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Material responses at micro- and macro-scales

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ABSTRACT

Material properties at micro- and macro-scales used in micromechanics and continuum mechanics are random and deterministic and so are the corresponding material responses. We view material properties and responses in continuum mechanics as approximations of those in micromechanics. Our premise is that solutions of problems using material properties at various scales must agree in some sense, e.g., continuum mechanics solutions should match on average micromechanics solutions. Continuum solutions with this property are said to be consistent. Theoretical arguments and numerical examples are presented to demonstrate that the continuum solutions may or may not be consistent and may miss essential features of material response depending on the problem and quantity of interest. The examples include beams with random stiffness and one- and two-dimensional specimens with random conductivity.

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1. Introduction

At small scale, material properties fluctuate randomly in space and can be characterized by random functions calibrated to microstructure images. An example is a Markov random field calibrated to measurements of atomic lattice orientations in aluminum polycrystals [6]. The representative volume element (RVE) and the assumption that the microstructure random field is ergodic provide the link between microscale and continuum descriptions. The size of the RVE is, theoretically, infinite relative to the scale of fluctuation of microstructure properties which means for a polycrystal specimen that its size is much larger than that of the constitutive grains. Material properties at the RVE scale, referred to as bulk, macroscopic, global, or effective properties, are deterministic, do not depend on boundary conditions, and are used to define the constitutive relations at the macroscale, i.e., the scale of continuum mechanics [16] (Chap. 7). Material properties on finite specimens that are large relative to their constituents, referred to as apparent, are random and depend on boundary conditions. These specimens are said to be of the scale of the statistical volume element (SVE).

There are numerous studies on the upscaling of microstructure properties to apparent and effective material properties [2,10,12–15]. They show that averages of apparent properties can be used to develop bounds on effective properties [12,15,13]. For linear elasticity problems, these bounds are in the sense of quadratic forms so that they can only be used to bound global material responses by, e.g., energy norms of the type considered in [17]. To reduce calculations and capture material properties at small scale, it has been proposed to use apparent, rather than effective, material properties for response analysis. The implementation of this approach for linear elastic problems requires to select the SVE size for calculating apparent properties, calculate bounds on effective material properties corresponding to essential and natural boundary conditions, and solve two finite element problems for these bounds. The approach had mixed success because two opposite requirements: small finite elements for numerical accuracy and large finite elements such that the bounds on effective properties based on SVEs of finite element size are not too wide. An extensive study on this matter can be found in [17].

Our work relates closely to existing studies on the dependence of material responses on the resolution used to represent microstructure features. However, we propose a new framework for quantifying differences between material responses at different scales, the framework provided by the theory of stochastic differential equations. In this framework, material responses at different scales are solutions of stochastic/deterministic equations with the same functional form but different coefficients, which depend on the resolution used to represent material properties. The approach is beneficial since the theory of stochastic differential equations provides bounds on differences between solutions of equations with the same functional form but different coefficients, i.e., the case of material responses at different scales. The bounds are obtained from differences between the coefficients of these equations; they are not based on bounds on effective material properties derived from apparent material properties, a common approach in the literature.

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Moreover, the bounds can be constructed on various response metrics so that they can capture differences between local response features, a useful feature since these responses are sensitive to microstructure features [5]. Also, recent advances on practical methods for solving stochastic equations, see, e.g., [8,7] (Chaps. 8 and 9), provide efficient methods for solving complex stochastic problems of the type encountered in micromechanics.

Let $U(x)$ and $u_0(x),\ x \in D$, be micro- and macro-scale material response fields, where D denotes the domain occupied by a material specimen. We assume throughout the paper that the probability law of the random field characterizing the microscale material properties is known and that $U(x)$ is the actual response. The microscale properties are used to infer effective material properties. The continuum mechanics solution $u_0(x)$ is viewed as an approximation of the microscale solution $U(x)$. If body forces and end conditions are deterministic, the micro- and macro-scale solutions are random and deterministic functions, so that it is only possible to compare $u_0(x)$, a deterministic function, with statistics of $U(x)$, a random function.

Our premise is that material responses based on material properties at different scales must agree in some sense, e.g., continuum mechanics solutions should match on average micromechanics solutions, i.e., $u_0(x) = E[U(x)],\ x \in D$, where $E[\cdot]$ denotes the expectation operator. Theoretical arguments and numerical examples are presented to evaluate the performance of the continuum solution $u_0(x)$ as an approximation of the microscale solution $U(x)$. The numerical examples include beams with random stiffness and one- and two-dimensional specimens with random conductivity, and are used to examine the consistency of the continuum solutions and quantify differences between continuum and microscale solutions. We focus on the lack of sensitivity of the continuum solution to some features of the material properties at small scale that affect significantly the microscale solution, e.g., the spatial correlation of the random field models for material properties at small scale, the difference and relationship between apparent and effective properties, and the inability of continuum solution to capture some relevant features of material response.

The following section presents two simple examples illustrating that the characterization of some quantities of interest require high resolution material models rather than bulk properties. Section 3 is somewhat technical. The first part of this section develops bounds on the discrepancy between material responses corresponding to material models with various resolutions and apply them to bound differences between $u_0(x)$ and $U(x)$. The second part of this section constructs approximate solutions $U_{\mathrm{perb}}(x)$ for the special case in which microstructure properties are small random perturbations about effective material properties and shows that $U_{\mathrm{perb}}(x)$ is superior to $u_0(x)$. Section 4 further explores the relationships between $u_0(x)$ and $U(x)$ in the context of two examples, a beam with random stiffness and one- and two-dimensional specimens with random conductivity. Section 5 summarizes our findings on features and limitations of the continuum solution as an approximation of the microscale solution. Concluding remarks are presented in Section 6.

2. Why microscale solutions

Let $\mathcal{D}_0$ and $\mathcal{D}$ denote the operators defining the equations for $u_0(x)$ and $U(x)$. Since $\mathcal{D}$ is a random operator, the microscale solution is a random field whose probability law is defined by this operator, source terms, and boundary conditions. Generally, it is not possible to derive analytically the probability law of $U(x)$. Statistics of $U(x)$ can be inferred from samples of this random field obtained numerically from samples of the random entries of $\mathcal{D}$ by using existing deterministic solvers. The continuum mechanics solution $u_0(x)$ is a deterministic function that satisfies an equation defined by $\mathcal{D}_0$. The operators $\mathcal{D}$ and $\mathcal{D}_0$ have the same functional form but different coefficients, which reflect material properties at small and large scales.

The following two examples show that continuum solutions may or may not be consistent depending on the quantities of interest. The first example discusses a rod with random stiffness in tension. The second examines a parallel systems with random fibers.

Example 1. Consider a rod with length $l > 0$ and random stiffness $A(x),\ 0 \leqslant x \leqslant l$, that is stretched at its ends by unit forces. The rod elongations $U(x)$ and $u_0(x),\ 0 \leqslant x \leqslant l$, satisfy the differential equations $\mathcal{D}[U(x)] := A(x)\,dU(x)/dx = 1$ and $\mathcal{D}_0[u_0(x)] := A_{\mathrm{eff}}\,du_0(x)/dx = 1$ with $U(0) = u_0(0) = 0$, and have the expressions $U(x) = \int_0^x dy/A(y) = \int_0^x B(y)\,dy$ and $u_0(x) = x/A_{\mathrm{eff}},\ 0 < x < l$, where $B(x) = 1/A(x)$ and A_{eff} denotes the effective stiffness. Suppose $B(x)$ is a homogeneous random field and let $\xi_c > 0$ denote its correlation distance. If $\xi_c \gg l$, the samples of $B(x)$ are nearly invariant along the rod so that $U(x) \simeq x\ B_0 = x/A_0$, where B_0 and A_0 denote random variables whose distributions are the marginal distributions of $B(x)$ and $A(x)$, respectively. The other limit, i.e., $\xi_c \ll l$, corresponds to the case in which the stiffness scale of fluctuation is much smaller that the rod length. If $B(x)$ is also ergodic, then $U(x) \simeq x\ E[B(\cdot)]$ for a sufficiently large x and resembles the functional form of the continuum solution $u_0(x) = x/A_{\mathrm{eff}}$. The continuum solution is consistent since it matches the expectation of the microscale solution, i.e., $u_0(x) = E[U(x)] = \int_0^x E[1/A(y)]\,dy = x\ E[1/A(\cdot)]$, provided $1/A_{\mathrm{eff}} = E[1/A(\cdot)] = E[B(\cdot)]$. The latter expectation coincides with the Reuss average, i.e., the limit of the spatial average $(1/l)\int_0^l B(x)\,dx$ as $l \to \infty$ provided the compliance field is ergodic.

The solid heavy lines and the thin dash lines in Fig. 1 show the continuum mechanics solution $u_0(x)$ and 50 samples of the microscale solution $U(x)$ for the homogeneous translation field $B(x) = a + (b-a)\,\Phi(G(x)),\ 0 \leqslant x \leqslant l,\ l = 1$, where $G(x)$ is homogeneous Gaussian field with mean 0 and variance 1. Samples of $G(x)$ have been generated at discrete spatial coordinates $x_i = i\,\Delta x,\ \Delta x > 0$, by the recurrence formula $G_i = \rho G\ i - 1 + \sqrt{1-\rho^2}\ W_i, i \geqslant 1$, where $G_i = G(x_i),\ \{W_i\}$ are independent standard Gaussian variables $N(0,1),\ |\rho| < 1$, and $G_0 \sim N(0,1)$ is independent of $\{W_i\}$. The left and right panels in the figure are for $\rho = 0.7$ and $\rho = 0.99$. The samples of $U(x)$ resemble the continuum mechanics solution $u_0(x)$ for $\rho = 0.99$ in agreement with our previous comments. However, their slopes are random following approximately the distribution of $B(0)$, rather than deterministic and equal to $1/A_{\mathrm{eff}}$. The plots show that the continuum mechanics solutions is consistent, e.g., $u_0(l) = 5.50$ and estimates of $E[U(l)]$ based on 1000 samples of $U(x)$ are 5.5045 for $\rho = 0.7$ and 5.6220 for $\rho = 0.99$. However, the solutions $U(x)$ and $u_0(x)$ can differ significant, e.g., the standard deviations of $U(l)$, which coincides with the square root of the error $E[(U(l) - u_0(l))^2]$, are 0.5795 for $\rho = 0.7$ and 2.1279 $\rho = 0.99$. The distribution of the tip displacement $U(l)$ depends strongly on the relationship between the scale of fluctuation of the compliance field $B(x)$, which is controlled by ρ and the rod length l. This random variable is approximately Gaussian for $\rho \leqslant 0.5$ and non-Gaussian for strong correlations, e.g., estimates of the skewness and kurtosis coefficients of $U(l)$ based on 1000 independent samples are -0.1844 and 3.0114 for $\rho = 0.5$ and -0.0703 and 2.0689 for $\rho = 0.99$.

These results show that the continuum mechanics solution with $A_{\mathrm{eff}} = 1/E[1/A(x)]$ is consistent. However, it provides no information on the variability of $U(x)$ about $u_0(x)$, which depends in a complex manner on the spatial correlation of the stiffness random field. The continuum solution cannot be used to, e.g., design rods with imposed limits on their elongations.

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