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Novel formulations of microscopic boundary-value problems in continuous multiscale finite element methods

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Abstract

This article explores the use of a homogenization method inspired by the classical Irving–Kirkwood procedure in the continuous multiscale modeling of elastic solids within the context of the finite element method. This homogenization method gives rise to a broad range of allowable boundary conditions for the RVE, which, in turn, yield a rich spectrum of estimates of the macroscopic stress response for two representative problems involving heterogeneous elastic bodies.
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1. Introduction

Many natural and engineered solids exhibit complex heterogeneous microstructures which may be challenging to characterize using classical macroscopic material constitutive laws. One approach in modeling such materials is to assume that macroscopic variables, such as stress and heat flux, are locally determined via homogenization of the appropriate microscopic variables. When both the macroscopic and the microscopic scale can be accurately analyzed using continuum modeling, computational homogenization may be effected by means of the so-called FE^2 method [1–5]. This explicitly resolves the material microstructure at select macroscopic points (which typically correspond to integration points of the macroscopic finite element mesh) using a finite element-based representative volume element (RVE), thus circumventing the need for full finite element resolution of the entire microstructure in a single scale. In recent years, the FE^2 method has been applied with success to polycrystalline materials [6], materials with voids [7], fiber-reinforced composites [8], and fabrics [9], as well as materials exhibiting coupled thermomechanical response [10] or microstructural phase transition [11].

The Hill–Mandel criterion [12,13] forms the theoretical basis of the vast majority of continuous multiscale modeling implementations to date. This criterion comprises intuitive *a priori* assumptions relating stress, deformation and virtual work across scales. Notwithstanding its widespread use, the Hill–Mandel criterion has several significant limitations. First, boundary conditions imposed on the RVE in the microscale must be consistent with the Hill–Mandel

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assumptions, resulting in a limited set of allowable such boundary conditions. Since the homogenized material response may depend strongly on the specific choice of RVE boundary conditions [14,15], this limitation may lead to inaccurate approximation of the true homogenized material response, especially when the latter deviates from periodicity (e.g., near exterior boundaries or interior surfaces of discontinuity). Second, the Hill–Mandel assumptions presume a quasi-static microscale relative to the macroscale dynamics based on time-scale separation arguments [11], which precludes the study of microscale inertial effects. Finally, the Hill–Mandel criterion appears to have no direct extension to thermal variables, thus necessitating the introduction of additional assumptions for thermomechanical homogenization problems. As Hill himself observed in connection with the definition of the macroscopic deformation and stress [13]: "It is not necessary, by any means, that macro-variables so defined should be unweighted volume averages of their microscopic counterparts. However, variables that do have this special property are naturally the easiest to handle analytically in the transition between levels". Indeed, there is no fundamental principle underlying the assumptions of the Hill–Mandel criterion other than analytical ease and conceptual plausibility.

Recently, a general continuum homogenization theory has been proposed [16] which is inspired by the classical Irving–Kirkwood procedure for upscaling atomistic variables to the continuum level [17]. The governing principle of this theory is that only fundamental extensive quantities of continuum thermomechanics (here, mass, momentum, and energy) should be volume-averaged over the microscale. As long as the continuum balance laws apply at both scales, this theory gives rise to expressions for the macroscopic stress and heat flux in terms of the microscopic kinematic and kinetic variables. The general framework of this theory allows the freedom to derive a broad range of RVE boundary conditions that communicate to the microscale sufficient evidence of the local macroscopic deformation, as well as to investigate the role of microscale thermal and inertial effects in the homogenized material response. Within the general theory, this article explores the RVE boundary-value problem and, in particular, the development of novel handshake conditions for the purely mechanical homogenization problem which transcend the Hill–Mandel criterion. Such conditions are formally derived both for finite and infinitesimal deformations and their practical implementation is considered within the context of the finite element method. In addition, it is shown that these conditions yield homogenized responses that differ from those obtained from the imposition of displacement, traction and periodic boundary conditions that are compatible with the Hill–Mandel criterion.

The remainder of this article is organized as follows: Section 2 summarizes the important ideas behind the continuum Irving–Kirkwood theory, and demonstrates its generality compared to the Hill–Mandel criterion. In Section 3, novel RVE boundary-value problems are introduced consistently with the continuum Irving–Kirkwood theory, and their finite element implementation is discussed. Section 4 includes two purely mechanical and quasistatic example problems which illustrate the homogenization properties of the proposed RVE boundary-value problems. This is followed by a reflection on the findings in Section 5.

2. Continuum homogenization theory

The theory proposed in [16] based on the classical Irving–Kirkwood procedure offers a rigorous and general approach to continuum homogenization. This theory relies on the following three fundamental assumptions:

1. The material of interest may be approximated as a continuum at the macroscopic and microscopic scales.
2. The conservation laws for mass, momentum, and energy hold at the macroscopic and microscopic scales.
3. Homogenization in the form of weighted averaging is effected on the three principal extensive quantities of continuum mechanics, that is, mass, linear momentum, and energy.

In the remainder of this section, the continuum Irving–Kirkwood theory is summarized and its relation to the Hill–Mandel approach is discussed.

2.1. Continuum balance laws

By way of background, the classical balance laws of continuum mechanics for purely mechanical processes are stated here in both spatial and referential form.

Consider a body $\mathcal{B}$ occupying a region $\mathcal{R}$ at time t. The integral forms of balance of mass and linear momentum for any region $\mathcal{P} \subset \mathcal{R}$ with boundary $\partial\mathcal{P}$ are

$$\frac{d}{dt}\int_{\mathcal{P}} \rho \, dv = 0 \tag{1}$$

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