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A set of enhanced formulations for existing nonlinear homogenization schemes and their evaluation

Amna Rekik [a,*], François Auslender [b], Michel Bornert [c]

[a] Univ. Orléans, INSA-CVL, PRISME, EA4229, 45072 Orléans, France
[b] Université Blaise Pascal, Institut Pascal, UMR CNRS 6602, BP 10448, 63000 Clermont-Ferrand, France
[c] Université Paris Est, Laboratoire Navier (ENPC/IFSTTAR/CNRS UMR 8205), ENPC, 6 et 8 avenue Blaise Pascal, 77455 Marne la Vallée Cedex, France

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ABSTRACT

On the basis of non-biased comparative evaluations of various linearization procedures used in nonlinear homogenization, performed both at the global and local scales for power-law composites (Rekik et al., 2005, 2007, 2012), we propose in this paper six *ad hoc* enhancements of some of the linearization procedures considered in Rekik et al. (2007). Both "stress–strain" approaches (the secant and affine formulations) or "variational formulations" (the tangent second-order method (Ponte Castañeda, 1996)) are considered. The main idea consists in proposing alternatives for the usual reference strains used by the secant, affine and tangent second-order procedures. The new linear comparison composites generated by the linearization step around the chosen alternative descriptors of the strain field statistics explicitly account for either intraphase strain fluctuations or both inter- and intraphase strain fluctuations. As a first illustration, the relevance and limitations of the enhanced linearization procedures are tested for rigidly-reinforced and porous power-law composites. For isochoric loadings, it is shown that two variants of the enhanced tangent second-order formulation lead to accurate estimates of the exact effective response which are in good agreement with the efficient second-order scheme of Ponte Castañeda (2002a). Further, the modified secant formulation provides good results for strongly nonlinear rigidly-reinforced composites away from low particulate volume fraction and the percolation threshold; however some new inherent limitations of secant formulations are also established. At last, a very discriminant situation is tested: it consists of a porous medium submitted to a pure hydrostatic loading at low pore concentrations. It is shown that one variant of the proposed enhanced second-order formulations leads to accurate estimates alike the efficient and more sophisticated formulations proposed in Bilger et al. (2002); Danas et al. (2008).

1. Introduction

Nonlinear homogenization techniques are powerful methods allowing the derivation of bounds or estimates for the effective properties of heterogeneous nonlinear composites from both their local constitutive laws and the statistical description of their microstructure. These techniques rely on two steps: the linearization and the linear homogenization. The first step, through the linearization of the phase constitutive relations defines a linear comparison composite (LCC) whose microstructure is in general taken to be similar to that of the nonlinear composite. In the literature, several expressions of the corresponding local linearized behavior have been proposed. For the secant method (Berveiller and Zaoui, 1979), the phases of the LCC are defined from the secant moduli $(9)_1$ of the actual phases. For the affine formulation due to Masson et al. (2000), thermoelastic comparison materials are defined from tangent operators $(9)_2$ of the phases. The classical secant and affine estimates are evaluated at the first-moment of the strain field over the phases and yield too stiff responses (Gilormini, 1995; Rekik et al., 2007). To improve the affine formulation, Chaboche and Kanouté (2003) proposed to replace the tangent anisotropic operator by a softer isotropic simplification. Simultaneously, Brenner et al. (2001) proposed a "modified affine" formulation that accounts for the intraphase heterogeneity, by analogy to the "modified secant" approach proposed by Suquet (1995) for the special case of power-law materials. The latter is equivalent to the variational approach developed by Ponte Castañeda (1991) which consists in the use of an optimally

* Corresponding author.
E-mail address: amna.rekik@univ-orleans.fr (A. Rekik).

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chosen LCC with reference to a variational formulation. It delivers bounds exact to the first-order in the heterogeneities contrast. The same author proposed in Ponte Castañeda (1996) an alternative approach relying on a second-order expansion of the strain energy of a constitutive phase around a reference strain taken as the strain average over this phase. This model yields estimates that are exact to the second-order in the contrast but which can violate the variational bounds in some special cases, as near the percolation phenomenon (Leroy and Ponte Castañeda, 2001). For this reason Ponte Castañeda (2002a) proposed an improved second order method that makes use of a generalized secant moduli incorporating both inter-and intra-phase strain fluctuations. However, one of the reference strain used in this new procedure is not fully defined by stationary conditions relying on the nonlinear composite and thus induces some limitations for the second order variant proposed in Ponte Castañeda (2002a). Accordingly, Idiart and Ponte Castañeda (2005); Idiart et al. (2006a) introduced an alternative prescription for this reference strain in a new and third variant of the second-order method which provides slightly improved estimates for the effective and local responses in comparison with the earlier prescription (Ponte Castañeda, 2002a). The new prescription for the reference strain field does still not ensure fully stationarity conditions. It is noteworthy that the second-order methods do not directly deliver an effective stress–strain relation but rather an effective strain-energy which needs to be differentiated. Moreover, the affine formulation is less accurate compared with the second-order methods. In particular, the affine scheme is not exact to second order in the contrast and, more critically, is not associated with an overall potential. To overcome these difficulties, Lahellec and Suquet (2004) proposed a new approximate scheme which closes the gap between the affine and the second order procedure and gives results exact to second order in the contrast.

As seen above, numerous linearization methods are available and their relative merits are not easy to understand to an unexperienced user. However, they have been accurately evaluated by different authors – e.g. Moulinec and Suquet (2004), Rekik et al. (2005, 2007, 2012), Lahellec and Suquet (2004) and Idiart et al. (2006b) – without any ambiguity related to the approximations induced by the linear homogenization estimates of the LCC. In particular, Rekik et al. (2005, 2007) proposed a methodology allowing the evaluation of the sole effect of linearization schemes without the classical bias present in earlier evaluations such as the use of linear homogenization schemes available in the literature for assessing the LCC behavior. It relies on an exact treatment of both the nonlinear and linear homogenization problems using the finite element method. In Rekik (2006); Rekik et al. (2007, 2012), various nonlinear homogenization schemes such as the classical secant scheme (referred to as SEC), the variational procedure (VAR), the original affine formulation (AFF-ANI) and its isotropic simplification (AFF-ISOT), the original (SOE-1) and improved (SOE-2) second-order procedures as well as the Lahellec and Suquet (LS) formulation were compared with regard to their predictions in terms of overall responses and local field statistics for the special case of power-law two-phase composites with different contrast between the phases ranging from the rigidly-reinforced composites to porous materials. Based on the main results of these comparisons, we propose in this paper some improvements for existent "stress–strain" approaches (SEC, AFF-ANI) or "potential-based" approaches such as the variational (VAR) and tangent second-order (SOE-1) formulations. The main idea consists in evaluating the secant shear modulus $\mu^r_{sct}(\varepsilon^r)$ of the secant $(9)_1$ or tangent $(9)_2$ stiffness tensor at a reference strain $\hat{\varepsilon}^r_{eq}$ $(14)_1$ incorporating both the inter- and intra-phase strain fluctuations. Such an incorporation of both the inter- and intra-phase strain fluctuations is applied to the SEC, AFF-ANI and SOE-1 approaches and aims to soften the secant and tangent operators associated with these approaches and thus to improve them since these procedures have been shown in Rekik et al. (2007, 2012) to provide too stiff estimates of the effective behavior. For the affine formulations (AFF-ANI and AFF-ISOT), it is also proposed to make use of a shear modulus which is intermediate between the standard secant $\mu^r_{sct}(\bar{\varepsilon}^r)$ and tangent $\mu^r_{tgt}(\bar{\varepsilon}^r)$ ones for the perpendicular direction F^r of the tangent operator (B.3). Such a linearization aims to improve the classical and simplified affine formulations especially for strong nonlinearities since numerical comparisons performed in Rekik et al. (2007) have shown that the exact solution lies between the AFF-ANI and AFF-ISOT responses. At last, for the tangent second-order procedure, we also propose to soften the secant shear modulus $\mu^r_{sct}(\bar{\varepsilon}^r_{eq})$ (resp. the tangent shear modulus $\mu^r_{tgt}(\bar{\varepsilon}^r_{eq})$) associated with the orthogonal direction F^r (resp. the parallel direction E^r) of the tangent operator by evaluating it at the second-order moment of the strain field in each phase $\bar{\bar{\varepsilon}}^r_{eq}$ $(13)_1$ or at the strain descriptor $\hat{\varepsilon}^r_{eq}$ $(14)_1$.

Then, in order to evaluate the efficiency of these proposed enhanced linearization schemes, we present a first comparative and non-biased study at the macroscopic scale with some of the most used or famous linearization procedures, i.e. the secant, affine, second-order formulations as well as the Lahellec and Suquet procedure. For that, we focus our attention on rigidly-reinforced and porous power-law materials. These materials are of extreme heterogeneity in the contrast and therefore constitute discriminating cases to study.

The structure of the paper is as follows. In Section 2, we briefly recall the various linearization schemes which will be used in the sequel either to design new linearization procedures or for comparative purposes. In Section 3, relying on some relevant observations and conclusions derived from non-biased comparative evaluations of the linearization schemes presented in Section 2, new and enhanced formulations are proposed. A first evaluation of their performances at the macroscopic scale is carried out in Section 4 where the new proposed linearization schemes are compared with some of the most used linearization procedures for nonlinear two-phase composites made of identical spherical inclusions – either pores or quasi-incompressible isotropic linear elastic particles – embedded in a nonlinear isotropic matrix following a Ramberg–Osgood law. Conclusions are summarized in Section 5.

The tensor notation used herein is a fairly standard one. Products containing dots denote summation over repeated indices. For example, $L{:}\varepsilon = L_{ijkl}\varepsilon_{kl}e_i \otimes e_j$ and $E{::}F = E_{ijkl}F_{klij}$ where e_i $(i = 1, 2, 3)$ is a time-independent orthogonal cartesian basis and the operation $\otimes$ denotes the classical tensorial diadic product.

2. Reminder of general principles of nonlinear homogenization schemes and their evaluation by a non-biased methodology

2.1. Nonlinear effective properties

The main objective of homogenization is to predict the macroscopic behavior of composite materials in terms of the behavior of their constituents and prescribed statistical information about their microstructure. In this framework, we consider composite materials made of N different homogeneous constituents, each occupying a volume $v_r{:}(r = 1,\ldots,N)$, "periodically or randomly" spatially distributed in a specimen occupying a volume $V = \cup^N_{r=1} V_r$, and submitted to mechanical loadings which are assumed to be macrohomogenous (Hill, 1967), thus making the scale transition possible. The constitutive behavior of each phase is characterized by a convex single potential or strain energy function w^r, such that the stress σ and strain ε tensors are related by