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Distribution-enhanced homogenization framework and model for heterogeneous elasto-plastic problems

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ABSTRACT

Multi-scale computational models offer tractable means to simulate sufficiently large spatial domains comprised of heterogeneous materials by resolving material behavior at different scales and communicating across these scales. Within the framework of computational multi-scale analyses, hierarchical models enable unidirectional transfer of information from lower to higher scales, usually in the form of effective material properties. Determining explicit forms for the macroscale constitutive relations for complex microstructures and nonlinear processes generally requires numerical homogenization of the microscopic response. Conventional low-order homogenization uses results of simulations of representative microstructural domains to construct appropriate expressions for effective macroscale constitutive parameters written as a function of the microstructural characterization. This paper proposes an alternative novel approach, introduced as the *distribution-enhanced homogenization framework* or DEHF, in which the macroscale constitutive relations are formulated in a series expansion based on the microscale constitutive relations and moments of arbitrary order of the microscale field variables. The framework does not make any a priori assumption on the macroscale constitutive behavior being represented by a homogeneous effective medium theory. Instead, the evolution of macroscale variables is governed by the moments of microscale distributions of evolving field variables. This approach demonstrates excellent accuracy in representing the microscale fields through their distributions. An approximate characterization of the microscale heterogeneity is accounted for explicitly in the macroscale constitutive behavior. Increasing the order of this approximation results in increased fidelity of the macroscale approximation of the microscale constitutive behavior. By including higher-order moments of the microscale fields in the macroscale problem, micromechanical analyses do not require boundary conditions to ensure satisfaction of the original form of Hill's lemma. A few examples are presented in this paper, in which the macroscale DEHF model is shown to capture the microscale response of the material without re-parametrization of the microscale constitutive relations.

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1. Introduction

Multi-scale modeling is a theme integral to the modeling of heterogeneous multi-phase materials. It offers a tractable means to model sufficiently large spatial domains of heterogeneous media without being impeded by the exorbitant computational overhead incurred due to detailed high-resolution modeling of variations in material morphology at the lower microscopic scale. The ability of these powerful computational methods to resolve material behavior at different scales and communicate across them is fostering unprecedented advances in multi-scale modeling. These models provide in-depth understanding of material deformation and failure that brings new insights to the integrated computational structure-material engineering paradigm.

Within the domain of computational multi-spatial scale analyses, two categories of methods have emerged, depending on the nature of coupling between the scales, namely, "hierarchical" and "concurrent" models. Hierarchical models enable bottom-up coupling for unidirectional transfer of information from lower to higher scales. The information transferred is usually in the form of effective material properties. This type of model is depicted in Fig. 1, where information about the polycrystalline microstructure would be used at the macroscale to determine the effective material response at a point in the macroscopic domain.

A number of different methods to achieve this transfer have been developed in the literature. Analytical models have been developed, e.g. for linear elasticity, to evaluate effective constitutive quantities at the macroscale based on characterization of the microstructure. However, microscale solutions are known analytically only for a very limited class of problems. The canonical example of this type of homogenization is the effective medium theory introduced by Eshelby (1957) to deal with isotropic ellipsoidal inclusions in an otherwise homogeneous isotropic medium. Other methods based on this approach can provide good approximations of certain material properties for simple microstructures, e.g. Mori and Tanaka (1973) and Mura (1987). These approaches are applicable to linear constitutive relations and simple inclusion/matrix morphologies. Extensions to a limited class of nonlinear materials have been achieved in the variational framework proposed in Ponte Castañeda (1991, 1992). This approach establishes absolute bounds for some nonlinear composites. The self-consistent method, originally developed by Kröner (1958) and Budiansky and Wu (1962), has been extended to the polycrystalline problems in Lebensohn and Tomé (1993), which simultaneously satisfies compatibility and equilibrium between each phase of a material and its surrounding homogeneous medium.

A subset of the hierarchical models has been branded as the "FE^2 multi-scale methods" by Feyel and Chaboche (2000) and Kouznetsova et al. (2001), where micro-mechanical RVE or unit cell models are solved in every increment to obtain homogenized properties for macroscopic analysis. The model does not require a closed form macroscale constitutive relation, rather, this relationship is implicit in the transfer of information from the microscale to the macroscale. However, this method can be very expensive, as it entails solving the RVE micromechanical problem for every element integration point in the computational domain. The macroscale discretization must be sufficiently coarse to achieve a computational advantage over a fully microscale discretization of the entire domain.

To overcome the limitations of prohibitive computational overhead, explicit forms for the macroscale constitutive relations have been developed in Ghosh et al. (2007) and Keshavarz and Ghosh (2015) from homogenization of RVE response at microscopic scales. This requires determination of the functional forms of the macroscale constitutive parameters with

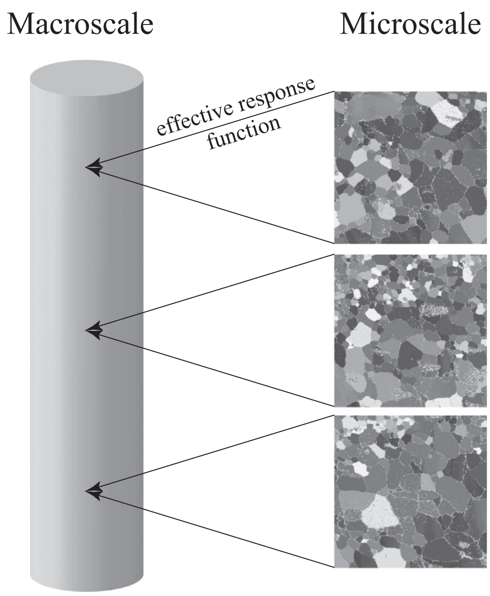

Fig. 1. Schematic representation of a hierarchical multi-scale model.