = \frac{1}{V} \oint_{\partial V} t_i^0 y_j \mathrm{d}S \tag{6}$$

because we know from elasticity that the stress field must satisfy the traction boundary condition: $t_i^0 = \sigma_{ik} n_k$ although t_i^0 might not be generated from a constant stress tensor according to $t_i^0 = \bar{\sigma}_{ik} n_k$.

3.2 Average Strain Theorem

If a continuous body with perfect bonding between constituents is subjected to applied displacement boundary conditions generated by a constant strain tensor $\bar{\varepsilon}_{ij}$ along the boundary such that $u_i^0 = y_j \bar{\varepsilon}_{ij}$ with y_j as the components of the position vector of a point on the boundary, the average of the infinitesimal strain field of the body is equal to $\bar{\varepsilon}_{ij}$.

In general the strain field, ε_{ij}, is not constant within the body, as the body could be formed by different constituents. However, the following is obvious:

$$\begin{aligned} \langle \varepsilon_{ij} \rangle &\equiv \frac{1}{V} \int_V \varepsilon_{ij} \mathrm{d}V = \frac{1}{2V} \int_V (u_{i,j} + u_{j,i}) \mathrm{d}V = \frac{1}{2V} \oint_{\partial V} (u_i^0 n_j + u_j^0 n_i) \mathrm{d}S \\ &= \frac{1}{2V} \oint_{\partial V} (\bar{\varepsilon}_{ik} y_k n_j + \bar{\varepsilon}_{jk} y_k n_i) \mathrm{d}S = \frac{1}{2V} \int_V (\bar{\varepsilon}_{ik} \delta_{kj} + \bar{\varepsilon}_{jk} \delta_{ki}) \mathrm{d}V = \bar{\varepsilon}_{ij} \end{aligned} \tag{7}$$

This is a fundamental result in micromechanics called *Average Strain Theorem*. What this theorem tells us is that when a continuous body, let it be formed by a single constituent or multiple different constituents, is subject to a prescribed displacement distribution according to $u_i^0 = y_j \bar{\varepsilon}_{ij}$, the infinitesimal field averaged over the entire body is the same as $\bar{\varepsilon}_{ij}$, regardless the complexity of the strain field within the body.

Eq. (7) also implies that the average strain of an RVE can be computed by the displacement values along the boundary although the displacement values might not be generated by a constant strain tensor according to $u_i^0 = y_j \bar{\varepsilon}_{ij}$.

4 Effective Stiffness and Compliance

To achieve the first aim of micromechanics, homogenization, we need to find the constitutive relations for the imaginary homogeneous material to replace the original heterogeneous material. Let us restrict to linear elastic behavior for illustrative purpose. We assume that the constituents of the original heterogeneous material obeys the following constitutive relations

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \qquad \varepsilon_{ij} = S_{ijkl} \sigma_{kl} \tag{8}$$

with σ_{ij} and ε_{kl} denoting the pointwise stress field and strain field of the original material, respectively. C_{ijkl} and S_{ijkl} are the corresponding stiffness tensor and compliance tensor,

respectively, which are functions of location for a heterogeneous material, assumed to be known. It is known that the inverse of the compliance is the stiffness: $C_{ijkl} = S^{-1}_{ijkl}$. σ_{ij} and ε_{kl} are also called as *microscopic stress and strain*, respectively.

Homogenization of the heterogeneous material implies that we need to obtain the following constitutive relations

$$\bar{\sigma}_{ij} = C^*_{ijkl}\bar{\varepsilon}_{kl} \qquad \bar{\varepsilon}_{ij} = S^*_{ijkl}\bar{\sigma}_{kl} \tag{9}$$

where $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ are the stress field and strain field of the homogeneous material, respectively, C^*_{ijkl} and S^*_{ijkl} represent the so-called effective stiffness tensor and compliance tensor, correspondingly. It is known that the inverse of the compliance is the stiffness: $C^*_{ijkl} = S^{*-1}_{ijkl}$. Note $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ are constant within the equivalent homogeneous material corresponding to the RVE (see Fig. 1) for the reason that they are considered as the stress and strain states of a material point in the macroscopic structural analysis. $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ are also called *macroscopic stress and strain*, respectively. Since the homogeneous material is imaginary, the macroscopic stress and strain are merely the volume average of the real stresses and strains within the constituents in the heterogeneous material. They are not real physical quantities experienced by the composites.

To compute C^*_{ijkl} or S^*_{ijkl}, we need to find a way to relate the microscopic stress and strain with the macroscopic stress and strain. Often in most micromechanics models, $\bar{\sigma}_{ij}$, $\bar{\varepsilon}_{ij}$, or a combination of their components are applied to the RVE, usually in terms of boundary conditions, to solve a boundary value problem to find the stress σ_{ij} and strain ε_{ij} field within the RVE.

4.1 Hill-Mandel Macrohomogeneity Condition

The celebrated Hill-Mandel macrohomogeneity condition in micromechanics addresses the following question: for a heterogenous body without body force in linear elastic static equilibrium, under what condition the average of the strain energy density is the same as the the strain energy density of homogeneous body occupying the same space with a uniform stress field and a uniform strain field? The uniform stress field and strain field of the homogeneous body is the same as the average stress field and strain field of the heterogeneous body.

For the heterogeneous body, let us denote the strain field as ε_{ij} and the stress field as σ_{ij}. They are not constant in general as the body is heterogeneous. The stress tensor is governed by the static equilibrium equations without body force. The strain energy density, $\frac{1}{2}\sigma_{ij}\varepsilon_{ij}$, is not constant. It is obvious that

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \bar{\varepsilon}_{ij}\sigma_{ij}dV = \frac{1}{V}\int_V \varepsilon_{ij}\bar{\sigma}_{ij}dV = \frac{1}{V}\int_V u_{i,j}\bar{\sigma}_{ij}dV \tag{10}$$

The question raised in the beginning of this section requires us to show under what condition we have $\langle\sigma_{ij}\varepsilon_{ij}\rangle = \bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$. To this end we need to find under what condition the

difference will vanish.

$$\begin{aligned}
\langle \sigma_{ij}\varepsilon_{ij} \rangle - \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} &= \frac{1}{V}\int_V \left(\sigma_{ij}u_{i,j} - \bar{\sigma}_{ij}u_{i,j} - \sigma_{ij}\bar{\varepsilon}_{ij} + \bar{\sigma}_{ij}\bar{\varepsilon}_{ij}\right) dV \\
&= \frac{1}{V}\int_V \left(\sigma_{ij} - \bar{\sigma}_{ij}\right)\left(u_{i,j} - \bar{\varepsilon}_{ij}\right) dV \\
&= \frac{1}{V}\int_V \left(\sigma_{ik} - \bar{\sigma}_{ik}\right)\left(u_{i,k} - \delta_{jk}\bar{\varepsilon}_{ij}\right) dV \\
&= \frac{1}{V}\int_V \left(\sigma_{ik} - \bar{\sigma}_{ik}\right)\left(u_{i,k} - y_{j,k}\bar{\varepsilon}_{ij}\right) dV \\
&= \frac{1}{V}\int_V \left[\left(\sigma_{ik} - \bar{\sigma}_{ik}\right)\left(u_i - y_j\bar{\varepsilon}_{ij}\right)\right]_{,k} dV \\
&= \frac{1}{V}\oint_{\partial V} n_k \left(\sigma_{ik} - \bar{\sigma}_{ik}\right)\left(u_i - y_j\bar{\varepsilon}_{ij}\right) dS
\end{aligned} \tag{11}$$

Note that $\left(\sigma_{ik} - \langle\sigma_{ik}\rangle\right)\left(u_{i,k} - y_{j,k}\bar{\varepsilon}_{ij}\right) = \left[\left(\sigma_{ik} - \langle\sigma_{ik}\rangle\right)\left(u_i - y_j\bar{\varepsilon}_{ij}\right)\right]_{,k}$ due to Eq. (3). We can observe from the equation in Eq. (11) that if the surface integral on the right hand side vanishes, we have $\langle \sigma_{ij}\varepsilon_{ij} \rangle = \bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$. This condition is called the *Hill-Mandel macrohomogeneity condition* in micromechanics. There are infinite many ways to vanish the surface integral. For example, the homogenous traction boundary conditions, the homogeneous displacement boundary conditions, or the periodic boundary conditions can satisfy this condition, the details of which will be later. So if such boundary conditions are applied to the RVE, the volume-averaged strain energy density of a heterogeneous material is equal to those obtained from the volume averages of the stresses and strains. Accordingly, homogenization can be interpreted as finding a homogeneous comparison material that is energetically equivalent to a given heterogeneous material. This idea can be used to define the effective properties of heterogeneous media. If the Hill-Mandel macrohomogeneity condition is satisfied, we can compute the average of strain energy of the RVE as

$$U = \frac{1}{2}\langle \sigma_{ij}\varepsilon_{ij} \rangle = \frac{1}{2}\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} \tag{12}$$

which implies the following

$$\bar{\sigma}_{ij} = \frac{\partial U}{\partial \bar{\varepsilon}_{ij}} \tag{13}$$

The effective elasticity tensor can be computed as

$$C^*_{ijkl} = \frac{\partial \bar{\sigma}_{ij}}{\partial \bar{\varepsilon}_{kl}} = \frac{\partial^2 U}{\partial \bar{\varepsilon}_{ij}\partial \bar{\varepsilon}_{kl}} \tag{14}$$

Using effective stiffness and compliance, the energy equivalence according to Hill-Mandel macrohomogeneity condition can also be expressed using the following formulas

$$\langle C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \rangle = C^*_{ijkl}\bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl} = S^*_{ijkl}\bar{\sigma}_{ij}\bar{\sigma}_{kl} \tag{15}$$

5 Rules of Mixtures

The simplest models of micromechanics are the rules of mixtures (ROMs) according to Voigt assumption and Reuss assumption, which are also frequently used in industry. Voigt assumed that the strain field within the RVE is constant, that is $\varepsilon_{ij} = \bar{\varepsilon}_{ij}$. We have the following

$$\bar{\sigma}_{ij} = \langle \sigma_{ij} \rangle = \langle C_{ijkl} \varepsilon_{kl} \rangle = \langle C_{ijkl} \bar{\varepsilon}_{kl} \rangle = \langle C_{ijkl} \rangle \, \bar{\varepsilon}_{kl} = C^*_{ijkl} \bar{\varepsilon}_{kl} \tag{16}$$

which implies

$$C^{V*}_{ijkl} = \langle C_{ijkl} \rangle \tag{17}$$

meaning that the effective stiffness is the volume average of the stiffness of the constituents. The superscript V indicates that the effective stiffness is computed according to Voigt rule of mixtures (ROM). Clearly the effective stiffness according to Voigt ROM features the same symmetry as the least symmetry of the constituent properties.

Reuss assumed that the stress field within the RVE is constant, that is $\sigma_{ij} = \bar{\sigma}_{ij}$. We have the following

$$\bar{\varepsilon}_{ij} = \langle \varepsilon_{ij} \rangle = \langle S_{ijkl} \sigma_{kl} \rangle = \langle S_{ijkl} \bar{\sigma}_{kl} \rangle = \langle S_{ijkl} \rangle \, \bar{\sigma}_{kl} = S^*_{ijkl} \bar{\sigma}_{kl} \tag{18}$$

which implies

$$S^{R*}_{ijkl} = \langle S_{ijkl} \rangle = \left\langle C^{-1}_{ijkl} \right\rangle \tag{19}$$

meaning that the effective compliance is the volume average of the compliance of the constituents. The superscript R indicates that the effective property is computed according to Reuss ROM. The Reuss ROM can also be expressed in terms of stiffness as

$$C^{R*}_{ijkl} = \left(S^{R*}_{ijkl} \right)^{-1} = \left\langle C^{-1}_{ijkl} \right\rangle^{-1} \tag{20}$$

Similarly, the effective properties, stiffness or compliance, according to Reuss ROM features the same symmetry as the least symmetry of the constituent properties.

It can be shown that the effective stiffness obtained using Voigt ROM is the upper bound and that obtained using Reuss ROM is the lower bound. In other words, if one uses another method to obtain the effective stiffess C^*_{ijkl}, it must satisfy the following

$$C^{R*}_{ijkl} \leq C^*_{ijkl} \leq C^{V*}_{ijkl} \tag{21}$$

These inequalities must be understood in the sense of the inequality for corresponding strain energy, which implies that for any set of strains ε'_{ij}, we have the following inequalities exist

$$\frac{1}{2} C^{R*}_{ijkl} \varepsilon'_{ij} \varepsilon'_{kl} \leq \frac{1}{2} C^*_{ijkl} \varepsilon'_{ij} \varepsilon'_{kl} \leq \frac{1}{2} C^{V*}_{ijkl} \varepsilon'_{ij} \varepsilon'_{kl} \tag{22}$$

It is emphatically pointed out that the inequality in Eq. (21) does not mean corresponding entries in the corresponding matrices satisfy this inequality. Nevertheless, it is easy to conclude that the corresponding eigenvalues and diagonal terms of the matrices will satisfy the inequality in Eq. (21).

The inequality in Eq. (22) can be proven as follows. Let us assume $\varepsilon_{ij} = \bar{\varepsilon}_{ij} + \varepsilon'_{ij}$, then due to the positive definiteness of C_{ijkl}, we have

$$\begin{aligned} 0 \leq \left\langle C_{ijkl}\varepsilon'_{ij}\varepsilon'_{kl} \right\rangle &= \langle C_{ijkl}(\varepsilon_{ij} - \bar{\varepsilon}_{ij})(\varepsilon_{kl} - \bar{\varepsilon}_{kl}) \rangle \\ &= \langle C_{ijkl}(\varepsilon_{ij}\varepsilon_{kl} - 2\bar{\varepsilon}_{ij}\varepsilon_{kl} + \bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl}) \rangle \\ &= C^*_{ijkl}\bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl} - 2\bar{\varepsilon}_{ij}\bar{\sigma}_{kl} + \langle C_{ijkl} \rangle \bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl} \\ &= \left(C^{V*}_{ijkl} - C^*_{ijkl} \right) \bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl} \end{aligned} \tag{23}$$

Here we used the Hill-Mandel macrohomogeneity condition in Eq. (15) and the effective properties definition in Eq. (9).

Similarly, let us assume $\sigma_{ij} = \bar{\sigma}_{ij} + \sigma'_{ij}$, then due to the positive definiteness of S_{ijkl} or C^{-1}_{ijkl}, we have

$$\begin{aligned} 0 \leq \left\langle S_{ijkl}\sigma'_{ij}\sigma'_{kl} \right\rangle &= \langle S_{ijkl}(\sigma_{ij} - \bar{\sigma}_{ij})(\sigma_{kl} - \bar{\sigma}_{kl}) \rangle \\ &= \langle S_{ijkl}(\sigma_{ij}\sigma_{kl} - 2\bar{\sigma}_{ij}\sigma_{kl} + \bar{\sigma}_{ij}\bar{\sigma}_{kl}) \rangle \\ &= S^*_{ijkl}\bar{\sigma}_{ij}\bar{\sigma}_{kl} - 2\bar{\sigma}_{ij}\bar{\varepsilon}_{kl} + \langle S_{ijkl} \rangle \bar{\sigma}_{ij}\bar{\sigma}_{kl} \\ &= \left(S^{R*}_{ijkl} - S^*_{ijkl} \right) \bar{\sigma}_{ij}\bar{\sigma}_{kl} \end{aligned} \tag{24}$$

Here we used the Hill-Mandel macrohomogeneity condition in Eq. (15) and the effective properties definition in Eq. (9). From Eq. (23) and (24), we can conclude the inequality in Eq. (22).

For a composite made of two orthotropic constituents, denoting as fiber and matrix, the effective stiffness according to the Voigt ROM can be computed as

$$C^{V*} = \begin{bmatrix} C^{V*}_{11} & C^{V*}_{12} & C^{V*}_{13} & 0 & 0 & 0 \\ C^{V*}_{12} & C^{V*}_{22} & C^{V*}_{23} & 0 & 0 & 0 \\ C^{V*}_{13} & C^{V*}_{23} & C^{V*}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C^{V*}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C^{V*}_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C^{V*}_{66} \end{bmatrix} \tag{25}$$

where $C^{V*}_{ij} = V^f C^f_{ij} + V^m C^m_{ij}$ with V^f and V^m denoting volume fraction of fiber and matrix, respectively, and C^f_{ij} and C^m_{ij} are corresponding stiffness matrices of fiber and matrix, respectively according to the Voigt engineering notation. Note $V^f + V^m = 1$. Based on C^{V*} we can compute the corresponding engineering constants.

The effective stiffness according to the Reuss ROM can be computed as

$$C^{R*} = \begin{bmatrix} \left\langle \frac{1}{E_1} \right\rangle & -\left\langle \frac{\nu_{21}}{E_2} \right\rangle & -\left\langle \frac{\nu_{31}}{E_3} \right\rangle & 0 & 0 & 0 \\ -\left\langle \frac{\nu_{12}}{E_1} \right\rangle & \left\langle \frac{1}{E_2} \right\rangle & -\left\langle \frac{\nu_{32}}{E_3} \right\rangle & 0 & 0 & 0 \\ -\left\langle \frac{\nu_{13}}{E_1} \right\rangle & -\left\langle \frac{\nu_{23}}{E_2} \right\rangle & \left\langle \frac{1}{E_3} \right\rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & \left\langle \frac{1}{G_{23}} \right\rangle & 0 & 0 \\ 0 & 0 & 0 & 0 & \left\langle \frac{1}{G_{13}} \right\rangle & 0 \\ 0 & 0 & 0 & 0 & 0 & \left\langle \frac{1}{G_{12}} \right\rangle \end{bmatrix}^{-1} \tag{26}$$

where $\left\langle \frac{\nu_{21}}{E_2} \right\rangle = V^f \frac{\nu_{21}^f}{E_2^f} + V^m \frac{\nu_{21}^m}{E_2^m}$, with $E_2^f, \nu_{21}^f, E_2^m, \nu_{21}^m$ denoting the properties for fiber and matrix, respectively.

If the composite is made of two isotropic constituents, with E^f and ν^f denoting the Young's modulus and Poisson's ratio for the fiber and with E^m and ν^m denoting the Young's modulus and Poisson's ratio for the matrix, we can solve for the effective Young's modulus and Poisson's ratio according to the Voigt ROM from the following two equations

$$C_{12}^{V*} = \frac{V^f \nu^f E^f}{(1+\nu^f)(1-2\nu^f)} + \frac{V^m \nu^m E^m}{(1+\nu^m)(1-2\nu^m)} = \frac{\nu^{V*} E^{V*}}{(1+\nu^{V*})(1-2\nu^{V*})} \tag{27}$$

$$C_{44}^{V*} = \frac{V^f E^f}{2(1+\nu^f)} + \frac{V^m E^m}{2(1+\nu^m)} = \frac{E^{V*}}{2(1+\nu^{V*})} \tag{28}$$

which can be used to solve for E^{V*} and ν^{V*} as

$$E^{V*} = V^f E^f + V^m E^m + \frac{2V^f V^m E^f E^m (\nu^f - \nu^m)^2}{V^f E^f (1+\nu^m)(1-2\nu^m) + V^m E^m (1+\nu^f)(1-2\nu^f)} \tag{29}$$

$$\nu^{V^*} = \frac{V^f E^f \nu^f (1+\nu^m)(1-2\nu^m) + V^m E^m \nu^m (1+\nu^f)(1-2\nu^f)}{V^f E^f (1+\nu^m)(1-2\nu^m) + V^m E^m (1+\nu^f)(1-2\nu^f)} \tag{30}$$

Eq. (28) implies that the effective shear modulus can be be computed using the following formula

$$G^{V*} = V^f G^f + V^m G^m \tag{31}$$

We can easily verify that the effective bulk modulus can be computed using

$$K^{V*} = V^f K^f + V^m K^m \tag{32}$$

This means that shear modulus and bulk modulus obey the commonly known ROMs. But neither Young's modulus nor Poisson's ratio obey the simple rules given below

$$E^* = V^f E^f + V^m E^m \qquad \nu^* = V^f \nu^f + V^m \nu^m \tag{33}$$

which is a a common mistake made in many textbooks and research papers on composites [28]. Young's modulus obeys the simple ROMs only if $\nu^f = \nu^m$ for the composites made of isotropic constituents. For composites made of transversely isotropic or orthotropic constituents, it is possible to obtain analytical formulas to express effective engineering constants in terms of constituent constants similar as those in Eq. (30) for isotropic constituents, although the formulas are very lengthy and not given here.

The Young's modulus, shear modulus, bulk modulus, and Poisson's ratio for a composite containing two isotropic components according to the Reuss ROM are obtained as

$$\frac{1}{E^{R*}} = \frac{V^f}{E^f} + \frac{V^m}{E^m} \tag{34}$$

$$\frac{1}{G^{R*}} = \frac{V^f}{G^f} + \frac{V^m}{G^m} \tag{35}$$

$$\frac{1}{K^{R*}} = \frac{V^f}{K^f} + \frac{V^m}{K^m} \tag{36}$$

$$\frac{1}{\nu^{R*}} = \frac{V^f E^m + V^m E^f}{V^f E^m \nu^f + V^m E^f \nu^m} \tag{37}$$

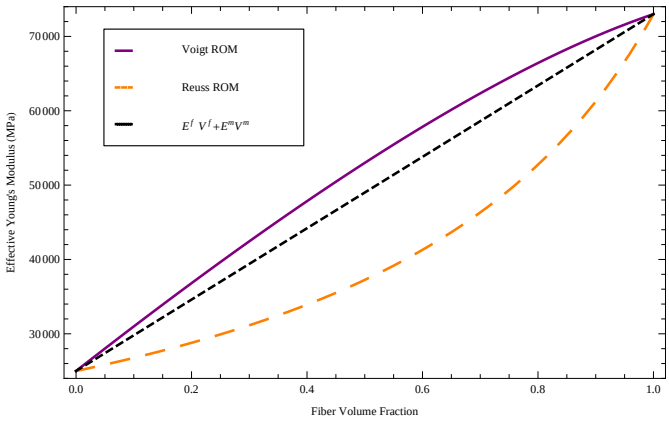

Figure 3: Young's modulus versus fiber volume fraction

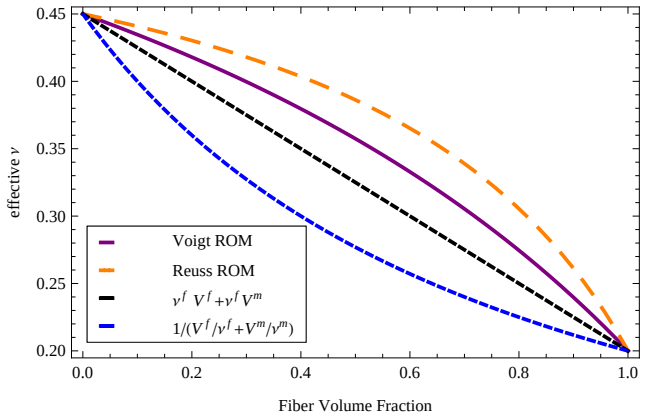

Figure 4: Poisson's ratio versus fiber volume fraction

Note that the Poisson's ratio does not obey the simplistic rule such as

$$\frac{1}{\nu^{R*}} = \frac{V^f}{\nu^f} + \frac{V^m}{\nu^m} \tag{38}$$

Assume $E^f = 73$ GPa, $E^m = 25$ GPa, $\nu^f = 0.22$, and $\nu^m = 0.45$, we can plot the prediction of Young's modulus and Poisson's ratio versus V^f using Voigt ROM, Reuss ROM, and the simple rules as shown in Figure 3 and Fig. 4. Clearly the simplistic rules might cause significant loss of accuracy.

6 RVE Analysis

RVE analysis is a very popular micromechanics method, partially due to the extensive acceptance of user friendly commercial FEA software. RVE analysis is a straightforward use of readily available commercial FEA packages such as ABAQUS or ANSYS to carry out a static analysis of the RVE subjected to a carefully crafted boundary conditions in terms of displacements and tractions. As FEA has achieved the maturity that practicing engineers believe it to be the golden standard, the only thing one needs to pay attention to

is the boundary conditions. Another reason of the popularity of RVE analysis is that the concept is deeply rooted in engineering. Although not as formalized as the RVE analysis in micromechanics, similar ideas have been used in practice for many decades, for example to obtain the torsional stiffness and bending stiffness needed in an aeroelastic design of a wing using beam representation, one usually subjects a segment of the wing to a unit torque or bending moment to obtain the corresponding twist or bending curvature. The sub-structuring and super-element techniques in FEA also have similar philosophical roots as the RVE analysis.

According to linear elasticity, we know the static equilibrium of the RVE without body force is given by Eq. (3). To have a well posed boundary value problem, boundary conditions in terms of displacement or traction along the RVE boundary are needed. As the objective is to compute the effective stiffness or compliance, Eq. (9), we need to apply the boundary conditions in terms of the macroscopic stress or strain $\bar{\sigma}_{ij}$, $\bar{\varepsilon}_{ij}$, then we can solve the boundary value problem using FEA to find the stress σ_{ij} and strain ε_{ij} field within the RVE which can be used to compute the effective properties. Assumed loads in terms of displacements, forces, or unit strains [29, 20], are often applied as boundary conditions to the RVE to complete the boundary value problem.

According to its definition, RVE should be chosen so that the effective properties will not depend on the boundary conditions. In other words, no matter which boundary conditions applies to the RVE, we will get the same effective properties. To be true to this definition, we need to chose RVEs with increasing sizes and subject to arbitrary boundaries to compute the effective properties until the effective properties are not changing with respect to the size of RVE and boundary conditions. However, in real practices, the size of such RVEs become so large that its computation is too expensive to exploit any advantage provided by micromechanics. Instead, the analyst chooses a RVE according to his/her own experience to carry out the analysis which usually does not satisfy the original definition of RVE. Thus the results are sensitive to the boundary conditions applied to the RVE. As RVE is essentially a material point in the macroscopic structural analysis, boundary conditions are artificially created to formulate a well-posed boundary value problem for FEA to solve. For virtual material characterization of material response under simple loading conditions, boundary conditions are usually applied in a way to mimic the real boundary conditions applied to the test coupon. For constitutive modeling needed to compute the complete set of effective material properties for the macroscopic structural analysis, many boundary conditions have been proposed in the past. Now, it is commonly accepted that the boundary conditions applied to a RVE should satisfy the Hill-Mandel macrohomogeneity condition so that the homogenized material is energetically equivalent to the original heterogeneous material.

Three types of boundary conditions are commonly applied to an RVE including homogeneous displacement boundary conditions, homogeneous traction boundary conditions, and periodic boundary conditions with details given below.

The *homogeneous displacement boundary conditions*, also called kinematically uniform boundary conditions, are given in terms of

$$u_i^0 = \bar{\varepsilon}_{ij} y_j \tag{39}$$

with $\bar{\varepsilon}_{ij}$ as constant along the boundary. Under these boundary conditions, the average

strain of a perfectly bonded RVE is the same as $\bar{\varepsilon}_{ij}$ according to the average strain theorem. Clearly these boundary conditions will vanish the surface integral in Eq. (11), thus satisfying the Hill-Mandel macro-homogeneity condition.

The *homogeneous stress boundary conditions*, also called statically uniform boundary conditions, are given in terms of

$$t_i^0 = \bar{\sigma}_{ij} n_j \tag{40}$$

with $\bar{\sigma}_{ij}$ as constant along the boundary. Under these boundary conditions, the average stress of the RVE is the same as $\bar{\sigma}_{ij}$ according to the average stress theorem. Clearly these boundary conditions will vanish the surface integral in Eq. (11), thus satisfying the Hill-Mandel macrohomogeneity condition. The reason the boundary conditions in Eqs. (39) and (40) are called homogeneous boundary conditions is that these boundary conditions, when applied to a homogeneous body, will generate a homogeneous (uniform) strain or stress field in the body.

The *periodic boundary conditions* are given in terms of

$$t_i^+ = -t_i^- \qquad \chi_i^+ = \chi_i^- \tag{41}$$

where

$$\chi_i = u_i - y_j \bar{\varepsilon}_{ij} \tag{42}$$

denoting the displacement fluctuations and superscripts + and − denote the quantities on the corresponding periodic boundaries. Basically periodic boundary conditions require that the tractions on the corresponding periodic boundaries equal and opposite in directions, and displacement fluctuations equal to each other on the corresponding periodic boundaries. Clearly the periodic boundary conditions will vanish the surface integral in Eq. (11), thus satisfying the Hill-Mandel macrohomogeneity condition.

It is proven that homogeneous displacement boundary conditions and homogenous traction boundary conditions lead to upper and lower estimates of the effective properties, respectively, compared to periodic boundary conditions. Predictions using homogeneous displacement and traction boundary conditions converge to those of periodic boundary conditions with increasing RVE size [30, 31, 32]. It is also theoretically justified and numerically confirmed that periodic boundary conditions provide the most reasonable estimates among the class of possible boundary conditions satisfying Hill-Mandel macrohomogeneity condition [33]. In other words, PBC is the best boundary conditions to use for RVE analysis. As most FEA is displacement based, only the the displacement fluctuations are required to be periodic and the periodic traction boundary conditions are automatically satisfied for a fine enough mesh with converged stress results. The periodic boundary conditions were originally given in [30]. However, periodic boundary conditions are not extensively used in the RVE analysis using commercial FEA software until the recent arrival of coupled equation constraints in these software packages which enables convenient application of these conditions.

In summary, substituting the constitutive relations in Eq. (8) along with the infinitesimal strain definition into Eq. (3), we can obtain the following displacement-based formulation for the RVE analysis

$$\left(C_{ijkl} u_{k,l}\right)_{,j} = 0 \tag{43}$$

subject to boundary conditions $(u_i - y_j\bar{\varepsilon}_{ij})^+ = (u_i - y_j\bar{\varepsilon}_{ij})^-$. In real analysis, we apply unit value to one component of the macroscopic strain, say $\bar{\varepsilon}_{11} = 1$, then write out these boundary conditions explicitly for each surfaces. Run FEA using these boundary conditions to carry out the static analysis to compute the stress field σ_{ij} within the RVE. Then we can compute the volume average of the stress $\bar{\sigma}_{ij}$, which corresponds to the first column of the effective stiffness matrix according to Eq. (9). Similarly applying unit value to the rest of five macroscopic strain components, we will obtain the corresponding column of the effective stiffness matrix. Six FEA analyses are needed to compute the 6×6 stiffness matrix.

7 Mathematical Homogenization Theory

Mathematical homogenization theory (MHT), also called asymptotic homogenization theory, despite its arcane mathematical derivation, is another popular micromechanics method. It is an application of the formal asymptotic method through a two-scale formulation [34, 16]. Its application in engineering has been popularized by its implementation using the finite element method [35, 18, 36, 19]. Although it was originally developed for periodic media formed by a unit cell, it can be applied to RVE because the material must be locally periodic for us to replace it with an effective homogenous material in the macroscopic structural analysis. For periodic media, the unit cell can be chosen as a RVE. In fact, it will be shown later that MHT is exactly the same as RVE analysis with periodic boundary conditions. Thus, we will use RVE only in later derivations with the understanding that RVE is chosen to be a unit cell for a periodic material.

The two-scale formulation assumes that a field function of the original structure can be generally written as a function of the macro coordinates x_k and the micro coordinates y_j. Following [16], the partial derivative of a function $f(x_k, y_j)$ can be expressed as

$$\frac{\partial f(x_k, y_j)}{\partial x_i} = \frac{\partial f(x_k, y_j)}{\partial x_i}|_{y_j=\text{const}} + \frac{1}{\delta}\frac{\partial f(x_k, y_j)}{\partial y_i}|_{x_k=\text{const}} \equiv f_{|i} + \frac{1}{\delta}f_{,i} \tag{44}$$

According to 3D elasticity, the mechanical behavior of the heterogeneous material $(u_i, \varepsilon_{ij}, \sigma_{ij})$ must satisfy the following governing equations at every point of the composite body

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = 0 \tag{45}$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{46}$$

$$\sigma_{ij} = C_{ijkl}\varepsilon_{ij} \tag{47}$$

along with boundary conditions in terms of displacements and tractions such as $u_i = \bar{u}_i$ and $\sigma_{ij}n_j = \bar{t}_i$. It is noted that these boundary conditions are not applied on the RVE boundary but on the boundary of the macroscopic structure.

MHT starts with the assumption that the displacement field can be expanded into an asymptotic series such that

$$u_i(x, y) = u_i^0(x, y) + \delta\ u_i^1(x, y) + \delta^2 u_i^2(x, y) + O(\delta^3) \tag{48}$$

Substituting Eq. (48) into Eq. (46) and considering Eq. (44), we obtain

$$\varepsilon_{ij}(x,y) = \frac{1}{\delta}\varepsilon_{ij}^{-1}(x,y) + \varepsilon_{ij}^{0}(x,y) + \delta\ \varepsilon_{ij}^{1}(x,y) + O(\delta^2) \tag{49}$$

with

$$\varepsilon_{ij}^{-1}(x,y) = u_{(i,j)}^{0} \tag{50}$$
$$\varepsilon_{ij}^{0}(x,y) = u_{(i|j)}^{0} + u_{(i,j)}^{1} \tag{51}$$
$$\varepsilon_{ij}^{1}(x,y) = u_{(i|j)}^{1} + u_{(i,j)}^{2} \tag{52}$$

where the subscript pairs with parenthesis denote the symmetric gradient defined as

$$u_{(i,j)}^{0} = \frac{1}{2}(u_{i,j}^{0} + u_{j,i}^{0}) \qquad u_{(i|j)}^{0} = \frac{1}{2}(u_{i|j}^{0} + u_{j|i}^{0}) \tag{53}$$

Substituting Eq. (49) into Eq. (47), we have

$$\sigma_{ij}(x,y) = \frac{1}{\delta}\sigma_{ij}^{-1}(x,y) + \sigma_{ij}^{0}(x,y) + \delta\ \sigma_{ij}^{1}(x,y) + O(\delta^2) \tag{54}$$

with

$$\sigma_{ij}^{-1}(x,y) = C_{ijkl}\varepsilon_{ij}^{-1} \tag{55}$$
$$\sigma_{ij}^{0}(x,y) = C_{ijkl}\varepsilon_{ij}^{0} \tag{56}$$
$$\sigma_{ij}^{1}(x,y) = C_{ijkl}\varepsilon_{ij}^{1} \tag{57}$$

Here MHT introduces the second assumption that the elasticity tensor C_{ijkl} is an order on function.

Substituting Eq. (54) into Eq. (45), we have

$$\frac{1}{\delta^2}\sigma_{ij,j}^{-1} + \frac{1}{\delta}\left(\sigma_{ij|j}^{-1} + \sigma_{ij,j}^{0}\right) + \sigma_{ij|j}^{0} + \sigma_{ij,j}^{1} + f_i + O(\delta) = 0 \tag{58}$$

Multiplying Eq. (58) by δ^2 and then taking the limit of δ approaching zero, one can obtain the leading order equilibrium. Similarly, we can obtain the equilibrium for other orders. The resulting equilibrium equations according to each asymptotic order are

$$\sigma_{ij,j}^{-1} = 0 \tag{59}$$

$$\sigma_{ij|j}^{-1} + \sigma_{ij,j}^{0} = 0 \tag{60}$$

$$\sigma_{ij|j}^{0} + \sigma_{ij,j}^{1} + f_i = 0 \tag{61}$$

Here MHT introduces the third assumption that the body force f_i and the boundary conditions $\bar{u}_i$ and $\bar{t}_i$ are order one functions.

Multiplying Eq. (59) by u_i^0, we have

$$0 = \int_V u_i^0 \sigma_{ij,j}^{-1} dV = \oint_{\partial V} u_i^0 \sigma_{ij}^{-1} n_j dS - \int_V u_{i,j}^0 \sigma_{ij}^{-1} dV \tag{62}$$

The surface integral over the boundary vanishes due to the assumption of periodic response over unit cell boundaries so that u_i^0 is equal on the corresponding periodic sides of the unit cell, while traction $\sigma_{ij}^{-1}n_j$ is equal with opposite sign on the corresponding periodic sides of the unit cell. Further substituting Eqs. (55) and (50) into Eq. (62), we have

$$\int_V u_{i,j}^0 C_{ijkl} u_{k,l}^0 dV = 0 \tag{63}$$

As C_{ijkl} is positive definite and has both minor and major symmetry, we conclude that for Eq. (63) to be satisfied, we must have $u_{i,j}^0 = 0$, which implies

$$u_i^0(x,y) = u_i^0(x) \equiv \bar{u}_i(x) \qquad \sigma_{ij}^{-1} = 0 \tag{64}$$

Here $\bar{u}_i$ is the volume average of u_i if we require

$$\left\langle u_i^1 \right\rangle = \left\langle u_i^2 \right\rangle = \ldots = 0 \tag{65}$$

Substituting Eqs. (64), (56), and (51) into Eq. (60), we have

$$\left(C_{ijkl}\left(\bar{\varepsilon}_{kl} + u_{k,l}^1\right)\right)_{,j} = 0 \tag{66}$$

with

$$\bar{\varepsilon}_{kl} = \bar{u}_{(k|l)} \tag{67}$$

Eq. (66) can be used along with the constraints in Eq. (65) to uniquely solve for u_k^1, which can be symbolically written as

$$u_k^1 = H_k^{mn} \bar{\varepsilon}_{mn} \tag{68}$$

As u_k^1 must be periodic, then H_k^{mn} must be periodic too.

The strain field ε_{ij}^1 can be obtained as

$$\varepsilon_{ij}^0(x,y) = \bar{\varepsilon}_{ij} + H_{(i,j)}^{mn} \bar{\varepsilon}_{mn} \tag{69}$$

It can be shown that

$$\bar{\varepsilon}_{ij} = \int_V \varepsilon_{ij}^0(x,y) dV \tag{70}$$

due to the periodicity of H_k^{mn}. The stress field σ_{ij}^0 can be obtained as

$$\sigma_{ij}^0(x,y) = C_{ijkl}\varepsilon_{kl}^0 = C_{ijkl}\left(\bar{\varepsilon}_{kl} + H_{(k,l)}^{mn}\bar{\varepsilon}_{mn}\right) = \left(C_{ijmn} + C_{ijkl}H_{(k,l)}^{mn}\right)\bar{\varepsilon}_{mn} \tag{71}$$

Lastly, we need to solve the equilibrium equation in Eq. (61). As the RVE is actually considered as a point in the macroscopic analysis, taking the volume average of this equation over the RVE domain and considering the periodicity of σ_{ij}^1, we have

$$\bar{\sigma}_{ij|j} + \bar{f}_i = 0 \tag{72}$$

with

$$\bar{\sigma}_{ij} = \left\langle \sigma_{ij}^0 \right\rangle = \left\langle \left(C_{ijmn} + C_{ijkl}H_{(k,l)}^{mn}\right)\bar{\varepsilon}_{mn} \right\rangle \equiv C_{ijmn}^* \bar{\varepsilon}_{mn} \tag{73}$$

with

$$C^*_{ijmn} = \left\langle C_{ijmn} + C_{ijkl} H^{mn}_{(k,l)} \right\rangle \tag{74}$$

Clearly, the 15 equations governing the macroscopic structural analysis consists of Eq. (72) for equilibrium, Eq. (73) for constitutive relations, and Eq. (67) for strain-displacement relations to solve for the 15 field variables including the macroscopic stress field $\bar{\sigma}_{ij}$, the macroscopic strain field $\bar{\varepsilon}_{ij}$, and the macroscopic displacement field $\bar{u}_i$. So according to MHT, the homogenization step is to solve Eq. (66) for a periodic u^1_i along with the constraint in Eq. (65) to find the effective properties C^*_{ijkl} using Eq. (74). Then the effective properties can be used to solve for the macroscopic behavior including $\bar{u}_i$, $\bar{\varepsilon}_{ij}$ and $\bar{\sigma}_{ij}$. The dehomogenization step is to obtain the local displacement field using

$$u_i(x, y) = \bar{u}_i(x) + \delta \; H^{mn}_i \bar{\varepsilon}_{mn} \tag{75}$$

Note here $\bar{u}_i$ should be interpreted as

$$\bar{u}_i = \bar{u}_i(x_{k_0}) + x_k \bar{u}_{i,k} \tag{76}$$

where x_{k_0} is the center of RVE and $\bar{u}_{i,k}$ is the gradient along x_k evaluated at x_{k_0}.

The local strain field can be obtained using

$$\varepsilon_{ij} = \bar{\varepsilon}_{ij} + H^{mn}_{(i,j)} \bar{\varepsilon}_{mn} \tag{77}$$

The local stress field can be obtained using

$$\sigma_{ij} = \left(C_{ijmn} + C_{ijkl} H^{mn}_{(k,l)} \right) \bar{\varepsilon}_{mn} \tag{78}$$

8 Mechanics of Structure Genome

Mechanics of structure genome (MSG) is a unified approach recently introduced for multi-scale constitutive modeling for all types of composites structures including beams, plates/shells, and 3D structures [23]. Structure Genome (SG) is defined as the *smallest mathematical* building block of the structure to emphasize the fact that it contains all the constitutive information needed for a structure the same fashion as the genome contains all the intrinsic information for an organism's growth and development. For 3D bodies, SG serves a similar role as the RVE concept in micromechanics (Figure 5). However, they are different. For example, for a structure made of composites featuring 1D heterogeneity (e.g. binary composites made of two alternating layers), SG will be a straight line with two segments denoting corresponding phases as one can mathematically repeat this line in plane to build the two layers of the binary composite, then repeat the binary composite out of plane to build the entire structure. For a structure made of composites featuring 2D heterogeneity (e.g. continuous fiber reinforced composites), the SG will be 2D, and for a structure made of composites featuring 3D heterogeneity (e.g. particle reinforced composites), the SG will be 3D. Despite that SG for 3D bodies could have different dimensions due to their heterogeneities, the effective properties should remain 3D for the 3D structural analysis. For example, for linear elastic analysis, one should be able to obtain the complete 6×6

stiffness matrix from an analysis of the 1D SG of the binary composite. Clearly, SG uses the lowest dimension, thus highest efficiency, to describe the heterogeneity, while RVE dimension is usually determined by heterogeneity and what type of properties required for the structural analysis. For example, if 3D properties are needed for 3D structural analysis of continuous fiber reinforced composites, a 3D RVE is usually required. Although unnecessary waste of computing resources, MSG can use SGs with higher dimensions to reproduce the results by SGs with dimensionality the same as that of the heterogeneity. For example, MSG can use 2D or 3D SGs to reproduce the results of 1D SGs for binary composites and 3D SGs to reproduce the results of 2D SGs for continuous fiber reinforced composites.

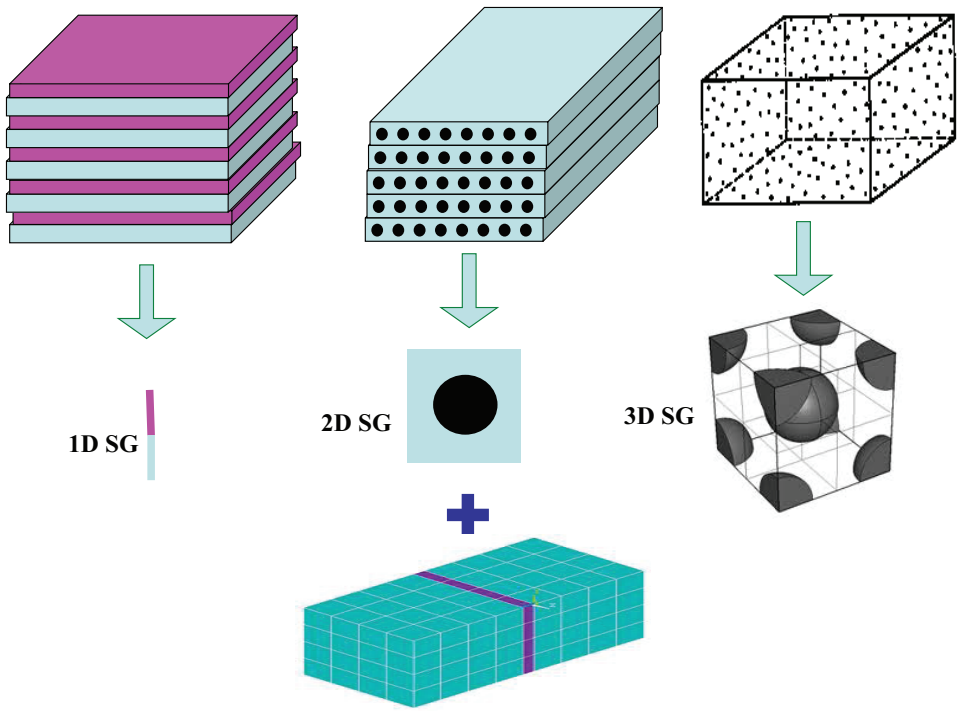

Figure 5: SG for 3D structure

MSG is based on the principle of minimum information loss which states that the homogenized model can be constructed through minimizing the information loss between the original model and the homogenized model. For linear elastic material, the information can be the strain energy density. According to MSG, we need to first express the kinematics of the original model in terms of the model to be constructed as

$$u_i(x, y) = \bar{u}_i(x) + \chi_i(x, y) \tag{79}$$

with u_i denoting the displacement field of the original model, $\bar{u}_i$ denoting the displacement of the homogenized model, and χ_i denoting the difference between these two fields, which is commonly called fluctuation function in micromechanics.

Then we can obtain the strain field of the original model as

$$\varepsilon_{ij}(x, y) = \bar{\varepsilon}_{ij}(x) + \frac{1}{\delta}\chi_{(i|j)} \tag{80}$$

Here the higher order term $\chi_{(i,j)}$ has been neglected according to the variational asymptotic method [37]. As we are constructing the homogenized model out of the original model, we need to define the kinematic variables of the homogenized model in terms of those of the original model. The natural choice is to define

$$\bar{u}_i = \langle u_i \rangle \qquad \bar{\varepsilon}_{ij} = \langle \varepsilon_{ij} \rangle \tag{81}$$

which implies the following constraints on the fluctuation functions

$$\langle \chi_i \rangle = 0 \qquad \left\langle \chi_{(i,j)} \right\rangle = 0 \tag{82}$$

The principle of minimum information loss seeks to minimize the difference between the strain energy of the original model and the homogenized model which is

$$\Pi = \left\langle \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right\rangle - \frac{1}{2} C^*_{ijkl} \bar{\varepsilon}_{ij} \bar{\varepsilon}_{kl} \tag{83}$$

To minimize Π, we consider the homogenized model as given (i.e., $C^*_{ijkl}, \bar{\varepsilon}_{ij}$ cannot be varied). Then χ_i can be solved from the following variational statement

$$\min_{\chi_i} \left\langle \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right\rangle = \min_{\chi_i \in \text{Eq. (82)}} \left\langle \frac{1}{2} C_{ijkl} \left(\bar{\varepsilon}_{ij} + \chi_{(i,j)} \right) \left(\bar{\varepsilon}_{kl} + \chi_{(k,l)} \right) \right\rangle \tag{84}$$

Using calculus of variations, we can conclude that χ_i must satisfy the following Euler-Lagrange equations

$$\left(C_{ijkl} \left(\bar{\varepsilon}_{kl} + \chi_{k,l} \right) \right)_{,j} = 0 \tag{85}$$

along with the constraints in Eq. (82), additional constraints can be incorporated as needed. For example, for periodic materials, χ_i must be periodic, and the second equation in Eq. (82) will be automatically satisfied. χ_i will be solved in terms of $\bar{\varepsilon}_{kl}$, which has the same symbolic form of Eq. (68).

$$\chi_k = H^{mn}_k \bar{\varepsilon}_{mn} \tag{86}$$

The volume average of the strain energy of the RVE can be obtained as

$$U = \left\langle \frac{1}{2} C_{ijkl} (\bar{\varepsilon}_{ij} + H^{mn}_{(i,j)} \bar{\varepsilon}_{mn}) (\bar{\varepsilon}_{kl} + H^{st}_{(k,l)} \bar{\varepsilon}_{st}) \right\rangle \tag{87}$$

The effective stiffness can be obtained using Eq. (14) as

$$C^*_{ijkl} = \left\langle C_{ijmn} + C_{ijkl} H^{mn}_{(k,l)} \right\rangle \tag{88}$$

9 Theoretical Connections of RVE Analysis, MHT and MSG

To show the theoretical connections among RVE analysis, MHT, and MSG, we need to first to change the formulation of the RVE analysis with periodic boundary conditions. From Eq. (42), we can obtain

$$u_i = \chi_i + y_j \bar{\varepsilon}_{ij} \tag{89}$$

Then the strain field within the RVE can be obtained as

$$\varepsilon_{ij} = \chi_{(i,j)} + \bar{\varepsilon}_{ij} \tag{90}$$

Substituting the constitutive relations in Eq. (8) along with the infinitesimal strain in Eq. (90) into Eq. (3), we can obtain the following displacement-based formulation for the RVE analysis

$$\left(C_{ijkl}(\bar{\varepsilon}_{kl} + \chi_{k,l})\right)_{,j} = 0 \tag{91}$$

with χ_i being periodic. This differential equation is the exactly same as that obtained by MSG in Eq. (85), and that obtained by MHT in Eq. (66) with a simple change of variable $u_k^1 = \chi_k$. In other words, for a heterogeneous material featuring a 3D RVE with periodic boundary conditions, RVE analysis, MHT and MSG will provide exactly the same results for both effective properties and local fields.

As far as efficiency is concerned, computing the complete stiffness matrix, RVE analysis requires solving the six static problems because the coefficient matrix of the linear system is affected by the coupled equation constraints used to apply the periodic boundary conditions. MHT and MSG can be implemented using the finite element method so that the linear system will be factorized once and solve for six load steps. Theoretically speaking, MHT and MSG could be five to six times more efficient than RVE analysis.

However, such equivalence does not exist for situations when periodic boundary conditions cannot be applied. MHT is not appicable for such cases. RVE analysis and MSG can still use whatever boundary conditions are appropriate but the results will differ from each other.

For materials featuring lower-dimensional heterogeneities such as binary composites or continuously reinforced composites, RVE analysis and MHT can only obtain properties and local fields with the same dimensionality as that of the RVE, while MSG can still obtain the complete set of 3D properties and local fields out of a 1D or 2D analysis. The main reason is that numerical implementation of MHT and RVE are based on weak form converted from the strong form of the boundary value problem in Eq. (66) and Eq. (43), while MSG directly solve the variational statement in Eq. (84).

MSG has the capability to directly construct models for beams/plates/shells based on the same principle of minimum information loss which is different from the RVE analysis and MHT although it is possible to modify RVE analysis and MHT to construct models for beams/plates/shells.

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