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Finite strain mean-field homogenization of composite materials with hyperelastic-plastic constituents

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ABSTRACT

A finite strain mean-field homogenization (MFH) formulation is proposed for a class of composites where multiple phases of solid inclusions or cavities are embedded in a continuum matrix. Local constitutive equations of each solid phase are based on a multiplicative decomposition of the deformation gradient onto elastic and inelastic parts and hyperelastic-plastic stress-strain relations. For the special situation of hyperelastic constituents, a mixed variational formulation is presented which handles both compressible and quasi-incompressible cases within the same framework. A special emphasis is put on the proper definition of various macroscopic stress measures and tangent operators. For an extended Mori-Tanaka MFH model, numerical algorithms were developed and implemented. The MFH predictions were extensively tested against direct finite element simulations of representative volume elements or unit cells, for several heterogeneous microstructures under various loadings.

1. Introduction

The prediction of the influence of the microstructure on the macroscopic or effective properties of heterogeneous materials is important both from scientific and engineering design viewpoints, and the aim of scale-transition methods is to understand and quantify this influence. In continuum mechanics, those methods rely on a separation of scales and belong to one of four categories (see for instance the reviews of Kanouté et al. (2009) and Geers et al. (2010) for references). First, there is the direct finite element (FE) analysis of representative volume elements (RVEs). Second, in the method of cells and subcells (which is related to the transformation field analysis), the RVE or unit cell is discretized with voxels (or pixels in 2D), and the boundary-value problem is solved using different approaches. Third, there is the asymptotic or mathematical theory of homogenization for periodic media, which ends up with problems on a unit cell which need to be solved with FE or voxel methods. The fourth and last category is mean-field homogenization (MFH) which is restricted to microstructures such that multiple phases of solid inclusions or cavities which are supposed to have an ellipsoidal shape are embedded in a continuum matrix. MFH is based on assumed relations between the mean values (volume averages) of strain or stress fields in each phase, and unlike the former three methods, it is not direct and it does not solve for the detailed micro fields. Compared to the three direct full-field methods, MFH is more restricted both in terms of microstructures that it can handle and the results it can

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deliver, however it is much easier to use and its computing time is several orders of magnitude smaller than that of direct scale-bridging methods, especially in the nonlinear regime.

MFH methods are based on the fundamental linear elastic solution developed by Eshelby (1957) for an ellipsoidal subdomain of an infinite matrix undergoing a uniform eigen or transformation strain. In linear elasticity, successful MFH models have been developed based on an approximate use of Eshelby's solution, typical examples being the Mori and Tanaka (1973) model and the self-consistent scheme (Kröner (1958); Hill (1965)).

A significant research effort has been devoted to extending MFH to the nonlinear regime. The major difficulty is that for nonlinear composites, even if each phase's material is homogeneous, the instantaneous stiffness operators are not uniform per phase. Consequently, Eshelby's results and MFH models cannot be extended directly from linear elasticity to the nonlinear realm, and in order to circumvent this difficulty, several methods each based on its own assumptions and approximations have been proposed. The unifying feature of those methods is the definition of a linear comparison composite (LCC) whose response approximates that of the nonlinear composite. Recent research trends focus on achieving two goals. First, for history-dependent materials, be able to simulate general non-monotonic and non-radial loading histories. Second, construct LCCs where besides mean field values, field fluctuations are taken into account, typically via per-phase second statistical moments (which measure the variance). Such recent proposals for small strain elasto(visco)plastic composites include the incremental variational formulations of Brassart et al. (2011, 2012) and Lahellec and Suquet (2013), the second-moment incremental tangent formulation of Doghri et al. (2011) and the second-moment incremental-secant formulation of Wu et al. (2015).

For finite strain elasto(visco)plastic heterogeneous materials, most MFH methods rely on local (micro) constitutive models which are based on the following two classical assumptions:

$$\boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p, \;\; \overset{\nabla}{\boldsymbol{\tau}} = \boldsymbol{c}^e : \boldsymbol{d}^e, \tag{1}$$

i.e., an additive decomposition of the rate of deformation tensor $\boldsymbol{d}$ onto elastic and inelastic parts, and a hypoelastic stress-strain relation, where $\overset{\nabla}{\boldsymbol{\tau}}$ is an objective rate of the Kirchhoff stress $\boldsymbol{\tau}$ (e.g., Jaumann's, Green-Naghdi-Mc Innis, Lie, etc.) Representative MFH proposals based on eq. (1) include, for polycrystalline metals: Nemat-Nasser and Obata (1986) and Segurado et al. (2012), for porous materials: Danas and Aravas (2012) and Aravas and Ponte Castaneda (2004), for solid propellants: Xu et al. (2008) and for metal-matrix composites: Pettermann et al. (2010).

It is well known that assumptions (1) are acceptable if the elastic strains are small, which is typical of metals. However, this is not the case for polymer materials, for which a better formulation is based on the following assumptions:

$$\boldsymbol{F} = \boldsymbol{F}^e \cdot \boldsymbol{F}^p, \;\; \boldsymbol{\tau} = 2\frac{\partial \psi}{\partial \boldsymbol{b}^e} \cdot \boldsymbol{b}^e, \tag{2}$$

i.e. a multiplicative decomposition of the deformation gradient $\boldsymbol{F}$ onto elastic and inelastic parts, and a hyperelastic stress strain relation between the Kirchhoff stress $\boldsymbol{\tau}$ and the elastic left Cauchy-Green strain $\boldsymbol{b}^e = \boldsymbol{F}^e \cdot (\boldsymbol{F}^e)^T$, derived from a specific free energy per unit reference volume ψ. Unless the elastic strains are small, eq. (1a) cannot be deduced and is not compatible with eq. (2a), see for instance Vladimirov et al. (2010). For heterogeneous materials with hyperelastic-viscoplastic constituents obeying to eq. (2), direct full-field homogenization methods have been proposed, e.g. Miehe et al. (1999) and Matous and Maniatty (2009) for polycrystals. However, the literature seems to lack finite strain MFH methods (e.g. extended Mori-Tanaka or self-consistent schemes) which are based locally on eq. (2).

For finite strain hyperelastic composites, several MFH formulations based on variational formulations and including field fluctuations have been proposed over the years by Ponte Castañeda, Suquet and their co-workers, reaching a high degree of accuracy, see for instance Ponte Castañeda and Tiberio (2000), Ponte Castañeda and Suquet (2002), Ponte Castañeda (2002) and Idiart et al. (2006).

The present article is concerned with the finite strain MFH of a class of composites where multiple phases of solid inclusions or cavities are embedded in a continuum matrix. Each solid phase obeys a hyperelastic-plastic material model built on the basic assumptions of eq. (2). For the special situation of hyperelastic constituents (i.e., when their initial yield stresses are not reached) a mixed variational formulation is proposed which handles both compressible and quasi-incompressible cases within the same framework. A special emphasis is put on the proper definition of various macroscopic stress measures and tangent operators. Numerical algorithms were developed and implemented for an extended Mori-Tanaka MFH model. The predictions were extensively tested against direct FE simulations of RVEs or unit cells.

The paper is organized as follows. Section 2 presents some basic results needed in all further developments. The MFH of composites with hyperelastic-plastic constituents is considered in Section 3, whereas the case of hyperelastic constituents is studied in Section 4. Comments about the proposed MFH are made in Section 5. Several numerical MFH predictions and their verification against direct FE simulations of RVEs or unit cells are presented and discussed in Section 6. Conclusions are given in Section 7. Numerical algorithms are presented in Appendix A.

Acronyms: FE: finite element, MF: mean-field, MFH: MF homogenization, RVE: representative volume element, VWT: virtual work theorem.