Nonlinear composites: a linearization procedure, exact to second-order in contrast and for which the strain-energy and affine formulations coincide

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Abstract

This Note presents a new approximate scheme for nonlinear composites. The approximation which is made preserves certain features of the original second-order scheme of Ponte Castañeda, exactness to second-order in the contrast and existence of an effective energy, but improves on one drawback, which is the gap between the strain-energy formulation and the affine formulation. A numerical example shows the accuracy of the present method. *To cite this article: N. Lahellec, P. Suquet, C. R. Mecanique 332 (2004).*

Résumé

Composites non linéaires : un schéma exact au second ordre pour lequel la formulation en énergie de déformation coïncide avec la formulation affine. Cette Note présente une nouvelle approximation pour l'homogénéisation de composites non linéaires. Cette approximation préserve certaines qualités de la méthode du second ordre de Ponte Castañeda, qui sont l'exactitude au second ordre par rapport au constraste des phases et l'existence d'une énergie effective, mais corrige l'un de ses défauts qui est l'écart entre la méthode de l'énergie et la méthode affine. Un exemple numérique où des résultats exacts sont comparés aux résultats de l'approximation proposée, montre la précision de l'approche. *Pour citer cet article : N. Lahellec, P. Suquet, C. R. Mecanique 332 (2004).*

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Cet article traite de l'homogénéisation de composites non linéaires. Les équations de comportement de chacune des phases du composite sont définies à partir d'un potentiel $w^{(r)}$ par (1). La méthode dévelopée est une extension de la méthode du second ordre initialement proposée par Ponte Castañeda [1].

Son principe est de remplacer dans la définition du comportement homogénéisé (déduit de l'expression (2)), le potentiel $w^{(r)}$ par son développement au *troisième ordre* donné par (3) autour d'une déformation de référence constante par phase $\boldsymbol{\varepsilon}^{(r)}$. Cette expression fait apparaître le développement au second ordre classique de Ponte Castañeda et un terme cubique que l'on approche par un terme linéaire faisant intervenir une seconde déformation de référence constante par phase $\hat{\boldsymbol{\varepsilon}}^{(r)}$ qui est définie par (4).

Les deux déformations de référence $\boldsymbol{\varepsilon}^{(r)}$ et $\hat{\boldsymbol{\varepsilon}}^{(r)}$ sont choisies de façon à rendre stationnaire le potentiel effectif défini par (6). Elles sont solutions des équations (9) et (10), dans lesquelles la déformation est solution du problème d'équilibre linéaire défini par (12). On montre que le choix précédent fait coïncider les estimations du comportement macroscopique données par la méthode énergétique et affine.

Le modèle proposé est testé sur un exemple numérique. Deux cellules de base constituées d'une matrice renforcée par des fibres longues aléatoirement réparties ($c^{(1)} = 0,218$ et $c^{(1)} = 0,5$) sont étudiées en déformations planes. Les constituants sont incompressibles et sont définis par le potentiel en loi puissance (19). Sur la Fig. 1 on compare l'estimation de la contrainte d'écoulement effective, définie par (21), donnée par notre modèle (la résolution de (12) étant réalisée par la méthode des Eléments Finis) avec la valeur exacte (résolution du problème non linéaire par E.F.). Les résultats donnés par notre méthode sont très proches des résultats exacts.

Pour finir, on montre que l'estimation proposée est exacte au second ordre par rapport au contraste et que dans le cas d'inclusions rigides elle correspond exactement à la procédure du second ordre de Ponte Castañeda [1].

1. Motivation

The present study is motivated by difficulties encountered in a separate study on composite materials with elasto-viscoplastic phases. In this study we applied the second-order method of Ponte Castañeda [1], one of the most accurate procedure available to predict the effective properties of nonlinear composites, to an incremental potential. The difficulties which were encountered (as described in [2]) are, by order of importance:

1. The second-order method does not deliver directly an effective stress-strain relation. This relation is obtained by taking the derivative of the effective strain-energy (or complementary energy when a dual approach is followed). When the effective energy $\widetilde{w}$ is not found in closed form, its derivative $\frac{\partial \widetilde{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}})$ has to be evaluated numerically by computing the energy for different values of the overall strain and then approximating the derivative of the energy by a difference quotient. Unfortunately, in the problem of interest in [2], the different terms in these difference quotients correspond to problems which are physically different from the original one (different strain-rates). This gives rise to a first inconsistency which is reflected for instance by the dependence of the results on the time-step in the time-integration of the underlying incremental equations. For the type of problems addressed in [2], the use of a different quotient should be avoided.
2. This difficulty was not encountered when the affine method [3,4] was used. The affine method delivers the effective stress-strain relations at a given strain, without having to compute the response of the composite at other overall strain states. It is based on the resolution of the same thermoelasticity problem as in the original second-order method, but the local stress and strain fields are used differently. In the affine approach the averages of these fields are taken, whereas in the second-order procedure the average of their energy is computed. Unfortunately, as is well-known [4], the results of these two averaging procedures are different and the affine method is less accurate than the second-order method. In particular it is not exact to second-order in the contrast and is not associated to an overall potential.

These observations led us to look for a modification of the original second-order procedure for which the energy approach and the affine approach would match. There are, however, nice features of the original second-order procedure of Ponte Castañeda which we would like to preserve in our modification: firstly, it is exact to second-order in the contrast, and secondly, the effective constitutive relations of the composite derive from an energy (as long as those for the individual phases derive from a potential).

2. Approximate expansion up to order 3 for the effective potential

The composites under consideration in this study are made of N different homogeneous constituents or *phases* $r = 1, \ldots, N$. In a representative volume element V of the composite the individual phases occupy different domains V_r with characteristic functions $\chi^{(r)}(\boldsymbol{x})$ and volume fraction $c^{(r)}$. The spatial average over r.v.e. V and the partial average over domains V_r are denoted with brackets as $\langle \cdot \rangle$ and $\langle \cdot \rangle_r$. The total and partial averages of a function f defined on V are denoted as $\bar{f} = \langle f \rangle$ and $\bar{f}^{(r)} = \langle f \rangle_r$.

The constitutive relations of the individual phases derive from a strain-energy potential $w^{(r)}$:

$$\boldsymbol{\sigma} = \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) \quad \text{in phase } r \tag{1}$$

In all cases considered in this study, the energy-functions $w^{(r)}$ are convex and four times differentiable.

The effective constitutive relations for the composite can be deduced [5] from the effective energy:

$$\widetilde{w}(\bar{\boldsymbol{\varepsilon}}) = \inf_{\boldsymbol{v} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \langle w(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})) \rangle, \quad \text{with } \mathcal{K}(\bar{\boldsymbol{\varepsilon}}) = \{\boldsymbol{v} = \bar{\boldsymbol{\varepsilon}} \cdot \boldsymbol{x} + \boldsymbol{v}^*, \ \boldsymbol{v}^* \text{ periodic on } \partial V\} \tag{2}$$

For simplicity periodic boundary conditions have been chosen on ∂V.

The potentials $w^{(r)}$ of interest in our study are nonquadratic. To simplify the variational problem (2), a Taylor expansion up to third-order of $w^{(r)}$ is taken about a reference strain $\boldsymbol{\varepsilon}^{(r)}$ which is uniform in each phase:

$$w^{(r)}(\boldsymbol{\varepsilon}) \simeq w^{(r)}(\boldsymbol{\varepsilon}^{(r)}) + \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}^{(r)}) : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) + \frac{1}{2}\frac{\partial^2 w^{(r)}}{\partial \boldsymbol{\varepsilon}^2}(\boldsymbol{\varepsilon}^{(r)}) :: (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)})$$
$$+ \frac{1}{6}\frac{\partial^3 w^{(r)}}{\partial \boldsymbol{\varepsilon}^3}(\boldsymbol{\varepsilon}^{(r)}) ::: (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \tag{3}$$

As such, this expansion does not simplify the variational problem (2) since the last term in (3) is cubic with respect to $\boldsymbol{\varepsilon}$.

A further approximation is introduced by linearizing this cubic term:

$$(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \simeq (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}) \tag{4}$$

The new term is now linear with respect to $\boldsymbol{\varepsilon}$ and involves a second 'reference strain' $\hat{\boldsymbol{\varepsilon}}^{(r)}$ which is uniform in each phase. The approximation of the potential $w^{(r)}$ now becomes approximately $w^{(r)}(\boldsymbol{\varepsilon}) \simeq w_{\text{toe}}^{(r)}(\boldsymbol{\varepsilon})$ where:

$$w_{\text{toe}}^{(r)}(\boldsymbol{\varepsilon}) = w^{(r)}(\boldsymbol{\varepsilon}^{(r)}) + \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}^{(r)}) : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) + \frac{1}{2}\frac{\partial^2 w^{(r)}}{\partial \boldsymbol{\varepsilon}^2}(\boldsymbol{\varepsilon}^{(r)}) :: (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)})$$
$$+ \frac{1}{6}\frac{\partial^3 w^{(r)}}{\partial \boldsymbol{\varepsilon}^3}(\boldsymbol{\varepsilon}^{(r)}) ::: (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}) \otimes (\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}) \tag{5}$$

An approximation of the effective potential $\widetilde{w}$ is obtained by substituting (5) into (2).

Following the procedure initiated by Ponte Castañeda and Willis [6] (see also Ponte Castañeda [7]), the approximate effective potential can be rendered stationary with respect to the variables $\boldsymbol{\varepsilon}^{(r)}$ and $\hat{\boldsymbol{\varepsilon}}^{(r)}$:

$$\widetilde{w}(\bar{\boldsymbol{\varepsilon}}) \simeq \underset{\boldsymbol{\varepsilon}^{(r)}}{\text{Stat}} \underset{\hat{\boldsymbol{\varepsilon}}^{(r)}}{\text{Stat}} \inf_{\boldsymbol{v} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \langle w_{\text{toe}}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})) \rangle \tag{6}$$

The stationarity condition with respect to $\boldsymbol{\varepsilon}^{(r)}$ can be written:

$$
\begin{aligned}
\frac{\partial^3 w^{(r)}}{\partial \boldsymbol{\varepsilon}^3}\big(\boldsymbol{\varepsilon}^{(r)}\big) &:: \left[\left\langle \frac{1}{2}\big(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}\big) \right\rangle_r - \frac{1}{6}\big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) \right. \\
&\left. - \frac{1}{3}\big(\langle \boldsymbol{\varepsilon} \rangle_r - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) \right] \\
&+ \frac{1}{6}\frac{\partial^4 w^{(r)}}{\partial \boldsymbol{\varepsilon}^4}\big(\boldsymbol{\varepsilon}^{(r)}\big) ::: \big(\langle \boldsymbol{\varepsilon} \rangle_r - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) = 0
\end{aligned}
\tag{7}
$$

The stationarity condition with respect to $\hat{\boldsymbol{\varepsilon}}^{(r)}$ can be written:

$$
\frac{\partial^3 w^{(r)}}{\partial \boldsymbol{\varepsilon}^3}\big(\boldsymbol{\varepsilon}^{(r)}\big) :: \big(\langle \boldsymbol{\varepsilon} \rangle_r - \boldsymbol{\varepsilon}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\varepsilon}^{(r)}\big) = 0
\tag{8}
$$

There exist different ways of solving the systems of nonlinear equations (7) and (8). The approach followed in the present study consists of identifying $\boldsymbol{\varepsilon}^{(r)}$ with the average strain over phase r:

$$
\boldsymbol{\varepsilon}^{(r)} = \langle \boldsymbol{\varepsilon} \rangle_r \stackrel{\text{def}}{=} \bar{\boldsymbol{\varepsilon}}^{(r)}
\tag{9}
$$

The equations (8) are then identically satisfied whereas (7) reduces to:

$$
\frac{1}{3}N^{(r)}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) :: \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \bar{\boldsymbol{\varepsilon}}^{(r)}\big) \otimes \big(\hat{\boldsymbol{\varepsilon}}^{(r)} - \bar{\boldsymbol{\varepsilon}}^{(r)}\big) = N^{(r)}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) :: \boldsymbol{C}_\varepsilon^{(r)}
\tag{10}
$$

where

$$
N^{(r)}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) = \frac{\partial^3 w^{(r)}}{\partial \boldsymbol{\varepsilon}^3}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big), \qquad \boldsymbol{C}_\varepsilon^{(r)} = \big\langle \big(\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}^{(r)}\big) \otimes \big(\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}^{(r)}\big) \big\rangle_r
\tag{11}
$$

Finally, the Euler equations associated with the minimization with respect to $\boldsymbol{v}$ in (2) correspond to a boundary value problem for a thermoelastic composite material:

$$
\boldsymbol{\sigma} = \boldsymbol{\tau}^{(r)} + \boldsymbol{L}^{(r)} : \big(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(r)}\big) \quad \text{in } V, \quad \text{div}\,\boldsymbol{\sigma} = 0 \quad \text{in } V, \quad \langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}
\tag{12}
$$

where

$$
\boldsymbol{\tau}^{(r)} = \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) + \frac{1}{2}N^{(r)}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) :: \boldsymbol{C}_\varepsilon^{(r)}, \qquad \boldsymbol{L}^{(r)} = \frac{\partial^2 w^{(r)}}{\partial \boldsymbol{\varepsilon}^2}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big)
\tag{13}
$$

An alternative expression of the effective energy can be obtained by taking the average of (5):

$$
\widetilde{w} = \sum_{r=1}^{N} c^{(r)} \left[w^{(r)}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) + \frac{1}{2}\frac{\partial^2 w^{(r)}}{\partial \boldsymbol{\varepsilon}^2}\big(\bar{\boldsymbol{\varepsilon}}^{(r)}\big) :: \boldsymbol{C}_\varepsilon^{(r)} \right]
\tag{14}
$$

This expression *has exactly the same form* as in the second-order procedure of Ponte Castañeda [1], except that the strain field from which the average strain $\bar{\boldsymbol{\varepsilon}}^{(r)}$ derives is the solution of a different thermoelastic problem.

3. Effective constitutive relations

Two (apparently) different expressions for the overall stress and for the effective constitutive relations can be derived from (6) and (12). The first expression is obtained by taking the derivative of the potential (6) with respect to $\bar{\boldsymbol{\varepsilon}}$, whereas the second expression is obtained by taking the average of the stress field solution of (12). Taking the derivative of the potential yields:

$$
\bar{\boldsymbol{\sigma}} = \frac{\partial \widetilde{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) \quad \text{with } \widetilde{w}(\bar{\boldsymbol{\varepsilon}}) = \underset{\boldsymbol{\varepsilon}^{(r)}}{\text{Stat}}\, \underset{\hat{\boldsymbol{\varepsilon}}^{(r)}}{\text{Stat}}\, \underset{\boldsymbol{v} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})}{\text{Inf}} \big\langle w_{\text{toe}}\big(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})\big) \big\rangle
\tag{15}
$$

It becomes:

$$\frac{\partial \widetilde{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) = \left\langle \frac{\partial w_{\text{toe}}}{\partial \boldsymbol{\varepsilon}} : \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\boldsymbol{\varepsilon}}} \right\rangle + \sum_{r=1}^{N} c^{(r)} \left[\left\langle \frac{\partial w_{\text{toe}}^{(r)}}{\partial \boldsymbol{\varepsilon}^{(r)}} \right\rangle_r : \frac{\partial \boldsymbol{\varepsilon}^{(r)}}{\partial \bar{\boldsymbol{\varepsilon}}} + \left\langle \frac{\partial w_{\text{toe}}^{(r)}}{\partial \hat{\boldsymbol{\varepsilon}}^{(r)}} \right\rangle_r : \frac{\partial \hat{\boldsymbol{\varepsilon}}^{(r)}}{\partial \bar{\boldsymbol{\varepsilon}}} \right] \tag{16}$$

The two last terms in the above expression vanish (stationarity of $\langle w_{\text{toe}} \rangle$ with respect to $\boldsymbol{\varepsilon}^{(r)}$ and $\hat{\boldsymbol{\varepsilon}}^{(r)}$). By Hill's lemma, and since $\langle \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\boldsymbol{\varepsilon}}} \rangle = \boldsymbol{I}$, the first term reduces to:

$$\left\langle \frac{\partial w_{\text{toe}}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) \right\rangle : \left\langle \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\boldsymbol{\varepsilon}}} \right\rangle = \left\langle \frac{\partial w_{\text{toe}}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) \right\rangle = \sum_r c^{(r)} \boldsymbol{\tau}^{(r)} \tag{17}$$

The comparison of (17) with (12) shows that $\frac{\partial \widetilde{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) = \langle \boldsymbol{\sigma} \rangle$, where $\boldsymbol{\sigma}$ is the stress field solution of (12).

In conclusion, it has been shown that the constitutive relations obtained by derivation of the effective strain-energy (6) *coincide* with the constitutive relations obtained by averaging the stress and strain fields solution of the thermoelastic problem (12). In short, the strain-energy procedure and the affine procedure coincide.

As a consequence, an alternative expression for the average stress predicted by the third-order expansion method can be obtained by taking the average of the stress field solution of the thermoelasticity problem (12)

$$\bar{\boldsymbol{\sigma}}_{\text{toe}} = \sum_r c^{(r)} \boldsymbol{\tau}^{(r)} = \sum_r c^{(r)} \left(\frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\bar{\boldsymbol{\varepsilon}}^{(r)}) + \frac{1}{2} N^{(r)}(\bar{\boldsymbol{\varepsilon}}^{(r)}) :: \boldsymbol{C}_{\varepsilon}^{(r)} \right) \tag{18}$$

It is seen that the second-order moment of the strain fluctuations $\boldsymbol{C}_{\varepsilon}^{(r)}$ appears explicitly in this expression.

4. A numerical example

The accuracy of the approximation provided by the third-order expansion (5) and the resulting scheme (6) can be assessed by comparing fully nonlinear Finite Element results with the predictions of the approximate scheme. To avoid further approximations which would complicate the understanding of the results, the local problem (12) is also solved numerically by the FEM. We consider two-dimensional composites, made of fibers dispersed in a surrounding matrix. Their microstructure is characterized by the two unit-cells shown in Fig. 1 corresponding to two different fiber volume fractions $c^{(1)} = 0.218$ and $c^{(1)} = 0.5$. Both phases are incompressible power-law materials with the same exponent:

$$w^{(r)}(\boldsymbol{\varepsilon}) = \frac{\sigma_0^{(r)} \varepsilon_0}{m+1} \left(\frac{\varepsilon_{\text{eq}}}{\varepsilon_0} \right)^{m+1} \quad \text{when } \operatorname{tr}(\boldsymbol{\varepsilon}) = 0, \quad +\infty \quad \text{otherwise} \tag{19}$$

The macroscopic loading condition imposed to the unit-cell is an in-plane deformation in the form:

$$\bar{\boldsymbol{\varepsilon}} = \bar{\varepsilon}_{11}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 - \boldsymbol{e}_2 \otimes \boldsymbol{e}_2) \tag{20}$$

Due to the lack of symmetry of the unit-cell the overall stress is a general in-plane stress (there is no longitudinal stress since the overall strain is a pure shear). An effective flow stress $\tilde{\sigma}_0$ for the composite can be defined as

$$\tilde{\sigma}_0 = \bar{\sigma}_{\text{eq}} \left(\frac{\varepsilon_0}{\bar{\varepsilon}_{\text{eq}}} \right)^m \tag{21}$$

The comparison are carried out for two specific unit cells. The predictions of the approximate scheme and of exact calculations are shown in Fig. 1 for a contrast $\sigma_0^{(1)}/\sigma_0^{(2)} = 5$ (phase 1 = fibers). The two sets of results can be hardly distinguished when $c^{(1)} = 0.218$ and are in good agreement when $c^{(1)} = 0.5$. Similar comparison for other values of the contrast and more general microstructures is left for future work.
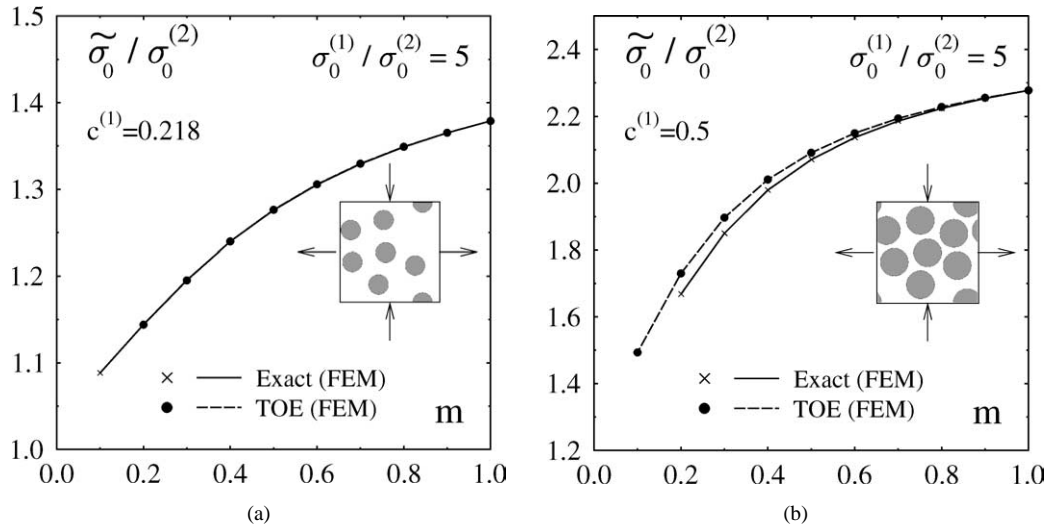
Fig. 1. Two-dimensional composites. Fibers stronger than the matrix $\sigma_0^{(1)}/\sigma_0^{(2)} = 5$. Effective flow-stress (21) as a function of the nonlinearity exponent m. (a) $c^{(1)} = 0.218$; (b) $c^{(1)} = 0.5$.

5. Comments

5.1. Composites with small contrast: exactness of the method to second-order in the contrast

The composites considered in this section have *a small contrast*. The energy functions $w^{(r)}$ deviate from a uniform energy w_0 by a small quantity characterized by a small parameter t.

$$w^{(r)}(\boldsymbol{\varepsilon}) = w_0(\boldsymbol{\varepsilon}) + t\delta w^{(r)}(\boldsymbol{\varepsilon})$$

An exact expansion in powers of t of the effective properties of the composite and of the local stress and strain fields as been performed by Ponte Castañeda and Suquet [8]. It reads as:

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}} + t\dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \frac{t^2}{2}\ddot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \mathrm{O}(t^3), \qquad \boldsymbol{\sigma}_t(\boldsymbol{x}) = \frac{\partial w^0}{\partial\bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) + t\dot{\boldsymbol{\sigma}}^0(\boldsymbol{x}) + \frac{t^2}{2}\ddot{\boldsymbol{\sigma}}^0(\boldsymbol{x}) + \mathrm{O}(t^3) \qquad (22)$$

The first order terms $\dot{\boldsymbol{\varepsilon}}^0$ and $\dot{\boldsymbol{\sigma}}^0$ solve the following linear thermoelastic problem

$$\dot{\boldsymbol{\sigma}}^0(\boldsymbol{x}) = \boldsymbol{L}^0 : \dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \boldsymbol{\tau}(\boldsymbol{x}), \quad \mathrm{div}(\dot{\boldsymbol{\sigma}}^0) = 0, \quad \langle\dot{\boldsymbol{\varepsilon}}^0\rangle = 0 \qquad (23)$$

where

$$\boldsymbol{L}^0 = \frac{\partial^2 w^0}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}(\bar{\boldsymbol{\varepsilon}}), \qquad \boldsymbol{\tau}(\boldsymbol{x}) = \frac{\partial}{\partial\boldsymbol{\varepsilon}}\delta w(\boldsymbol{x})(\bar{\boldsymbol{\varepsilon}})$$

Similarly the second-order terms $\ddot{\boldsymbol{\varepsilon}}^0$ and $\ddot{\boldsymbol{\sigma}}^0$ solve another linear thermoelastic problem

$$\ddot{\boldsymbol{\sigma}}^0(\boldsymbol{x}) = \boldsymbol{L}^0 : \ddot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \boldsymbol{\theta}(\boldsymbol{x}), \qquad \mathrm{div}(\ddot{\boldsymbol{\sigma}}^0) = 0, \quad \langle\ddot{\boldsymbol{\varepsilon}}^0\rangle = 0, \quad \text{where} \qquad (24)$$

$$\boldsymbol{\theta}(\boldsymbol{x}) = 2\delta\boldsymbol{L}(\boldsymbol{x}) : \dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \boldsymbol{N}^0\dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) \otimes \dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}), \quad \delta\boldsymbol{L}(\boldsymbol{x}) = \frac{\partial^2}{\partial\boldsymbol{\varepsilon}^2}\delta w(\boldsymbol{x}, \bar{\boldsymbol{\varepsilon}}), \quad \boldsymbol{N}^0 = \frac{\partial^3 w^0}{\partial\boldsymbol{\varepsilon}^3}(\bar{\boldsymbol{\varepsilon}}) \qquad (25)$$

A similar expansion can be performed for the approximate stress and strain fields solution of the thermoelasticity problem (12) (reference to the fact that these fields are solution of the approximate thermoelastic problem obtained by the third-order expansion is added for clarity):

$$\boldsymbol{\varepsilon}_{\text{toe}}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}} + t\dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + \frac{t^2}{2}\ddot{\boldsymbol{\varepsilon}}^0_{\text{toe}}(\boldsymbol{x}) + \mathrm{O}(t^3), \qquad \boldsymbol{\sigma}_{\text{toe}}(\boldsymbol{x}) = \frac{\partial w^0}{\partial\bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) + t\dot{\boldsymbol{\sigma}}^0(\boldsymbol{x}) + \frac{t^2}{2}\ddot{\boldsymbol{\sigma}}^0_{\text{toe}}(\boldsymbol{x}) + \mathrm{O}(t^3) \qquad (26)$$

The terms of order 0 and 1 coincide with the corresponding terms in the exact expansion (22). The terms of order 2 $\ddot{\boldsymbol{\varepsilon}}^0_{\text{toe}}$ and $\ddot{\boldsymbol{\sigma}}^0_{\text{toe}}$ solve the following system

$$\ddot{\boldsymbol{\sigma}}^0_{\text{toe}} = \boldsymbol{L}^0 : \ddot{\boldsymbol{\varepsilon}}^0_{\text{toe}} + \boldsymbol{\theta}_{\text{toe}}, \quad \operatorname{div}(\ddot{\boldsymbol{\sigma}}^0_{\text{toe}}) = 0, \quad \langle\ddot{\boldsymbol{\varepsilon}}^0_{\text{toe}}\rangle = 0 \qquad (27)$$

where the eigenstress $\boldsymbol{\theta}_{\text{toe}}$ in phase r reads:

$$\boldsymbol{\theta}_{\text{toe}}(\boldsymbol{x}) = 2\delta\boldsymbol{L}^{(r)} : \dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) + 2\boldsymbol{N}^0(\bar{\boldsymbol{\varepsilon}}) :: \left[\dot{\bar{\boldsymbol{\varepsilon}}}^{0(r)} \otimes \left(\dot{\boldsymbol{\varepsilon}}^0(\boldsymbol{x}) - \dot{\bar{\boldsymbol{\varepsilon}}}^{0(r)}\right)\right] + \boldsymbol{N}^0(\bar{\boldsymbol{\varepsilon}}) : \langle\dot{\boldsymbol{\varepsilon}}^0 \otimes \dot{\boldsymbol{\varepsilon}}^0\rangle_r \qquad (28)$$

It is readily seen that $\langle\boldsymbol{\theta}_{\text{toe}}\rangle_r = \langle\boldsymbol{\theta}\rangle_r$ and therefore that $\langle\ddot{\boldsymbol{\sigma}}^0_{\text{toe}}\rangle_r = \langle\ddot{\boldsymbol{\sigma}}^0\rangle_r$. Then it results from the second-order expansions (22) and (26) that $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\sigma}}_{\text{toe}}$ coincide up to second-order in t.

5.2. Two-phase rigidly-reinforced composites

We consider now the case of two-phase rigidly-reinforced composites (the contrast between the phases is therefore infinite). In this case the average strain in the phases is completely determined:

$$\bar{\boldsymbol{\varepsilon}}^{(1)} = \boldsymbol{0}, \qquad \bar{\boldsymbol{\varepsilon}}^{(2)} = \frac{1}{c^{(2)}}\bar{\boldsymbol{\varepsilon}} \qquad (29)$$

where phase 1 is the rigid phase. The second moments of the strain field in the deformable phase can be deduced from the effective energy of the thermoelastic composite as:

$$\langle\boldsymbol{\varepsilon}\otimes\boldsymbol{\varepsilon}\rangle_2 = \frac{1}{c^{(2)}}\bar{\boldsymbol{\varepsilon}} : \frac{\partial\tilde{\boldsymbol{L}}}{\partial\boldsymbol{L}^{(2)}} : \bar{\boldsymbol{\varepsilon}}, \quad \boldsymbol{C}^{(r)}_\varepsilon = \frac{1}{c^{(2)}}\bar{\boldsymbol{\varepsilon}} : \frac{\partial\boldsymbol{\Delta}\tilde{\boldsymbol{L}}}{\partial\boldsymbol{L}^{(2)}} : \bar{\boldsymbol{\varepsilon}}, \quad \text{where} \quad \boldsymbol{\Delta}\tilde{\boldsymbol{L}} = \tilde{\boldsymbol{L}} - \frac{1}{c^{(2)}}\boldsymbol{L}^{(2)} \qquad (30)$$

Finally the effective energy predicted by the present method can be written as:

$$\tilde{w}(\bar{\boldsymbol{\varepsilon}}) = c^{(2)}w\left(\frac{1}{c^{(2)}}\bar{\boldsymbol{\varepsilon}}\right) + \frac{1}{2}\bar{\boldsymbol{\varepsilon}} : \boldsymbol{\Delta}\tilde{\boldsymbol{L}} : \bar{\boldsymbol{\varepsilon}} \qquad (31)$$

It coincides with the effective energy predicted by the second-order procedure [1].

5.3. Further comments

- As shown by relation (5.30) in Ponte Castañeda and Suquet [5] (see also relation (35) in [4]), the difference between the macroscopic stress predicted by the standard affine procedure and the original second-order procedure can be expressed in terms of $\boldsymbol{N}^{(r)}$, $\boldsymbol{C}^{(r)}_\varepsilon$ and an additional term $\mathrm{d}\bar{\boldsymbol{\varepsilon}}^{(r)}/\mathrm{d}\bar{\boldsymbol{\varepsilon}}$ which is not explicit, as:

$$\bar{\boldsymbol{\sigma}}_{\text{soe}} = \sum_r c^{(r)}\left[\frac{\partial w^{(r)}}{\partial\boldsymbol{\varepsilon}}(\bar{\boldsymbol{\varepsilon}}^{(r)}) + \frac{1}{2}\boldsymbol{N}^{(r)}(\bar{\boldsymbol{\varepsilon}}^{(r)}) :: \boldsymbol{C}^{(r)}_\varepsilon : \frac{\mathrm{d}\bar{\boldsymbol{\varepsilon}}^{(r)}}{\mathrm{d}\bar{\boldsymbol{\varepsilon}}}\right] \qquad (32)$$

This relation suggests that one way to close the gap between the affine and the second-order procedure would be to add a term involving $\boldsymbol{N}^{(r)}$ and $\boldsymbol{C}^{(r)}_\varepsilon$ to the polarization stress field $\partial w^{(r)}/\partial\boldsymbol{\varepsilon}(\bar{\boldsymbol{\varepsilon}}^{(r)})$ defining the thermoelastic problem in the original second-order procedure. This is exactly what the present method does through (13) which leads to (18).

- The present method makes use of the average of the second-order fluctuations of the strain field in each phase (see Eq. (10)) as in the new second-order method of Ponte Castañeda [7]. However the predictions of the present method seem to be closer to the original second-order method [1].
- When the contrast between the phases is varied, the above results show that the present method coincides with the original second-order procedure of Ponte Castañeda in the two limiting cases of small contrast (coincidence up to second-order) and in the case of rigidly-reinforced composites (the case of voided materials has not been investigated so far). Therefore we do not expect large differences between the predictions of the two methods regarding the effective properties of the composite, even at intermediate values of the contrast. The main advantage of the method is, in our opinion, that it combines the advantages of the energy formulation (exactness to second-order) with the advantages of the affine procedure in which the approximate local stress and strain fields are defined as the solutions of (12).
- As shown above, the present method has no gap between the strain-energy formulation and the affine formulation. However, there exists a gap between the strain-energy formulation and the complementary energy formulation.

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