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A random field-based method to estimate convergence of apparent properties in computational homogenization

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Highlights

- Convergence rate of apparent properties in computational homogenization is computed.
- Rate is determined from analysis of only one statistical volume element size.
- Higher order terms affecting variance of apparent properties are derived.
- Omission of higher order terms leads to extrapolation errors in predicting RVE size.
- Methodology is demonstrated for a 3D crystal plasticity finite element model.

Abstract

This work addresses the challenge of efficiently determining the representative volume size in computational homogenization by exploiting the requirement that mechanical response quantities are statistically homogeneous and ergodic random fields. The proposed computational homogenization approach focuses on empirically determining the autocorrelation functions of output response quantities through post processing finite element analyses. Once the autocorrelation functions are known, only trivial computations are needed to determine the variance of apparent properties as a function of domain size without any additional finite element computation by utilizing a simple formula relating the autocorrelation function to the variance of spatially averaged quantities. This approach improves upon the current established approach by circumventing the need to analyze numerous successively larger domains in order to determine convergence of apparent properties, which can be computationally prohibitive. Furthermore, similar previous analytical expressions for the variance of apparent properties are asymptotic with respect to domain size while the expression in the proposed approach is exact. After presenting the formulation, the method is first demonstrated for a one-dimensional bar model where analytical expressions can be derived. Then the approach is demonstrated on two numerical examples: (1) a plane strain, linear elastic domain with a lognormal random field describing its compliance, and (2) a stochastic polycrystalline microstructure of a Nickel super alloy having a crystal plasticity model for its constitutive law.
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Keywords: Computational homogenization; Crystal plasticity; Statistical volume element; Representative volume element; Stochastic simulation

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1. Introduction

Computing and post processing the mesoscale mechanical response through the finite element solution of a boundary value problem (BVP) formulated on the scale of material heterogeneity is of great interest in the areas of computational homogenization, multiscale methods, and, more recently, materials by design. The primary goal of these methods is to relate the effects of material heterogeneity, e.g., polycrystalline morphology, crystallography, and constituents, to macroscopic material properties. For computational homogenization and multiscale methods, mesoscale mechanical response quantities are spatially averaged to obtain macroscopic properties. On the other hand, materials design is primarily focused on relating the effects of underlying deformation mechanisms on mesoscale mechanical response in order to understand how microstructural features give materials their idiosyncratic properties (i.e., microstructure–property correlations [1]).

The mesoscale, as defined in this work, is the smallest length scale that encompasses material heterogeneity with statistical significance, which, for polycrystalline metals, is typically 100 μm to 1000 μm, containing on the order of thousands of grains. For this reason, the mesoscale will be denoted as the microscale for the remainder of this paper. This definition of the microscale, often described as the representative volume element (RVE), leads to an ambiguous definition of its size, which is strongly sensitive to the particular mechanical response quantity of interest. In response, the concept of the statistical volume element (SVE) was introduced by recognizing that spatially averaged response quantities, denoted as apparent properties, are random variables that converge to deterministic quantities asymptotically with respect to the size of the spatial domain of the microscale BVP [2,3]. The random apparent properties are a direct consequence of the stochastic nature of microstructure configurations, notably morphology, crystallography, and constitution.

There is extensive literature in recent years on sampling based methods to compute apparent properties as a function of SVE size, e.g., [4–28]. These methods follow the general framework of simulating numerous statistically equivalent microstructures, solving a BVP under admissible set of BCs satisfying the Hill–Mandel condition, evaluating statistics of the apparent properties, and assessing the number of microstructural features required to obtain convergence of apparent properties to effective properties within some tolerance. For example, in [5] a thorough study was done computing variability of Von-Mises yield criteria through Monte Carlo (MC) simulation for ductile, porous metals using J_2-type plasticity for identically-sized spherical pores of varying number and volume fraction. One of the most commonly recommended procedures to determine RVE size is to observe the decrease in variation of apparent properties by performing MC simulation for increasing SVE sizes [9,12,29]. In [12], an empirical power law form for the variance of apparent properties as a function of SVE size was introduced whose parameters are fit via the series of numerical experiments described above for specifically chosen SVE sizes. This approach, and similar variants (e.g., [9]), are considered to be the only alternative to simply performing MC simulation of the BVP on increasing size SVEs until convergence is obtained. However, this approach is still a prohibitively large computational task for challenging problems and a more efficient means to determine the convergence of apparent to effective properties is desired.

There are numerous sampling-based studies on computational homogenization and only a few have been highlighted above. For a more complete overview, the reader is referred to the review paper [19] for explicit treatment of material randomness, [30] for review of deterministic treatment of classical, second order, and discontinuous homogenization methods, and [6] for general overview of computational homogenization and multiscale methods.

In this paper, the requirement in homogenization theory that micromechanical response quantities are statistically homogeneous random fields is exploited to introduce an efficient and systematic approach to determine convergence of apparent properties as a function of SVE size (e.g., see [19] for a discussion on the requirements of statistical homogeneity and ergodicity in computational homogenization). Micromechanical simulations are performed with the target of obtaining convergence of empirically determined autocorrelation functions of response quantities. Based on these results, the variance of the spatial average of a response quantity, (i.e., apparent property) is easily computed as a function of SVE size. The need to perform repeated, costly experiments of MC simulation of SVEs of increasing size is circumvented. Instead, only one judiciously selected SVE size is required to estimate the random field properties. This SVE size is significantly smaller than the RVE size. Therefore, the main contribution of this paper is the introduction of a more efficient approach to predict the convergence behavior of apparent properties than the established brute-force approach. This novel approach utilizes a simple analytical and exact expression relating the autocorrelation function of a random field with the variance of its spatial average. Additionally, this analytical form reveals that the known convergence rate, which states that the variance of apparent properties is proportional to L^{-d} (e.g., [31]), is only