Differences between VAMUCH and FEA-based Micromechanics Approaches

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I. Introduction

The purpose of this short note is to articulate the differences between VAMUCH and FEA-based micromechanics approaches. VAMUCH stands for a new micromechanics approach, namely *variational asymptotic method for unit cell homogenization*, recently developed by the author and his student (Tian Tang). FEA-based approaches carry out a conventional finite element analysis of a RVE (or unit cell) with specially designed boundary conditions under specifically designed loads. Although VAMUCH is as versatile as FEA-based approaches, VAMUCH is dramatically different from FEA-based approaches, both from the view point of theoreticians and from the view point of practicing engineers.

II. Differences from the View Point of Theoreticians

Taking advantage of the smallness of the microstructure of heterogeneous materials, VAMUCH formulates a variational statement of the unit cell through an asymptotic analysis of the energy functional by invoking only two essential assumptions within the concept of micromechanics of heterogeneous materials with identifiable UCs.

- **Assumption 1** The exact solutions of the field variables have volume averages over the UC.
- **Assumption 2** The effective material properties obtained from the micromechanical analysis of the UC are independent of the geometry, the boundary conditions, and loading conditions of the macroscopic structure, which means that effective material properties are assumed to be the intrinsic properties of the material when viewed macroscopically.

Please note these assumptions are not restrictive. The mathematical meaning of the first assumption is that the exact solutions of the field variables are integrable over the domain of UC, which is true almost all the time. The second assumption implies that we can neglect the size effects and loading effects of the material properties in the macroscopic analysis, which is an assumption often made in the conventional continuum mechanics. Note to deal with nonlinear materials, one has to relax the second assumption. *All the other assumptions such as particular shape and arrangement of the constituents, specific boundary conditions, and prescribed relations between local fields and global fields are convenient but not essential.*

It has shown that the governing differential equations of Mathematical Homogenization Theory (MHT), which achieves the best available accuracy for periodic composites, can be derived from the variational statement of VAMUCH.[1] The main differences between VAMUCH and MHT are:

- The periodic boundary conditions are derived in VAMUCH, while they are assumed *a priori* in MHT. MHT also assumes periodic functions, which is shown to be unnecessary in VAMUCH.

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- The fluctuation functions are determined uniquely in VAMUCH, while they can only be determined up to a constant in MHT.
- VAMUCH has an inherent variational nature which is convenient for numerical implementation, while virtual quantities should be carefully chosen to make MHT variational as shown in [2].

Although the theory of VAMUCH can be compactly written as the variation of a functional, it is easier to look at the corresponding differential statement derivable from the variational statement to find out the theoretical differences between VAMUCH and FEA-based approaches. The corresponding differential statement of VAMUCH for elastic materials includes the following governing differential equation (GDE) and boundary conditions.

$$\frac{\partial}{\partial y_l} C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) = 0 \quad \text{in} \quad \Omega \tag{1}$$

$$\chi_i(\mathbf{x}; d_1/2, y_2, y_3) = \chi_i(\mathbf{x}; -d_1/2, y_2, y_3) \tag{2}$$

$$\chi_i(\mathbf{x}; y_1, d_2/2, y_3) = \chi_i(\mathbf{x}; y_1, -d_2/2, y_3) \tag{3}$$

$$\chi_i(\mathbf{x}; y_1, y_2, d_3/2) = \chi_i(\mathbf{x}; y_1, y_2, -d_3/2) \tag{4}$$

$$C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_1 = d_1/2} = C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_1 = -d_1/2} \tag{5}$$

$$C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_2 = d_2/2} = C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_2 = -d_2/2} \tag{6}$$

$$C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_3 = d_3/2} = C_{ijkl} \left(\bar{\epsilon}_{ij} + \chi_{(i|j)} \right) |_{y_3 = -d_3/2} \tag{7}$$

$$\langle \chi_i \rangle = 0 \tag{8}$$

where Eq. (1) is the governing differential equations, Eqs. (2)-(4) are the periodic boundary conditions for fluctuation functions, and Eqs. (5)-(7) are the periodic boundary conditions for local stresses. All these equations are identical to those of MHT, as listed in [3] except Eq. (8) which ensures a unique solution for the fluctuation functions χ_i.

The GDE of FEA-based approaches for elastic properties is the 3D equilibrium equation without body force

$$\frac{\partial}{\partial y_l} C_{ijkl} \left(u_{i,j} + u_{j,i} \right) = 0 \quad \text{in} \quad \Omega \tag{9}$$

Comparing this equation with the VAMUCH GDE in Eq. (1), one clearly observes that the fundamental variables of VAMUCH are fluctuation functions while those of FEA-based approaches are the macroscopic displacements. Furthermore, the boundary conditions for FEA-based approaches are applied on the macroscopic variables such as displacements. Different sets of displacement boundary conditions are needed for calculating different properties. Since these boundary conditions are applied a priori based on engineering intuition, it is not surprising to find out that different researchers introduced different boundary conditions for calculating the same property, see Ref. 4 for a detailed discussion on the boundary conditions for RVE. It is known that the predicted effective properties are very sensitive to boundary conditions. Another theoretical difference is that the dimensionality of VAMUCH analysis is based on the periodicity of the microstructure. For example, we can use 1D UC to model binary composites, 2D UC to model fiber reinforced composites, and 3D UC to model particle reinforced composites. No special treatment is necessary for these different types of microstructures. However, it is not the case with FEA-based approaches, to get the complete set of 3D material properties, one has to use 3D UCs, let it be a binary composite, fiber reinforced composite, or particle reinforced composite. For example, according to the author's understanding, Sun and Vaidya[4] derived the most rigorous FEA-based approach for elastic properties, which requires 3D RVE for fiber reinforced composites.

III. Differences from the View Point of Practicing Engineers

Although there are significant theoretical difference between VAMUCH and FEA-based approaches, practicing engineers are usually more concerned with the convenience and efficiency. To use a FEA-based approach, one has to carry out multiple runs with different sets of boundary conditions and external loads for predicting different material properties. And postprocessing steps such as averaging stresses or averaging strains are needed for calculating the effective properties. If one is also interested in the local fields within the microstructure, one more run is necessary to predict local stress/strain field if the global stress/strain state is different from that used to obtain the effective properties. Comparing to FEA-based approaches, VAMUCH has the following advantages:

1. VAMUCH can obtain the complete set of material properties within one analysis without applying any load and any boundary conditions, which is far more efficient and less labor intensive than those approaches requiring multiple runs under different boundary and load conditions. It is also noted that VAMUCH can even obtain the complete set of 3D material properties using a one-dimensional analysis of the 1D UC for binary composites. It is impossible for FEA-based approaches.

2. VAMUCH calculates effective properties and local fields directly with the same accuracy as the fluctuation functions. No postprocessing calculations which introduce more approximations, such as averaging stress and electric displacement field, are needed, which are indispensable for FEM-based approaches.

3. VAMUCH can recover the local fields using a set of algebraic relations obtained in the process of calculating the effective properties. Another analysis of the microstructures which is needed for FEA-based approaches is not necessary for VAMUCH.

It is also emphasized here that VAMUCH calculation is conceptually different from automating the multiple runs including postprocessing steps of FEA-based approaches using a macro language such as APDL of ANSYS. VAMUCH is not just a different postprocessing approach.

IV. Conclusion

At this stage, we are confident to claim that VAMUCH achieves the most mathematical rigor and consequently the best available accuracy with invoking only the very essential assumptions within the micromechanics concept. VAMUCH is as versatile as FEA-based approaches because it can deal with arbitrary UC with arbitrary number of inclusions with arbitrary shape made of general anisotropic material. VAMUCH is much more convenient and efficient than FEA-based approaches. In fact, one just needs to provide a mesh with corresponding constituent properties, VAMUCH will produce the complete set of material properties with one run, which takes just a very small faction of both the model preparation time and the computational time of a FEA-based approach. Also to obtain the complete set of properties of fiber reinforced composites or binary composites, FEA-based approaches need to use 3D UC, while VAMUCH will only need to use 2D UC and 1D UC, respectively. The time saving in this dimensionality reduction is dramatic.

References

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