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A consistent nonlocal scheme based on filters for the homogenization of heterogeneous linear materials with non-separated scales

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ABSTRACT

In this work, the question of homogenizing linear elastic, heterogeneous materials with periodic microstructures in the case of non-separated scales is addressed. A framework if proposed, where the notion of mesoscopic strain and stress fields are defined by appropriate integral operators which act as low-pass filters on the fine scale fluctuations. The present theory extends the classical linear homogenization by substituting averaging operators by integral operators, and localization tensors by nonlocal operators involving appropriate Green functions. As a result, the obtained constitutive relationship at the mesoscale appears to be nonlocal. Compared to nonlocal elastic models introduced from a phenomenological point of view, the nonlocal behavior has been fully derived from the study of the microstructure. A discrete version of the theory is presented, where the mesoscopic strain field is approximated as a linear combination of basis functions. It allows computing the mesoscopic nonlocal operator by means of a finite number of transformation tensors, which can be computed numerically on the unit cell.

1. Introduction

Classical homogenization theory assumes separation between scales, i.e., that the overall strain and stress fields have a characteristic wavelength which is much larger than that of the microscopic fluctuations fields. When this assumption is not met, e.g., when the wavelength associated with the applied load is comparable with that of strain and stress fluctuations, the material behavior at a point is influenced by the deformation of neighboring points and the assumption of scale separation is no more valid. In that case, homogenized models able to capture the effects of a non-uniform overall strain are required. In addition, the notion of *mesoscopic models* has recently emerged in the literature. By mesoscopic models, we refer to a description of the behavior halfway between a fully (microscopic) detailed one and a fully homogenized (macroscopic) one using a constant effective tensor. In that sense, mesoscopic models correspond to equivalent behaviors when scales are not separated.

Two main classes of approaches have been proposed in the last decades to model homogenized media when scales are not separated.

The first class of methods uses generalized continuum mechanics by including gradient of strain or higher derivatives of the strain. Generalized continuum mechanics theories have been proposed since the works of Toupin (1962), Mindlin (1964) and Mindlin and Eshel (1968). These approaches are phenomenological and do not derive from a micromechanical analysis. Furthermore, they require identifying a large number of coefficients associated with higher-order tensors.

In Kouznetsova et al. (2002), Kouznetsova et al. used an extension of the classical computational homogenization techniques to a full geometrically non-linear gradient approach. Macroscopic equations are derived based on the work of Toupin (1962) and Koiter (1964) for the couple-stress continuum and generalized by Mindlin and Eshel (1968), see also Fleck and Hutchinson (1997) for a full gradient variational principle. In Ostoja-Starzewski et al. (1999), Ostoja-Starzewski et al. and Bouyge et al. (2001) have used the unit cell model with a different type of boundary conditions to calculate the overall moduli and characteristic length of a homogenized couple-stress model composed of classically linearly elastic constituents. de Felice and Rizzi (2001) and Yuan and Tomita (2008) have extended the classical homogenization scheme (Suquet, 1985) based on the Hill-Mandel macro homogeneity condition to the Cosserat medium. Other works (Bouyge et al., 2001; Bouyge et al., 2002; Kouznetsova et al., 2002; Kouznetsova et al., 2004; Yuan and Tomita, 2008) derive the constitutive equations of generalized continuum models through higher-order boundary conditions on the unit cell and use a generalization of the Hill-Mandel condition. As mentioned in Yuan and Tomita (2008), these approaches can lead to unphysical results in some situations due to an over-evaluation of the macroscopic internal energy of the medium. In addition, when the cell is homogeneous, the resulting

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macroscopic behavior remains in some cases a gradient elastic model which is obviously unsatisfying.

In Forest and Sab (1998) Forest and Sab have proposed a framework to derive an effective linear Cosserat continuum from a heterogeneous classical continuum microscopic model, and from a linear Cosserat microscopic model in Forest et al. (1999). In Forest et al. (2001), the asymptotic homogenization method,classically used for periodic heterogeneous materials, has been applied to linearly elastic Cosserat microstructural constituents.

In the case of periodic microstructures, Gambin and Kroener (1989), Boutin (1996), Triantafyllidis and Bardenhagen (1996), and Smyshlyaev and Cherednichenko (2000) have studied the influence of high-order terms of the series expansion on the macroscopic behavior of linear elastic composites, initiated by Bensoussan et al. (1978) and Sanchez-Palencia (1980). When the expansion parameter associated with the length ratio is no more small compared to one, then a rigorous framework can be established to introduce the effects of strain and stress gradients on the local response of heterogeneous composites.

Following Boutin (1996) and Smyshlyaev and Cherednichenko (2000), Tran et al. (2012) proposed a more systematic framework to define the coefficients of strain gradient elasticity in a series expansion framework. At the microscopic scale the phases are locally elastic but as the separation of scales no more holds, the material obeys strain gradient elasticity. The authors have shown that depending on the truncation order, strain gradient theory of Toupin (1962), Toupin (1964), Mindlin (1964), Mindlin and Eshel (1968), or a general theory of Green and Rivlin (1964) can be recovered.

A second class of theories uses nonlocal approaches to model the equivalent homogenized medium. Diener et al. (1981), Diener et al. (1982), Diener et al. (1984) and later Drugan and Willis (1996) derived a nonlocal constitutive model from the Hashin–Shtrikman variational principle. Other approaches provide a nonlocal constitutive equation relating the mean stress and strain fields (Beran and McCoy, 1970; Willis, 1983; Furmanski, 1997). Luciano and Willis (2000) introduced nonlocal constitutive behavior of an infinite laminated composite. The nonlocal elasticity theory can be traced back to Kröner et al. (1972), Kröner (1967) who formulated a continuum theory for classical materials with long range cohesive forces. Eringen (1972), Eringen (1972), Eringen (1976), Eringen and Edelen (1972) produced nonlocal elasticity theories characterizing the presence of nonlocality residues of fields (like body forces, mass, entropy, internal energy...). Eringen and Kim (1974), Eringen et al. (1977) simplified the above mentioned theory for linear homogeneous isotropic nonlocal elastic solids in such a way that the nonlocal theory differs from the classical one in the stress–strain constitutive relations only, with the elastic modulus being a simple function of the Euclidean distance between the strain and stress points. One serious issue is that this theory cannot take into account the presence of cracks or voids in the nonlocal model. In Eringen (1983) Eringen proposed a differential form to compute the nonlocal operator. However, this model is empirical and does not derive from microstructural considerations. In Gao (1999), an asymmetric theory of nonlocal elasticity is provided, and it is shown that the higher gradient model can be deduced from the nonlocal theory. In Polizzotto (2001) a thermodynamic and variational framework is proposed in the context of the nonlocal elasticity theory of Eringen (1972), Eringen (1972), Eringen (1976) and provided a nonlocal FEM based methodology as well as a treatment for the presence of cracks in the nonlocal model by replacing the Euclidean distance by a geodetical distance. A special mention may be made of nonlocal macroscopic behavior described by using wave-vectors dependent behavior in Fourier domain for conduction (Furmanski, 1997), which clearly indicates that separation of scale is no more achieved, but without a clear methodology for describing the kernel appearing in the constitutive behavior.

The framework proposed in this study belongs to the second class of theories, i.e., nonlocal approaches. However, compared to numerous previous works based on a phenomenological approach of the macroscopic behavior, a systematic methodology is provided to derive the nonlocal relations of the effective continuum including naturally all the effects of microstructural constituents. The present methodology then defines a *consistent nonlocal homogenization* procedure, without any empirical model. We first define the mesoscopic fields by means of nonlocal smoothing (filters) operators acting on the fine scale fluctuations of the microscopic fields. Then, we introduce a splitting of the strain field into a mesoscopic (filtered) part and the remaining fluctuation. A localization problem can be defined on a unit cell, as a function of the mesoscopic strain field, which appears as a non-uniform eigenstrain. Using an appropriate Green's tensor, the nonlocal mesoscopic constitutive relationship can be derived.

The paper content is as follows. In Section 2, the definitions of mesoscopic fields and of the localization problem in the context of non-separated scales are introduced. In Section 3, the homogenized quantities are defined, and analogies with classical homogenization are drawn. In Section 4, we show that the present theory matches the classical homogenization when the scales are separated, and that we recover classical (local) elastic media when the material is homogeneous. In Section 5, a discrete theory is provided, to set the problems to be solved in the unit cell in a numerical context. Guidelines for numerical computations are provided, even though finite element implementation details are left to a separated forthcoming study. Numerical examples are presented in Section 6 for illustration.

2. Localization problem for consistent nonlocal homogenization

2.1. Definition of mesoscopic fields through filters

We consider a domain $\Omega \in \mathbb{R}^3$, whose external boundary is denoted by $\partial\Omega$. The material is supposed to be linearly elastic. We assume that the domain Ω is associated with a unit cell of a periodic microstructure characterized by its size whose order is λ and therefore wave-number (or frequency) $\omega = 2\pi/\lambda$. We associate this size to a scale that we call microscopic scale, denoted by $\mathcal{S}$. Now let us define another scale $\hat{\mathcal{S}}$ related to a characteristic wavelength $\hat{\lambda} > \lambda$ and frequency $\hat{\omega} = 2\pi/\hat{\lambda}$, where $\hat{\lambda}$ is not necessarily much larger compared to λ. This characteristic wavelength is representative of an applied loading (external or body forces) on Ω. We denote by $\hat{\boldsymbol{\varepsilon}}(\mathbf{x})$ and $\hat{\boldsymbol{\sigma}}(\mathbf{x})$ the strain and stress fields related to the scale $\hat{\mathcal{S}}$, called *mesoscopic* strain and stress fields. Similarly to the classical homogenization scheme, this mesoscopic field will induce fluctuations at the scale of the microstructure which will have a wavelength λ. The microscopic strain and stress, resulting in superposition of the applied mesoscopic fields and of the local fluctuations in Ω, are denoted by $\boldsymbol{\varepsilon}(\mathbf{x})$ and $\boldsymbol{\sigma}(\mathbf{x})$, respectively.

In the present work, we consider that mesoscopic fields are related to microscopic ones through appropriate low-pass filters, e.g., by means of a convolution product:

$$\hat{\boldsymbol{\varepsilon}}(\mathbf{x}) = \gamma_\alpha(\mathbf{x}) * \boldsymbol{\varepsilon}(\mathbf{x}) = \int_{\Omega_\infty} \gamma_\alpha(\mathbf{x}-\mathbf{y})\boldsymbol{\varepsilon}(\mathbf{y})d\mathbf{y}, \quad (1)$$

$$\hat{\boldsymbol{\sigma}}(\mathbf{x}) = \gamma_\alpha(\mathbf{x}) * \boldsymbol{\sigma}(\mathbf{x}) = \int_{\Omega_\infty} \gamma_\alpha(\mathbf{x}-\mathbf{y})\boldsymbol{\sigma}(\mathbf{y})d\mathbf{y}, \quad (2)$$

where $d\mathbf{y}$ means that integration is carried out with respect to $\mathbf{y}$, and Ω_∞ is the (convex) infinite domain in which Ω is embedded.