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Exterior statistics based boundary conditions for representative volume elements of elastic composites

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ABSTRACT

Statistically equivalent representative volume elements or SERVEs are representations of the microstructure that are used for micromechanical simulations to generate homogenized material constitutive responses and properties (Swaminathan et al., 2006a; Ghosh, 2011). Typically, a SERVE is generated from the parent microstructure as a statistically equivalent region, whose size is determined from the requirements of convergence of macroscopic properties. Standard boundary conditions, such as affine transformation-based displacement boundary conditions (ATDBCs), uniform traction boundary conditions (UTBCs) or periodic boundary conditions (PBCs) are conventionally applied on the SERVE boundary for micromechanical simulations. However, when the microstructure is characterized by arbitrary, nonuniform distributions of heterogeneities, these simple boundary conditions do not represent the effect of regions exterior to the SERVE. Improper boundary conditions can result in significantly larger than optimal SERVE domains, needed for converged properties. In an attempt to overcome the limitations of the conventional boundary conditions on the SERVE, this paper explores the effect of boundary conditions that incorporate the statistics of the exterior region on the SERVE of elastic composites. Using Green's function based interaction kernels, coupled with statistical functions of the microstructural characteristics like one-point and two-point correlation functions, a novel *exterior statistics-based boundary condition* or ESBC is derived for the SERVE. The advantages of the ESBC are established by comparing with results of simulations using conventional boundary conditions. Results of the SERVE simulations subjected to ESBCs are also compared with those from other popular methods like statistical volume element (SVE) and weighted statistical volume element (WSVE). The proposed ESBCs offer significant advantages over other methods in the SERVE-based analysis of heterogeneous materials.

1. Introduction

Composite materials have gained wide commercial acceptance due to their superior effective thermal and mechanical properties. These properties depend not only on properties of individual constituents but also on the local microstructural morphology like fiber volume fraction, inclusion size and shape, and spatial dispersion of fibers. Effective properties are

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Nomenclature

RVE	representative volume element
SERVE	statistically equivalent representative volume element
ESBC	exterior statistics-based boundary condition
ATDBC	affine transformation-based displacement boundary condition
UTBC	uniform traction boundary condition
PBC	periodic boundary condition
SIGF	statistically informed Green's function
SVE	statistical volume elements
WSVE	weighted statistical volume element
MVE	microstructural volume element

evaluated by methods of homogenization or averaging of microscopic variables like stresses and strains, with various assumptions on the representative microstructural domain. A number of analytical models have evolved within the framework of small deformation elasticity theory (Eshelby, 1957; Benvensite, 1987; Hill, 1965; Hashin and Shtrikman, 1963; Hashin, 1983; Mura, 1987) to predict homogenized macroscale constitutive response of heterogeneous materials. Their underlying principle is the Hill–Mandel condition of homogeneity (Hill, 1965, 1967; Mandel, 1971), which states that for largely separated microscopic and macroscopic length scales, the volume-averaged strain energy is obtained as the product of the volume-averaged stresses and strains in representative microstructural domain. Hierarchical models, involving computational micromechanical analysis, have become increasingly popular for transfer of information from lower to higher scales, usually in the form of effective material properties (Böhm, 2004; Chung et al., 2000; Fish and Shek, 2000; Ghosh et al., 1995, 1996; Guedes and Kikuchi, 1991; Kouznetsova et al., 2002; Terada and Kikuchi, 2000; Ghosh, 2011; Willoughby et al., 2012). A number of hierarchical models incorporate the asymptotic homogenization theory with computational micromechanics models, based on scale-separation with assumptions of macroscopic homogeneity and microscopic periodicity. Uncoupling of governing equations at different scales is achieved through the incorporation of specific boundary conditions, e.g. uniform displacement, periodicity, etc., on the microscopic *representative volume elements* or RVEs. FE^2 multi-scale methods in Feyel and Chaboche (2000) solve micro-mechanical RVE models for every element integration point in the computational domain to obtain homogenized properties.

Determination of effective material properties necessitates the establishment of a microstructural representative volume element or RVE (Stroeven et al., 2004; Thomas et al., 2008; Heinrich et al., 2012). The concept of RVE was introduced in Hill (1963) as a microstructural subregion that is representative of the entire microstructure in an average sense. This was extended in Hashin and Shtrikman (1963), Jones (1975), and Drugan and Willis (1996) to a reference volume that is small compared to the entire body, for which the volume average of state variables such as strains, stresses, etc., may be taken to be the same as those for the entire body. The RVE can vary with the material property of interest, even for the same microstructure. A large number of studies have been conducted with unit cells as the RVE, consisting of a single heterogeneity in a regular (square, cubic, hexagonal, etc.) matrix (Zeman and Sejnoha, 2007). The underlying assumption in these studies is that the microstructure is a uniform, periodically repetitive array of heterogeneities and the body is subjected to homogeneous boundary conditions. The occurrence of perfect uniformity or periodicity is however rare for many heterogeneous microstructures, as shown in the composite microstructure of Fig. 1(a) (Shan and Gokhale, 2002). For these non-uniform microstructures it is difficult or even impossible to identify RVEs following the strict definitions. In these cases, it is important to identify *statistically equivalent RVEs* or SERVEs for meaningful simulation of microscopic regions. Methods of identifying the SERVE from morphological considerations, using a combination of statistical and computational analyses, have been proposed in Swaminathan et al. (2006a,b) and Ghosh (2011). The SERVE is identified as the smallest, statistically equivalent region of the microstructure, e.g. the micrograph in Fig. 1, that exhibits the following characteristics.

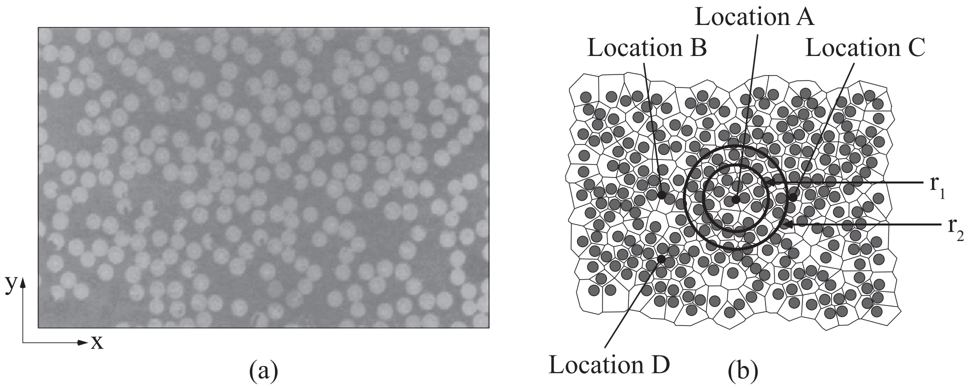

Fig. 1. (a) Optical micrograph of a fiber-reinforced composite microstructure; (b) computer simulated microstructure tessellated into Voronoi cells showing microstructural RVE regions.