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A micromechanics theory for homogenization and dehomogenization of aperiodic heterogeneous materials

Bo Peng, Wenbin Yu*

School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907-2045, USA

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ABSTRACT

Based on the recently discovered mechanics of structure genome, a micromechanics theory is developed for computing the effective properties and local fields of aperiodic heterogeneous materials. This theory starts with expressing the displacements of the heterogeneous material in terms of those of the corresponding homogeneous material and fluctuating functions. Integral constraints are introduced so that the kinematics including both displacements and strains of the homogeneous material can be defined as the average of those of the heterogeneous material. The principle of minimum information loss is used along with the variational asymptotic method to formulate the governing variational statement for the micromechanics theory. As this theory does not require conditions applied on the boundaries, it can handle microstructures of arbitrary shapes. This theory can also straightforwardly model periodic materials by enforcing the equality of the fluctuating functions on periodic edges. This theory provides a rational approach for avoiding the difficulty of creating periodic meshes and automatically captures finite dimension effects. Furthermore, this theory can model heterogeneous materials with partial periodicity. We have used several examples to verify and demonstrate the capability of this theory.

1. Introduction

Micromechanics seeks to model heterogeneous material as an equivalent homogenous material which includes predicting the effective macroscopic properties, commonly called homogenization, and predicting the local fields such as stress and strain fields within the microstructure from the macroscopic behavior, commonly called dehomogenization or localization. Dehomogenization is very important for evaluating the strength of heterogeneous materials.

In addition to the governing equations established in continuum mechanics, most micromechanics models need to choose an analysis domain, commonly called the representative volume element (RVE), and prescribe boundary conditions (BCs). On one hand, RVE must be large enough to be representative, while on the other hand, it must be small enough to be justified as a material point for the macroscopic structural analysis. For periodic materials, the smallest RVE can be the repeating unit cell (UC) of the material if periodic boundary conditions (PBCs) are applied. For aperiodic materials, RVEs are usually chosen out of practical considerations despite the requirements of a rigorous RVE based on the ergodic principle.

The current study consists of two concerns. The first concern is the constraints applied on a RVE. The boundary conditions we can apply to a RVE is governed by the Hill-Mandel macrohomogeneity condition so that the homogenized material is energetically equivalent to the original heterogeneous material under the assumed boundary conditions. Three types of boundary conditions satisfying the Hill-Mandel macrohomogeneity condition are commonly used: statically uniform boundary conditions (SUBCs), kinematically uniform boundary conditions (KUBCs), and PBCs. Pindera et al. [1] summarized the literature which numerically investigated the influence of the RVE size and boundary conditions. SUBCs and KUBCs lead to lower and upper estimates of the effective properties, respectively, compared to PBCs. In addition, predictions using SUBCs and KUBCs converge to those of PBCs with increasing analysis domain size. Mesarovic and Padbidri [2] proposed Minimal Kinematic Boundary Conditions (MKBCs) with linearized kinematics for simulations of disordered microstructures based on the Cauchy continuum. It has later been proved that the first-order homogenization schemes based on the MKBCs predicts uniform traction on the boundary of RVE if no body force is included [3]. Blanco et al. [4] proposed a generalized unified micromechnics theory, in which the Hill-Mandel condition is reformulated as the principle of multiscale virtual power by requiring the virtual power of the heterogeneous materials to be the same as the virtual power of the homogenized material. This principle is used to study various nonlinear problems such as dynamics, high order strain effects, and material failure.

In the other aspect, the standard way of implementing PBCs requires

* Corresponding author.
E-mail address: wenbinyu@purdue.edu (W. Yu).

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identical meshes on opposite RVE boundaries, which cannot always be guaranteed, resulted in non-periodic meshes. Larsson et al. [5] proposed a weak enforcement of PBCs. The BCs are applied by independent finite element discretization of boundary tractions, which allows for a parameterized transition between the strongest form (PBCs) to the weakest form (SUBCs). Nguyen et al. [6] developed a method to apply PBCs based on polynomial interpolation of the displacement field of two opposite RVE sides. Glüge et al. [7] proposed a generalized framework of the three classical BCs based on partitioning of the boundary of the RVE which allows smoothly adjusting the stiffness of the RVE. This method can also be used in spherical RVE which has shown a better convergence regarding to the effective material behavior as the RVE size increases when compared with cubical RVE [8]. Surface-to-surface constraints [9] can be used to apply PBCs approximately in ABAQUS, which is currently available in the micromechanics plugin of SIMULIA [10], also allowing multiple part meshes. Similar function has also been developed by Jacques et al. [11] in their in–house developed ORAS software. All of these methods require special treatment on the nodes at the RVE boundaries.

Another concern in multiscale simulation is the selection of RVE. For the dimensional reducible structures with one or two dimensions much smaller than the remaining dimensions (such as plates/shells or beams), since the periodicity does not exist in all the three directions, the finite cross-section dimensions of beams and the finite thickness of plates/shells should be considered, we call them as finite dimension effect for simplicity. Wang et al. [12] solved the axial Young's modulus of beam and Nasution et al. [13] solved the in-plane effective properties including Young's modulus, Poisson's ratio and coefficients of thermal expansion. In both papers, asymptotic homogenization method (AHM) is used, the periodic boundary conditions are only applied in the remaining dimensions of the homogenized beam/plate model while the traction-free boundary conditions are applied in the other dimensions. Therefore the other effective properties cannot be retrieved due to the absence of the constraints associated with the aperiodic directions. To obtain all the effective properties, Espadas-Escalante et al. [14] studied woven composites using mixed BCs in which PBCs are applied in the in-plane directions of the unit cell and uniform tractions are applied in the thickness direction.

In this paper, we developed a theory based on the recently discovered mechanics of structure genome (MSG) [15]. This theory starts with expressing the displacements of the heterogeneous material using the displacements of the corresponding homogeneous material and fluctuating functions. Integral constraints are introduced so that the kinematics including both displacements and strains of the homogeneous material can be defined as the average of those of the heterogeneous material. The principle of minimum information loss (PMIL) is used along with the variational asymptotic method to formulate the micromechanics theory. As this theory does not require conditions applied on the boundaries, it can handle microstructures of arbitrary shapes. This theory can also straightforwardly model periodic materials by enforcing the equality of the fluctuating functions on periodic edges. This theory also provides a rational approach for avoiding the difficulty of creating periodic meshes and automatically captures finite dimension effects. Furthermore, this theory can model heterogeneous materials with partial periodicity. We have implemented this theory using the finite element method into the general-purpose multiscale constitutive modeling code called SwiftComp™. A few typical examples including periodic materials, aperiodic materials, and partially periodic materials are studied to verify and demonstrate the capability of this theory and the companion SwiftComp™ code.

2. Formulation of the micromechanics theory

2.1. Concept of structure genome

SG [15] generalizes from the RVE or unit cell concepts in micromechanics with the two fundamental differences. First, SG allows a direct connection with macroscopic structures such as beams, plates, and shells so that one can compute equivalent structural properties such as bending stiffness and torsional stiffness from a SG. Second, it is the smallest mathematical building block of the structure. As long as one can use a domain to mathematically construct the heterogenous material, this domain can be chosen as a SG. For example, if the macroscopic structural analysis uses a three-dimensional (3D) model (Fig. 1), SG is not necessarily 3D and its dimensionality depends on the heterogeneity of the microstructure. If the structure is heterogeneous in one direction, such as a layered composite, we can choose the SG to be a straight line because one can sweep this line in both in-plane directions to mathematically construct the layered composite, then we can repeat the layered composite out of plane to build the entire structure. For a structure having a microstructure featuring two-dimensional (2D) heterogeneity such as unidirectional fiber reinforced composites, one can

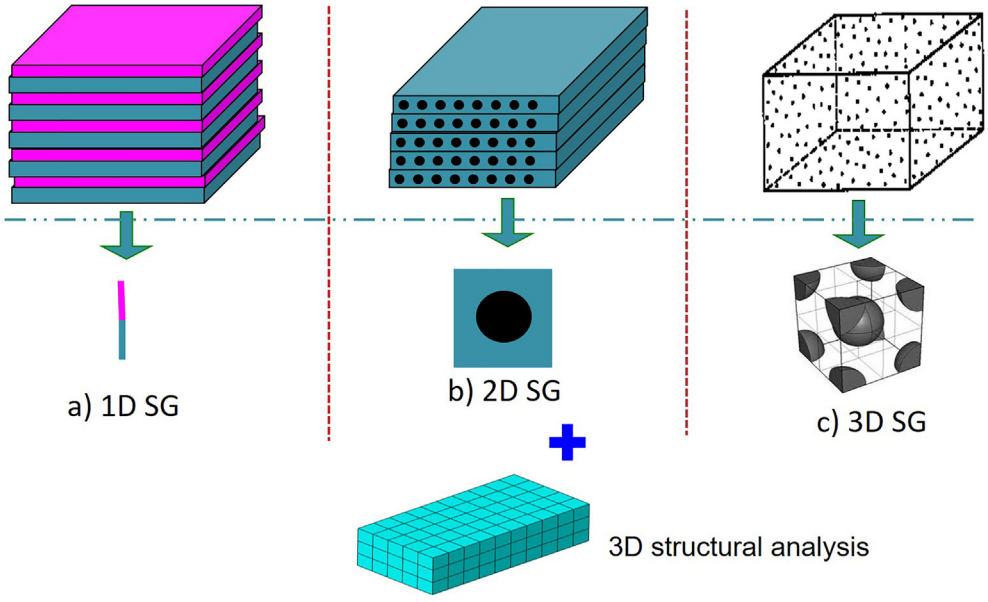

Fig. 1. SG for 3D structure (cited from Ref. [15]).