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Homogenization of high-frequency wave propagation in linearly elastic layered media using a continuum Irving-Kirkwood theory

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ABSTRACT

This article presents an application of a recently developed continuum homogenization theory, inspired by the classical work of Irving and Kirkwood, to the homogenization of plane waves in layered linearly elastic media. The theory explicitly accounts for the effects of microscale dynamics on the macroscopic definition of stress. It is shown that for problems involving high-frequency wave propagation, the macroscopic stress predicted by the theory differs significantly from classical homogenized stress definitions. The homogenization of plane waves is studied to illustrate key aspects and implications of the theory, including the characteristics of the homogenized macroscopic stress and the influence of frequency on the determination of an intermediate asymptotic length scale. In addition, a method is proposed for predicting the homogenized stress field in a one-dimensional bar subjected to a frequency-dependent forced vibration using only knowledge of the boundary conditions and the material's dispersion solution. Furthermore, it is shown that due to the linearity of the material, the proposed method accurately predicts the homogenized stress for any time-varying displacement or stress boundary condition that can be expressed as a sum of time-periodic signals.

1. Introduction

The properties of heterogeneous materials are often characterized in an average or effective sense. This is a particularly relevant approach when the physical length scale of the material heterogeneity is much smaller than the macroscopic body under consideration. Continuum homogenization theories represent one class of methodologies capable of predicting effective material properties from knowledge of the microstructural response. These theories typically assume that the macroscopic material behavior and properties can be defined through volume averages of appropriate microscopic quantities. For example, the seminal paper by Hill (1972) proposes relations between the deformation gradient, stress, and a work-like quantity across scales through volume averages over the microscale. Computational homogenization, which typically uses the finite element method in a multiscale setting, has leveraged these so-called Hill-Mandel relations with success in modeling a variety of heterogeneous materials as homogenized media (Feyel and Chaboche, 2000; Kouznetsova et al., 2001; Miehe et al., 2002; Sengupta et al., 2012).

While the Hill-Mandel homogenization approach is reasonable and has yielded good results in a variety of applications, it is by no means the only way in which homogenization relations may be defined. Recently, a continuum homogenization theory was proposed in which only the principal extensive quantities (mass, momentum, and energy) at a given macroscopic point are defined as weighted averages of their microscopic counterparts in a neighborhood around that point (Mandadapu et al., 2012). This theory is motivated by the seminal work of Irving and Kirkwood (1950), which proposed an upscaling method from atomistics to continuum; as such, it is henceforth referred to as the continuum Irving-Kirkwood theory. The theory is appealing in its reliance on a minimal number of assumptions, its natural extension to thermal processes, and its flexibility in accommodating a richer spectrum of microscopic deformations compared to the Hill-Mandel theory (Mercer et al., 2015). In fact, it is shown in Mandadapu et al. (2012) that the Hill-Mandel theory is recovered from the continuum Irving-Kirkwood theory under an additional set of assumptions.

For the purpose of this work, of particular interest is the definition of homogenized stress in the continuum Irving-Kirkwood

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theory. As shown in Mandadapu et al. (2012), the homogenized stress depends on the volume-averaged microscopic stress as well as a kinetic stress term which accounts for the effect of microscopic dynamics on the macroscopic stress. This kinetic stress term depends on the microscopic velocity fluctuations about the macroscopic velocity at a given point akin to the dependence of pressure on velocity fluctuations in ideal fluids. These fluctuations are negligible when the wavelengths generated by the imposed loading are long compared to the representative size of the material microstructure. However, as these wavelengths become shorter, the contribution of the kinetic stress to the overall stress becomes increasingly dominant. Therefore, a practical problem in which the continuum Irving-Kirkwood theory is indispensable is the homogenization of waves propagating through heterogeneous elastic media at high frequency, where the term "high frequency" is used to indicate a frequency which generates wavelengths whose size is on the order of the characteristic microstructural length scale for a material. The presence of band gaps in these materials is one of the primary reasons for the recent interest in wave propagation in composites and heterogeneous media (Nemat-Nasser and Srivastava, 2011; Shen and Cao, 2000; Sheng et al., 2007).

To better understand the effects of microscale dynamics on the homogenized stress within the context of the continuum Irving-Kirkwood theory, this work relies on analytical solutions of time-harmonic plane wave propagation in infinite media consisting of alternating layers of isotropic linearly elastic material. It is shown that for waves at high frequency, the kinetic stress term becomes dominant, thus establishing its importance in the determination of the macroscopic stress at a given point. Additionally, the existence of an intermediate asymptotic scale is demonstrated, and is shown to depend on both the microstructural length scale and the wavelengths induced by the loading. These scales characterize the size of the averaging region required to yield a converged macroscopic stress.

The utility of the continuum Irving-Kirkwood theory is greatest if it can be applied to predict the homogenized stress response for a given initial boundary-value problem. To this end, such an initial boundary-value problem is posed and a methodology is developed for predicting the homogenized stress field induced by the boundary conditions. This methodology does not rely on a macroscopic mesh, as in the FE^2 approach, since a macroscopic mesh is not capable of efficiently resolving the propagation of the microstructure-sized wavelengths through the system. Rather, the methodology exploits *a priori* knowledge of the analytical solution of plane wave propagation at a particular frequency, as well as the nature of the applied loading, to accurately predict the homogenized stress field.

The organization of this article is as follows: Section 2 summarizes the important aspects of the continuum Irving-Kirkwood theory developed in Mandadapu et al. (2012). In Section 3, the analytical solutions for time-harmonic wave propagation in layered media in one and two dimensions are reviewed, and the salient aspects of the procedure for computing the homogenized stress response is these systems are presented. Section 4 presents a boundary-value problem involving plane wave propagation in one dimension. The problem is first solved using the finite element method to explicitly model the layered microstructure, and subsequently the homogenized stress field is calculated from the resulting solution. A general methodology is then presented for estimating the homogenized stress field without performing the finite element analysis, and excellent agreement between the two methods is obtained. Conclusions are offered in Section 5.

2. Continuum Irving-Kirkwood homogenization theory

The methods used in this work are based on the continuum homogenization theory presented in Mandadapu et al. (2012). In this section, the most important details of this theory are reviewed in the context of purely mechanical processes.

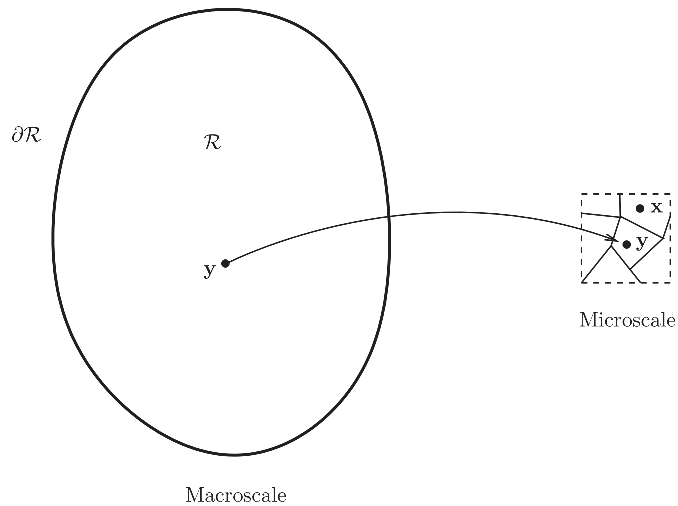

Fig. 1. Schematic of the representation of the two scales, with positions in each denoted by the vectors **y** and **x**.

2.1. Balance laws

Consider a body $\mathcal{B}$ occupying a region $\mathcal{R}$ at time t. It is assumed that there exists a microscopic ("fine") scale and a macroscopic ("coarse") scale with the properties of the latter being derived by homogenization from the former. Additionally, it is assumed that the material can be modeled accurately as a continuum at both scales. A typical macroscopic point will be denoted **y**, and a microscopic point in its neighborhood will be denoted **x**, as in Fig. 1.

Since the material in each scale is assumed to behave as a continuum, the standard continuum balance laws apply to both scales. Specifically, conservation of mass for the macroscale is written as

$$\dot{\rho}^M(\mathbf{y},t) + \rho^M(\mathbf{y},t)\frac{\partial}{\partial \mathbf{y}}\cdot \mathbf{v}^M(\mathbf{y},t) = 0, \tag{1}$$

and for the microscale as

$$\dot{\rho}^m(\mathbf{x},t) + \rho^m(\mathbf{x},t)\frac{\partial}{\partial \mathbf{x}}\cdot \mathbf{v}^m(\mathbf{x},t) = 0, \tag{2}$$

where ρ is the mass density and **v** the velocity. Here and henceforth, superscripts M and m refer to variables in the macroscopic and microscopic scales, respectively. Also, $\frac{\partial}{\partial \mathbf{y}}\cdot(\cdot)$ and $\frac{\partial}{\partial \mathbf{x}}\cdot(\cdot)$ denote the divergence operators in each scale, while $\dot{\overline{(\cdot)}}$ stands for the material time derivative of $(\,\cdot\,)$.

The balance of linear momentum for the macroscale is expressed as

$$\rho^M(\mathbf{y},t)\dot{\mathbf{v}}^M(\mathbf{y},t) = \frac{\partial}{\partial \mathbf{y}}\cdot \mathbf{T}^M(\mathbf{y},t) + \rho^M(\mathbf{y},t)\mathbf{b}^M(\mathbf{y},t), \tag{3}$$

and for the microscale as

$$\rho^m(\mathbf{x},t)\dot{\mathbf{v}}^m(\mathbf{x},t) = \frac{\partial}{\partial \mathbf{x}}\cdot \mathbf{T}^m(\mathbf{x},t) + \rho^m(\mathbf{x},t)\mathbf{b}^m(\mathbf{x},t). \tag{4}$$

Here, **T** is the Cauchy stress and **b** is the body force per unit mass.

In general, all macroscopic variables are functions of **y** and t, and microscopic variables are functions of **x** and t, but these function dependencies may be omitted for brevity in subsequent equations.