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Third-order bound of nonlinear composites and porous media under hydrostatic deformation

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1. Introduction

The earliest nonlinear models of heterogeneous materials dealt with crystal plasticity and two elementary bounds of Taylors and Sachs were given corresponding to Voigt's and Reuss' bounds for linear-elastic composites. Following the breakthrough of Eshelby's ellipsoidal solution (Eshelby, 1957) in micromechanics, various nonlinear models have been proposed since 1960s, which are roughly classified into following two groups, mean-field models and variational models.

1.1. Mean-field models

The mean-field models basically apply the Eshelby's ellipsoidal solution to evaluate the first-order moment or averaged phase strain or stress, similar to Mori–Tanaka scheme in linear-elastic micromechanics. One of the first self-consistent models was proposed by Kröner (1958) where local stress and plastic strain are assumed to be uniform in the grains, while individual plasticity of grains is assimilated into the overall equivalent medium

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ABSTRACT

In this study the third-order variational bound is explicitly derived for nonlinear composites subject to hydrostatic deformation. By formulating the stochastic extreme principle for nonlinear boundary value problems, the third-order upper bound of the potential is derived for nonlinear two-phase composites, which is further explicitly specialized to porous media. Examples of application are provided by applying the derived bound to various cases of composites and porous media characterized with power law nonlinearity. © 2013 Elsevier Ltd. All rights reserved.

> self-consistently. To account for anisotropic plastic interactions among crystals, an incremental self-consistent model was proposed by Hill (1965) with stiff responses close to Taylor's upper bound due to the assumption of uniform tangent moduli in the matrix. The Hill's model was later extended to rigid viscoplasticity by Hutchinson (1976). To reduce the errors accumulated in the incremental process, Molinari et al. (1987) developed a non-incremental tangent model, which was later generalized to an affine formulation (e.g., Masson et al., 2000). The self-consistent model using phase-uniform secant moduli was proposed by Berveiller and Zaoui (1979), which is also called the classical secant model. In dealing with various effects due to thermal, plastic, damage, phase transformation, etc., Dvorak (1992) proposed a so-called transformation field analysis where the transformation strain is assumed uniform in each phase. In the mean-field models, there is however a lack of clear link between the statistics of microstructure and properties, e.g. the third and higher-order correlation functions are not accounted for. Unlike the variational bounds providing a range of overall properties to account for various statistics of microstructure, a meanfield model leads to a deterministic estimate that corresponds to a certain type of microstructure only, e.g. most of self-consistent approximations are limited to weakly





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inhomogeneous materials such as dilute cases. For highly heterogeneous materials many mean field models may result in violation of theoretical bounds as shown e.g. in Gilormini (1996). Mean-field models normally lead to over-stiff responses, and a typical defect is no yielding for hydrostatic deformation of a dry porous medium.

1.2. Variational and 2nd-order models

A great advantage of variational models is by providing rigorous bounding properties, the bounds are generally applicable to a wide class of materials. By incorporating statistics of microstructure into the models, nonlinear variational bounds account for the second and higher order statistical moments of field fluctuations beyond phase averages. A nonlinear variational model was first proposed by Talbot and Willis (1985), following which a major attempt was made to extend the linear Hashin-Shtrikman (HS) bound to the nonlinear regime (Ponte Castañeda, 1991). Qiu and Weng (1992) showed that the fluctuations of strain in the matrix can be accounted for by using an energy concept to define the effective stress, instead of average stress in the mean field models. Suguet (1993) proposed variational bounds for power law materials. A number of works were explicitly devoted to the second-order estimates, e.g. (Hu, 1996; Buryachenko, 1996; Ponte Castañeda, 2002) among others. There was also a multiple scattering solution to account for higher-order effects beyond mean field approximations (Talbot and Willis, 1997). In Nan and Yuan (1993) further efforts were made to incorporate third-order statistics into variational models.

In this study the third-order bounds are explicitly derived in terms of the third order geometric parameters for nonlinear composites subject to hydrostatic deformation. In Section 2, following the linear principles formulated in Xu (2009) the stochastic extreme principle is formulated for nonlinear boundary value problems. In Section 3, the third-order upper bound of the potential is derived for nonlinear two-phase composites, which is explicitly specialized to porous media. In Section 4, the variational bound is applied to various cases of composites and porous media characterized with power law nonlinearity.

2. Stochastic extreme principle

The potential and the dual of a nonlinear phase i are defined as

$$\phi_i(\hat{\boldsymbol{\varepsilon}}) = \int_0^{\hat{\boldsymbol{\varepsilon}}} \boldsymbol{\sigma} d\boldsymbol{\varepsilon}$$
(1)

$$\phi_i^*(\hat{\boldsymbol{\sigma}}) = \int_0^{\hat{\boldsymbol{\sigma}}} \boldsymbol{\varepsilon} d\boldsymbol{\sigma}$$
(2)

which are complementary to each other in that

$$\phi_i(\hat{\boldsymbol{\varepsilon}}) + \phi_i^*(\hat{\boldsymbol{\sigma}}) = \hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\varepsilon}}$$
(3)

where $\frac{\partial \phi_i(\boldsymbol{\varepsilon})}{\partial \boldsymbol{\varepsilon}}\Big|_{\boldsymbol{\varepsilon}=\hat{\boldsymbol{\varepsilon}}} = \hat{\boldsymbol{\sigma}}$ and $\frac{\partial \phi_i^*(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}\Big|_{\boldsymbol{\sigma}=\hat{\boldsymbol{\sigma}}} = \hat{\boldsymbol{\varepsilon}}$, and the two are conjugated to each other. In nonlinear elasticity the functions (1)–(3) correspond to free energy. For elastoplasticity problems, the energy consists of both free energy and dissipated or plastic energy.

To homogenize the energy potential of a random twophase composite, let the unit volume composite body be subjected to a displacement boundary condition $\tilde{\mathbf{u}}$. Assume the characteristic size of heterogeneity is sufficiently small compared with the unit volume domain *D*. The total potential of the Dirichlet boundary value problem is written, accordingly, as

$$I(\boldsymbol{\varepsilon},\omega) = \int_{D} \phi(\boldsymbol{\varepsilon}; \mathbf{x}, \omega) dV - \int_{\partial D_{u}} \tilde{\mathbf{u}} \mathbf{t} dS$$
(4)

where the potential consists of the contribution from each phase

$$\phi(\boldsymbol{\varepsilon}; \mathbf{X}, \boldsymbol{\omega}) = \phi_1(\boldsymbol{\varepsilon}_1) + \phi_2(\boldsymbol{\varepsilon}_2) \tag{5}$$

with

$$\boldsymbol{\varepsilon}_1 = \boldsymbol{\varepsilon} \boldsymbol{\chi}_1 \quad \boldsymbol{\varepsilon}_2 = \boldsymbol{\varepsilon} \boldsymbol{\chi}_2 \tag{6}$$

The random morphological functions χ_i (\mathbf{x}, ω) = 1 when $x \in D_i$ and 0 otherwise, i = 1, 2, with ω indicating a sample in random space Ω . When the characteristic size of heterogeneity is sufficiently smaller than the unit volume domain D, i.e. the scales are separated or decoupled, and the random microstructure satisfies the statistical homogeneity and ergodicity condition, the randomness argument disappears on the left side of (4) by noting

$$\int_{D} \phi(\boldsymbol{\varepsilon}, \mathbf{x}, \omega) dV = \int_{\Omega} \phi(\boldsymbol{\varepsilon}, \mathbf{x}, \omega) dP(\omega)$$

or simply

$$\langle \phi(\boldsymbol{\varepsilon}, \mathbf{X}, \boldsymbol{\omega}) \rangle = \phi(\boldsymbol{\varepsilon}, \mathbf{X}, \boldsymbol{\omega}) \tag{7}$$

The first order variation of the total potential $(4)\delta I$ directly leads to the strong form equilibrium equation and the displacement boundary condition. Assume the potential function of each phase satisfies the positive definiteness of the tangent moduli

$$\frac{\partial^2 \phi_i(\boldsymbol{\varepsilon})}{\partial^2 \boldsymbol{\varepsilon}} > 0 \tag{8}$$

The second-order variation of (4) yields that

$$\frac{\delta^2 I}{\delta^2 \boldsymbol{\varepsilon}} = \chi_1 \frac{\partial^2 \phi_1(\boldsymbol{\varepsilon}_1)}{\partial^2 \boldsymbol{\varepsilon}_1} + \chi_2 \frac{\partial^2 \phi_2(\boldsymbol{\varepsilon}_2)}{\partial^2 \boldsymbol{\varepsilon}_2} > 0$$
(9)

which leads to the stochastic minimization principle

$$I^{E}(\bar{\boldsymbol{\varepsilon}}) = \underset{\boldsymbol{\varepsilon} \in \mathbf{E}}{\operatorname{Min}} \overline{I(\boldsymbol{\varepsilon})}$$
(10)

Where $\bar{\epsilon}$ denotes the macroscopic strain resulting from the boundary condition $\tilde{\mathbf{u}}$, and E the function space for all the admissible strain functions satisfying the displacement boundary condition.

Correspondingly, the effective potential is obtained as

$$\phi^{E}(\bar{\boldsymbol{\varepsilon}}) = \underset{\boldsymbol{\varepsilon} \in E}{\operatorname{Min}} \overline{\phi(\boldsymbol{\varepsilon})}$$
(11)

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