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Variational formulation of the equivalent eigenstrain method with an application to a problem with radial eigenstrains

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ABSTRACT

In this paper a variational formulation of the equivalent eigenstrain method is established. A functional of the Hashin–Shtrikman type is proposed such that the solution of the equivalent eigenstrain equation is a unique minimizer of the functional. Moreover, it is also shown that the equivalent eigenstrain equation is the Euler–Lagrange equation of the potential energy of the inclusions. An approximate solution of the equivalent eigenstrain equation is then found as a minimizer of the functional on a finite dimensional span of basic eigenstrains. Special attention is paid to possible symmetries of the problem. The variational formulation is illustrated by determination of effective linear elastic properties. In particular, material with a simple cubic microstructure is considered in detail. A solution for the polynomial radial basic eigenstrains approximation is found. In particular, for the homogeneous eigenstrain approximation, the effective moduli are derived in an exact closed form.

1. Introduction

The equivalent eigenstrain method/principle is a cornerstone of micromechanics. It states the equivalence of the stress state in a heterogeneous linearly elastic solid and in a homogeneous solid of the same shape, under the same loading, when the heterogeneities are replaced by an appropriate distribution of eigenstrains (transformation strains). The method, also known as the equivalent inclusion method (Mura, 1991), was first formulated and used by Eshelby in his seminal paper (Eshelby, 1957). However, the resulting equivalent eigenstrain equation is exactly solvable only for an isolated ellipsoidal inhomogeneity in an infinite solid. As a consequence, numerous approximate approaches have been developed.

The most direct approach uses Taylor series expansions of the eigenstrains (Moschovidis and Mura, 1975). In addition to a convergence problem, a drawback of the expansion is that the exterior part of the Eshelby operator does not map polynomial eigenstrains into polynomial strains. Therefore, another level of approximation, another Taylor series expansion, collocation method or finite element method, is needed. Another pertinent problem with the Eshelby operator is that its action is explicitly known, apart from some special cases, only for an ellipsoidal inclusion in an infinite domain. Thus non-elliptical inclusions and finite domains must be treated by approximate methods. To simplify the problem, the homogeneous eigenstrain approximation is commonly used as the first level of approximation. Examples of higher order Taylor series expansion are Fond et al. (2001) and Benedikt et al. (2006). For problems with periodic micro-structure a Fourier series expansion is a viable alternative (Nemat-Nasser and Hori, 1999); however, not without difficulties. The problem is that a Fourier series expansion of a discontinuous function, and here the eigenstrain and elasticity tensor are discontinuous across the material interfaces, is not absolutely convergent, and thus convergence of the Cauchy product of Fourier series expansions of the eigenstrain and elasticity tensor is not guaranteed. This problem is usually avoided by using a homogeneous eigenstrain approximation. The rather slow convergence of the Fourier series expansion can then be improved by using Fast Fourier Transformations (Moulinec and Suquet, 1998). A recent review of different approaches is given in Zhou et al. (2013).

The aim of this paper is to overcome the difficulties mentioned above. First, to find in principle a convergent approximation of the eigenstrains, and then to demonstrate, by a particular example of an application of the equivalent eigenstrain principle, that an exact solution can be found without further simplifications. The first aim is achieved by a variational formulation of the equivalent eigenstrain equation, and the second aim by taking into account the symmetry of the problem and developing an analysis that replaces a finite domain by an infinite domain.

The paper has the following structure. Section 2 sets out the mathematical notation. In Section 3 a variational formulation of the eigenstrain equation is established. A functional, similar to the Hashin–Shtrikman functional, is defined such that a solution of the equivalent eigenstrain equation is a unique minimizer of this functional. Then, restricting the minimization of the functional to a

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finite dimensional linear space of admissible eigenstrains, an approximate solution of the equivalent eigenstrain equation is found. It is shown that the eigenstrain approximation inherits the symmetry of the problem. The section is concluded with an observation that several functionals, each having its own merits, give rise to an equivalent eigenstrain equation. In Section 4 the determination of the effective linear elastic material properties is discussed. It is explained what modifications are needed to justify the replacement of the finite domain Eshelby tensor with the infinite domain tensor. In Section 5 the method is illustrated for the example of a simple cubic structure of spherical inclusions. Using a radial eigenstrain approximation the Eshelby tensor of the simple cubic structure is found in a closed form. Computation of the influence tensor is also explained in detail. It is proved that a general radial eigenstrain approximation gives the same effective bulk modulus of the cubic structure as the homogeneous eigenstrain approximation. Determination of the effective shear moduli is developed in Section 6 where a polynomial radial eigenstrain approximation is used. It is shown that the optimal radial approximation is given by a linear span of the homogeneous and quadratic eigenstrains. Using only the homogeneous approximation, the effective moduli first given by Cohen and Bergman (2003) are recovered, but here in an exact form. The paper concludes with a list of possible generalizations. Two appendices derive the Eshelby tensors and their volume averages for radial eigenstrains.

2. Notation preliminaries

Direct tensor notation is used throughout the paper. Vectors, second and fourth order tensors are denoted by $\underline{a}, \underline{\underline{a}}$, and $\underline{\underline{A}}$. In component notation with respect to the Cartesian basis vectors $\underline{e}_i$ they are $\underline{a} = a_i\underline{e}_i, \underline{\underline{a}} = a_{ij}\underline{e}_i \otimes \underline{e}_j$ and $\underline{\underline{A}} = A_{ijkl}\underline{e}_i \otimes \underline{e}_j \otimes \underline{e}_k \otimes \underline{e}_l$. The summation convention over repeated tensor indices is used. A vector space of n-th order tensors is denoted by $\mathcal{T}^n$.

The identity second order tensor is denoted by $\underline{\underline{i}}$ and the fourth order symmetric identity by $\underline{\underline{I}}$. The symmetric tensor product of two vectors $\underline{a}$ and $\underline{b}$ is denoted by $sym(\underline{a} \otimes \underline{b}) = \frac{1}{2}(\underline{a} \otimes \underline{b} + \underline{b} \otimes \underline{a})$. Symmetrization of a tensor $\underline{\underline{A}}$ with respect to indices i and j is denoted by $\mathrm{sym}_{ij}\underline{\underline{A}}$. In particular $\mathrm{sym}_{12}\underline{\underline{A}} = A_{ijkl}sym(\underline{e}_i \otimes \underline{e}_j)\underline{e}_k \otimes \underline{e}_l$. Transposition of a tensor $\underline{\underline{A}}$ with respect to indices i and j is denoted by $\mathrm{tran}_{ij}\underline{\underline{A}}$. Thus $\mathrm{tran}_{24}\underline{\underline{A}} = A_{ijkl}\underline{e}_i \otimes \underline{e}_l \otimes \underline{e}_k \otimes \underline{e}_j$. If $\mathrm{tran}_{ij}\underline{\underline{A}} = \underline{\underline{A}}$, we say that $\underline{\underline{A}}$ is $i \leftrightarrow j$ symmetric. Symmetric fourth order tensors have by definition $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$ symmetry. The symmetric part of a second order tensor $\underline{\underline{a}}$ is denoted by $\mathrm{sym}\underline{\underline{a}}$. The dot product of two tensors, a single contraction, is denoted by a single dot, and a double contraction by a colon. The gradient of a tensor field $\underline{\underline{a}} = \underline{\underline{a}}(\underline{x})$ is given by $\mathrm{grad}\underline{\underline{a}} = \partial\underline{\underline{a}}/\partial\underline{x}$. In Cartesian coordinates x_i we have $\mathrm{grad}\underline{\underline{a}} = \partial\underline{\underline{a}}/\partial x_i \otimes \underline{e}_i$. The divergence of a tensor field is given as $\mathrm{div}\underline{\underline{a}} = \mathrm{grad}\underline{\underline{a}} : \underline{\underline{i}}$. For example, $\mathrm{div}\underline{\underline{a}} = a_{ij,j}\underline{e}_i$ where the index j after the comma denotes partial differentiation with respect to x_j.

A group of orthogonal second order tensors is denoted by $\mathcal{O}$. Its subgroup of rotations that rotates a cube into itself is called the octahedral or cubic group and is denoted by $\mathcal{C}$. (Bradley and Cracknell, 2010). For example, $R(\underline{e}_i, \pi/2)$ and $R((\underline{e}_1 + \underline{e}_2 + \underline{e}_3)/\sqrt{3}, 2\pi/3)$ are among its elements. Here $R(\underline{e}, \theta)$ is a rotation with the axis $\underline{e}$ and the angle of rotation θ. The Rayleigh product (e.g. Bertram, 2005, Ch. 1) of tensor $\underline{\underline{A}}$ with $Q \in \mathcal{O}$ is denoted by $Q * \underline{\underline{A}}$ and is defined by

$$Q * \underline{\underline{A}} = Q * A_{ijkl}\underline{e}_i \otimes \underline{e}_j \otimes \underline{e}_k \otimes \underline{e}_l = A_{ijkl}Q\underline{e}_i \otimes Q\underline{e}_j \otimes Q\underline{e}_k \otimes Q\underline{e}_l.$$

By direct calculation it follows that

$$Q * \left(\underline{\underline{A}} : \underline{\underline{a}}\right) = \left(Q * \underline{\underline{A}}\right) : \left(Q * \underline{\underline{a}}\right) =: Q * \underline{\underline{A}} : Q * \underline{\underline{a}} \tag{1}$$

for arbitrary tensors $\underline{\underline{A}}, \underline{\underline{a}}$ and $Q \in \mathcal{O}$. Let $\mathcal{G}$ be a subgroup of $\mathcal{O}$. A tensor function $\underline{x} \mapsto \underline{\underline{A}}(\underline{x})$ is $\mathcal{G}$ symmetric if $\underline{\underline{A}}(Q\underline{x}) = Q * \underline{\underline{A}}(\underline{x})$ for all $Q \in \mathcal{G}$. In particular, if $\mathcal{G} = \mathcal{O}$ or $\mathcal{G} = \mathcal{C}$, it is called an isotropic or a cubic tensor function, respectively. If $\mathcal{A}$ is a linear operator that maps a tensor field $\underline{\underline{a}} : \underline{y} \mapsto \underline{\underline{a}}(\underline{y})$ into a tensor field $\mathcal{A}\underline{\underline{a}} : \underline{x} \mapsto \mathcal{A}\underline{\underline{a}}(\underline{x}) \in \mathcal{T}^2$, then $\mathcal{A}$ is called a $\mathcal{G}$ symmetric operator if

$$\mathcal{A}\underline{\underline{a}}(Q\underline{x}) = Q * \left(\mathcal{A}Q^T * \underline{\underline{a}}(Q\bullet)\right)(\underline{x}) \tag{2}$$

for all $\underline{\underline{a}}$ and $\underline{x}$. If $\underline{\underline{a}}$ is a constant tensor, then $\mathcal{A}$ acts as a fourth order tensor field $\underline{\underline{A}}(\underline{x})$ which is a $\mathcal{G}$ symmetric tensor function. Needless to say, all the above definitions naturally extend to tensors of arbitrary orders.

The space of fourth order tensors with the minor symmetry is an algebra where the multiplication is understood as the double contraction. It is well known, see for example Walpole (1981) or Jarić et al. (2008), that the subalgebra of tensors with both the cubic and major symmetry is three dimensional. However, assumption of major symmetry is redundant as the cubic and minor symmetry imply the major symmetry. Symmetric fourth order tensors with cubic symmetry are called cubic tensors. The space of cubic tensors is thus three dimensional. Its basis tensors are denoted by $\underline{\underline{E}}_i, i = 1, 2, 3$, chosen such that the components of a cubic tensor $\underline{\underline{A}}$ are just its Cartesian components A_{1111}, A_{1122} and A_{1212}. Thus

$$\underline{\underline{A}} = A_{1111}\underline{\underline{E}}_1 + A_{1122}\underline{\underline{E}}_2 + A_{1212}\underline{\underline{E}}_3.$$

Multiplication is given by

$$a_i\underline{\underline{E}}_i : b_j\underline{\underline{E}}_j = (a_1b_1 + 2a_2b_2)\underline{\underline{E}}_1 + (a_1b_2 + a_2b_1 + a_2b_2)\underline{\underline{E}}_2 + 2a_3b_3\underline{\underline{E}}_3, \tag{3}$$

where the summation convention over the repeated indices i and j is used. Therefore the algebra of fourth order symmetric tensors with cubic symmetry is isomorphic to an algebra $(\mathbb{R}^3, +, :)$ with multiplication given by

$$a_1, a_2, a_3) : (b_1, b_2, b_3) = (a_1b_1 + 2a_2b_2, a_1b_2 + a_2b_1 + a_2b_2, 2a_3b_3). \tag{4}$$

Clearly, the algebra is commutative. In the cubic basis an isotropic tensor $\lambda\underline{\underline{i}} \otimes \underline{\underline{i}} + 2\mu\underline{\underline{I}}$ has a representation

$$(\lambda + 2\mu)\underline{\underline{E}}_1 + \lambda\underline{\underline{E}}_2 + \mu\underline{\underline{E}}_3. \tag{5}$$

A cubic tensor $\underline{\underline{Z}} = z_i\underline{\underline{E}}_i$ has three eigenvalues, $\zeta_1 = z_1 + 2z_2, \zeta_2 = z_1 - z_2$ and $\zeta_3 = z_3$. The corresponding eigentensors are $\underline{\underline{w}}_1 = \underline{\underline{i}}$ for $\zeta_1, \underline{\underline{w}}_2^{(1)} = \underline{e}_1 \otimes \underline{e}_1 - \underline{e}_2 \otimes \underline{e}_2$ and $\underline{\underline{w}}_2^{(2)} = \underline{e}_1 \otimes \underline{e}_1 - \underline{e}_3 \otimes \underline{e}_3$ for ζ_2 and $\underline{\underline{w}}_3^{(1)} = sym(\underline{e}_1 \otimes \underline{e}_2)$, $\underline{\underline{w}}_3^{(2)} = sym(\underline{e}_1 \otimes \underline{e}_3)$ and $\underline{\underline{w}}_3^{(3)} = sym(\underline{e}_2 \otimes \underline{e}_3)$ for ζ_3. Note that the eigentensors are universal; all cubic tensors have the same eigentensors. They are called cubic eigentensors. To simplify the notation we now write $\underline{\underline{w}}_2$ and $\underline{\underline{w}}_3$ instead of $\underline{\underline{w}}_2^{(1)}$ and $\underline{\underline{w}}_3^{(1)}$. Expressing the components z_i with the eigenvalues we have

$$\underline{\underline{Z}} = \frac{1}{3}(\zeta_1 + 2\zeta_2)\underline{\underline{E}}_1 + \frac{1}{3}(\zeta_1 - \zeta_2)\underline{\underline{E}}_2 + \zeta_3\underline{\underline{E}}_3. \tag{6}$$

The space of the symmetric fourth order isotropic tensor functions is six dimensional. Here we use the following base:

$$\begin{aligned}
&\underline{\underline{X}}_1 = \underline{\underline{i}} \otimes \underline{\underline{i}},\\
&\underline{\underline{X}}_2 = \underline{\underline{I}},\\
&\underline{\underline{X}}_3(\underline{r}) = \underline{\underline{i}} \otimes \underline{r} \otimes \underline{r},\\
&\underline{\underline{X}}_4(\underline{r}) = \underline{r} \otimes \underline{r} \otimes \underline{\underline{i}},\\
&\underline{\underline{X}}_5(\underline{r}) = sym(\underline{r} \otimes \underline{e}_i) \otimes sym(\underline{r} \otimes \underline{e}_i),\\
&\underline{\underline{X}}_6(\underline{r}) = \underline{r} \otimes \underline{r} \otimes \underline{r} \otimes \underline{r}.
\end{aligned} \tag{7}$$