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On the bounds of applicability of two-step homogenization technique for porous materials

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ABSTRACT

We discuss applicability of the two-step homogenization procedure to microstructures formed by spherical pores of two distinct sizes with total porosity of 40%. Results of one- and two-step homogenizations utilizing Non-Interaction Approximation (NIA), Mori–Tanaka–Benveniste Scheme (MTB) and Differential Scheme (DS) are compared with numerical data obtained by finite element simulations. A modified collective rearrangement method powered by computationally efficient hierarchical k-means tree algorithm is developed for generating microstructures containing spherical pores of different sizes with prescribed partial porosities. Two-step procedure turns to be almost commutative with respect to the sequence of homogenization step showing 0.2% as a maximum relative error. Sensitivity of approximated overall elastic properties to the size difference of spherical inhomogeneities is observed with the shear modulus showing stronger dependence than the bulk modulus. The two-step MTB can be used to approximate effective properties of solids with spherical pores of distinct size as long as this size difference between pore families is larger than 10 times.

1. Introduction

The problem of the effective properties of heterogeneous materials plays a key role in material characterization providing the tools for analysis of both naturally occurring and man-made materials. Many modern materials are characterized by complex structure that require detailed representation, providing significant challenges in the modeling procedure. Direct numerical simulation requires fine-scale resolution and thus leads to great computational costs mostly not achievable even for supercomputers. Exact analytical solutions are very limited due to the complexity of boundary value problem and, therefore, most of the available studies use homogenization procedure, based on the solution for a single inhomogeneity, to find overall properties of a heterogeneous material. Generally, this approach can be applied in one- and multi-step homogenization models.

The idea of two-step (or, generally, multi-step) homogenization is intuitively very clear when there are two distinct scales of heterogeneity and is rooted in classical concepts of Navier and Cauchy (see historical remarks in the review of Markov (2000)). Implicitly, all the homogenization schemes use this technique. For example, when we apply micromechanical approximations to calculate overall properties of a, say, metal matrix reinforced with ceramic particles, we assume that the

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matrix material (consisting of randomly oriented crystalline with various defects) is homogeneous. Thus, this process contains two steps: (A) implicit first step, at which the properties of the matrix are obtained (this step may be experimental) and (B) explicit second step when the overall properties of the composite are calculated.

To the best of our knowledge, the idea of multi-step homogenization procedure attracted attention of many researchers in late 1990s since it allows one to avoid the reported problems appearing in application of Mori–Tanaka–Benveniste scheme to anisotropic multiphase composites—loss of symmetry and positive definiteness of the effective compliance tensor (Benveniste, 1987; Ferrari, 1991; Norris, 1989; Weng, 1990). Indeed, if the multi-step homogenization technique is used, the material can be considered as a two-phase one at each step. Dai, Huang & Wang (1998) used two-step homogenization technique to predict overall properties of multiphase hybrid composites. Thermo-mechanical properties for compression molded composites parts were considered by Lielens, Pirotte, Couniot, Dupret & Keunings (1998). The representative volume was decomposed into the set of aggregates having the same fiber orientation and volume fraction. Finally, effective properties were found by averaging reference composites with different fiber orientations. Lu & Weng (1998, 2000) used two-step homogenization to calculate overall properties of polymer composite shape-memory alloy (SMA) reinforced where the SMA itself consisted of the parent austenite and transformed martensite. Pierard, Friebel & Doghri (2004) applied multi-step technique for thermo-elastic composites with representative volume element characterized by a set of initially homogenized grains. Overall properties were calculated using Voight and Reuss models, due to physically unacceptable results of Mori–Tanaka–Benveniste scheme for multi-phase composites. Effective properties of short-fiber reinforced polymer composites were analyzed by Dray, Gilormini & Régnier (2007). Firstly, Mori–Tanaka–Benveniste scheme was used to predict properties of aggregate containing identically oriented fibers. At the second step, overall properties of the composite containing different fiber orientations were predicted by stiffness averaging and orthotropic closure approximations. Gruescu, Giraud, Homand, Kondo & Do (2007) considered two-step homogenization procedure to predict effective thermal conductivity of partially saturated rocks containing solid and porous inhomogeneities. Multi-step homogenization technique was applied for metal-ceramic composites with lamellar domains by Ziegler, Neubrand & Piat (2010), who compared numerical approach against micromechanical modeling. Barai & Weng (2011) used two-step homogenization to study plasticity strength of carbon nanotube-reinforced metal composites. Nguyen, Giraud & Grgic (2011) used two-step homogenization procedure to calculate effective elastic properties of the porous rocks characterized by an assemblage of grains (oolites) embedded in a calcite matrix. Pores on micro-scale were firstly homogenized to approximate effective properties using composite sphere assemblage model (Hashin, 1962). Shen, Kondo, Dormieux & Shao (2013) used multi-step homogenization procedure to formulate macroscopic plastic behavior of Callovo Oxfordian argillite containing porous clay matrix reinforced with linear elastic mineral inhomogeneities. Effective stiffness of polymer-clay nanocomposites with aligned inhomogeneities were analyzed by Pahlavanpour, Hubert & Lévesque (2014). Authors compared one- and two-step homogenization procedures (both analytical and numerical) against direct 3D FEA modeling and experimental data extracted from the literature. It was concluded that the analytical multi-coated inclusion models result in more accurate approximations. Giraud, Sevostianov, Chen & Grgic (2015) obtained effective thermal conductivity of oolitic limestones using two-step homogenization procedure, where the self-consistent scheme and Maxwell's scheme have been applied in the first and second steps, respectively.

As it follows from this literature review, multi-step homogenization technique is widely used for materials containing distinct families of inhomogeneities. However, to the best of our knowledge, the framework of the applicability of this technique has never been discussed in the literature. We address this problem focusing on the simplest case of a material containing spherical pores at two distinct sizes and compare results of finite element simulations with the predictions of micromechanical schemes.

2. Two-step homogenization in various one-particle approximations

2.1. Compliance contribution tensor

Compliance contribution tensors have been first introduced in the context of pores and cracks by Horii & Nemat-Nasser (1983) (see also detailed discussion in the book of Nemat-Nasser, Hori & Achenbach, 1993). Components of this tensor were calculated for 2-D pores of various shape and 3-D ellipsoidal pores in isotropic material by Kachanov, Tsukrov & Shafiro (1994). For general case of ellipsoidal elastic inhomogeneities, these tensors were formally defined and calculated by Sevostianov & Kachanov (1999, 2002). Following these works, we consider a homogeneous elastic material (matrix) with the compliance tensor $\mathbf{S}_0$ containing an isolated inhomogeneity of volume V_1 having different compliance tensor $\mathbf{S}_1$. The compliance contribution tensor of the inhomogeneity is a fourth-rank tensor $\mathbf{H}$ that gives the extra strain (per reference volume V) due to its presence:

$$\Delta\,\varepsilon = \frac{V_1}{V}\mathbf{H}{:}\sigma^0, \text{or, in components,}\quad \Delta\varepsilon_{ij} = \frac{V_1}{V}H_{ijkl}\sigma^0_{kl}, \tag{2.1}$$

where σ^0_{kl} are remotely applied stresses that are assumed to be uniform within V in the absence of the inhomogeneity. For an ellipsoidal inhomogeneity, its compliance contribution tensor is expressed in terms of Hill's tensor $\mathbf{P}$ (Hill, 1965; Walpole, 1969) as

$$\mathbf{H} = \left[(\mathbf{S}_1 - \mathbf{S}_0)^{-\mathbf{1}} + \mathbf{C}_0{:}(\mathbf{J} - \mathbf{P}\,{:}\mathbf{C}_0)\right]^{-1}. \tag{2.2}$$