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Consistency of homogenization schemes in linear poroelasticity

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Abstract

In view of extending classical micromechanics of poroelasticity to the non-saturated regime, one has to deal with different pore stresses which may be affected by the size and the shape of the pores. Introducing the macrostrain and these pore stresses as loading parameters, the macrostress of a representative volume element of a porous material can be derived by means of Levin's theorem or by means of the direct formulation of the stress average rule, respectively. A consistency requirement for a given homogenization scheme is obtained from the condition that the two approaches should yield identical results. Classical approaches (Mori–Tanaka scheme, self-consistent scheme) are shown to be only conditionally consistent. In contrast, the Ponte Castañeda–Willis scheme proves to provide consistent descriptions both of porous matrix-inclusion composites and of porous polycrystals. ***To cite this article: B. Pichler, L. Dormieux, C. R. Mecanique 336 (2008).***

Résumé

Cohérence des approches d'homogénéisation en poroélasticité linéaire. En vue d'étendre l'approche micromécanique de la poroélasticité dans le régime non saturé, il convient de prendre en compte différentes contraintes dans les pores, en fonction de leur forme et de leur taille. En adoptant la déformation macroscopique et ces contraintes de pores comme paramètres de chargement, la contrainte macroscopique peut être formulée à partir du théorème de Levin, ou bien en explicitant directement la règle de moyenne sur les contraintes. Une condition de cohérence du schéma d'homogénéisation retenu est obtenue en écrivant l'égalité des résultats de ces deux approches. On montre que les schémas classiques (Mori–Tanaka et autocohérent) ne satisfont cette condition que dans des cas particuliers. En revanche, elle est toujours vérifiée par le schéma de Ponte Castañeda et Willis. ***Pour citer cet article : B. Pichler, L. Dormieux, C. R. Mecanique 336 (2008).***

Keywords: Porous media; Micromechanics; Levin's theorem; Mori–Tanaka scheme; Self-consistent scheme; Ponte Castañeda–Willis scheme

Mots-clés : Milieux poreux ; Micromécanique ; Théorème de Levin ; Schéma de Mori–Tanaka ; Schéma autocohérent ; Schéma Ponte Castañeda–Willis

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1. Introduction

Drying of deformable porous media results in their shrinkage, and it may even cause cracking when shrinkage deformations are hindered by kinematic constraints. The description of drying requires consideration of partially saturated conditions. Because of the related surface tensions which are to be considered in all interfaces between solid, liquid, and gaseous matters, average pore stresses depend both on pore shape and on pore size (Section 2). Micromechanics-based drying analyses may raise the need to consider *different* pore morphologies exhibiting *different* average pore stresses on the *same* level of observation. This is the motivation for the present work, where we deal with a representative volume element (RVE) of a microheterogeneous porous material, satisfying the separation of scales requirement. The work is carried out within the framework of linear poroelasticity. Introducing the macrostrain and average pore stresses as loading parameters, we study the capability of different micromechanical homogenization schemes to provide reliable estimates of average phase quantities such as averages of stresses or of strains.

First, the Mori–Tanaka [1,2] and the self-consistent scheme [3,4] are considered, which can be interpreted as being directly related to generalized Eshelby problems, see, e.g., [5,6]. By analogy to [7], the consistency of both schemes is investigated, (i) by expressing the macrostress of the RVE based on Levin's theorem [8,9] as well as based on the direct implementation of the stress average rule, and (ii) by comparing these model predictions which, doubtlessly, should be equal (Section 3).

Secondly, the Ponte Castañeda–Willis scheme [10] is considered, i.e. generalized Hashin–Shtrikman estimates [11] resting on phase distribution statistics with ellipsoidal symmetries. We implement this approach with phase prestresses, and we prove its consistency with Levin's theorem (Section 4).

2. Porous materials under partially saturated conditions

Let Ω denote the domain occupied by an RVE of a microheterogeneous material, comprising n_s solid phases ($i = 1, \ldots, n_s$) capturing the solid domain Ω^s and n_p pore families ($j = n_s + 1, \ldots, n_\alpha = n_s + n_p$) constituting the pore space Ω^p. As loading parameters, we introduce the uniform macrostrain $\boldsymbol{E}$ and the average pore stresses $\boldsymbol{\pi}^j$, $j - n_s = 1, \ldots, n_p$. The stress field $\boldsymbol{\sigma}$, the strain field $\boldsymbol{\varepsilon}$, and the displacement field $\underline{\xi}$, characterizing the response of the RVE in linear poroelasticity, satisfy

$$
\begin{aligned}
&\operatorname{div} \boldsymbol{\sigma} = 0 \quad (\Omega), && \boldsymbol{\sigma} = \mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon} + \boldsymbol{\pi}(\underline{x}) \quad (\Omega) \\
&\underline{\xi} = \boldsymbol{E} \cdot \underline{x} \quad (\partial\Omega), && \boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \underline{\xi} + {}^t\,\nabla \underline{\xi}) \quad (\Omega)
\end{aligned}
\tag{1}
$$

where $\partial\Omega$ stands for the boundary of the RVE. We consider both the microheterogeneous stiffness tensors $\mathbb{C}(\underline{x})$ and the prestress tensors $\boldsymbol{\pi}(\underline{x})$ to be phase-wise constant:

$$
\mathbb{C}(\underline{x}) = \begin{cases} \mathbb{C}^i & (\Omega^i \subseteq \Omega^s), \\ 0 & (\Omega^p), \end{cases} \qquad \boldsymbol{\pi}(\underline{x}) = \begin{cases} 0 & (\Omega^s) \\ \boldsymbol{\pi}^j & (\Omega^j \subseteq \Omega^p) \end{cases}
\tag{2}
$$

Given ellipsoidal pores shapes in the considered framework of partially saturated conditions, a part of the volume of each pore is liquid-occupied, while the rest of the pore is gas-filled. The prestress tensor $\boldsymbol{\pi}^j$ of the j-th pore family accounts (i) for the average pore pressure (the pore-volume average over liquid and gas pressures) and for the surface tensions prevailing in all interfaces between solid, liquid, and gaseous matters [12]. Consequently, all $\boldsymbol{\pi}^j$ are symmetric ($\pi^j_{k\ell} = \pi^j_{\ell k}$), but anisotropic for non-spherical pores, see, e.g., [13] for the average pore stress of a partially saturated penny-shaped crack.

Average pore stresses within spherical pores are pore size-dependent, because the intensity of the surface tension effects depends on the pore radius. The description of *progressive* drying shrinkage with decreasing liquid saturation requires consideration of several pore sizes. Since the pore radii spectrum remains commonly on *one* scale of observation, spherical pores of different sizes are introduced in one homogenization step [14]. The size-dependent average pore stresses, in turn, raise the need to introduce spherical pores of *different* sizes as *distinct* phases. Accordingly, pores of *one family* are considered in the following to exhibit not only the same shape and the same orientation, but also the same size.

Denoting the average of a (tensorial) quantity $\mathbb{Q}$ over the volume of the RVE as $\overline{\mathbb{Q}}$, and using Levin's theorem [8,9] to express the RVE-related macrostress $\boldsymbol{\Sigma} = \bar{\boldsymbol{\sigma}}$, the first state equation of poroelasticity is obtained in the form

$$\boldsymbol{\Sigma} = \mathbb{C}^{\text{hom}} : \boldsymbol{E} + \overline{\boldsymbol{\pi} : \mathbb{A}}, \qquad \mathbb{C}^{\text{hom}} = \overline{\mathbb{C} : \mathbb{A}} \tag{3}$$

where $\mathbb{A}$ denotes the microheterogeneous strain concentration tensor. Since during the derivation of (3) repeatedly use is made of Hill's theorem (see, e.g., [12]), the validity of Levin's theorem (3) requires the microscopic displacement field $\underline{\xi}$ to be kinematically admissible and the stress field $\boldsymbol{\sigma}$ to be statically admissible, which is noted for later reference. Eq. (3) can be interpreted as an elegant way of writing the stress average rule, the direct formulation of which reads—under consideration of (2)—as

$$\boldsymbol{\Sigma} = \sum_{r=1}^{n_\alpha} \varphi_r \bar{\boldsymbol{\sigma}}^r = \sum_{i=1}^{n_s} \varphi_i \mathbb{C}^i : \bar{\boldsymbol{\varepsilon}}^i + \sum_{j=(n_s+1)}^{n_\alpha} \varphi_j \boldsymbol{\pi}^j. \tag{4}$$

$\bar{\boldsymbol{\sigma}}^r$ stands for the volume average of $\boldsymbol{\sigma}$ over Ω^r (intrinsic phase average) and φ_r denotes the volume fractions of the r-th material phase. Eqs. (3) and (4) are rigorously equivalent from a theoretical viewpoint.

3. Consistency of homogenization schemes based on generalized Eshelby problems

In general, analytical expressions for strain concentration tensors are not available. As a remedy, they are estimated based on homogenization schemes. Regarding approaches which are directly related to generalized Eshelby problems, the following ansatz for the average phase strains $\bar{\boldsymbol{\varepsilon}}^r$ is made [5,6,12]:

$$\bar{\boldsymbol{\varepsilon}}^r = \mathbb{A}^r_\infty : \left(\boldsymbol{E}^0 - \mathbb{P}^r : \boldsymbol{\pi}^r\right), \quad \mathbb{A}^r_\infty = \left[\mathbb{I} + \mathbb{P}^r : (\mathbb{C}^r - \mathbb{C}^0)\right]^{-1}, \quad \forall r = 1, \ldots, n_\alpha \tag{5}$$

$\bar{\boldsymbol{\varepsilon}}^r$ can be interpreted as the spatially constant strain prevailing in an ellipsoidal inclusion (with elastic stiffness $\mathbb{C}^r$ and with prestress $\boldsymbol{\pi}^r$) which is embedded in an infinite matrix of elastic stiffness $\mathbb{C}^0$ subjected (at infinity) to Hashin-type [15] displacement boundary conditions referring to uniform strain $\boldsymbol{E}^0$. Accordingly, $\mathbb{P}^r$ stands for the Hill tensor of this ellipsoidal inclusion and $\mathbb{I}$ denotes the symmetric 4-th order identity tensor. The auxiliary strain $\boldsymbol{E}^0$ is related to the RVE-related macrostrain $\boldsymbol{E}$ such that the strain average rule $\boldsymbol{E} = \bar{\boldsymbol{\varepsilon}}$ is satisfied

$$\boldsymbol{E}^0 = \mathbb{L} : (\boldsymbol{E} + \boldsymbol{E}^p), \quad \mathbb{L}^{-1} = \overline{\mathbb{A}_\infty}, \quad \boldsymbol{E}^p = \sum_{j=(n_s+1)}^{n_\alpha} \varphi_j \mathbb{A}^j_\infty : \mathbb{P}^j : \boldsymbol{\pi}^j \tag{6}$$

Inserting (6) into (5) delivers the average phase strains as

$$\bar{\boldsymbol{\varepsilon}}^r = \mathbb{A}^r_{\text{esh}} : (\boldsymbol{E} + \boldsymbol{E}^p) - \mathbb{A}^r_\infty : \mathbb{P}^r : \boldsymbol{\pi}^r, \qquad \mathbb{A}^r_{\text{esh}} = \mathbb{A}^r_\infty : \mathbb{L} \tag{7}$$

where $\mathbb{A}^r_{\text{esh}}$ stands for the strain concentration tensor of schemes related to generalized Eshelby problems.

3.1. Remarks on the diagonal symmetry of homogenized stiffness tensors of porous media

Stiffness estimates follow from inserting $\mathbb{A}^r_{\text{esh}}$ from (7) into Eq. $(3)_2$. Mori–Tanaka estimates for matrix-inclusion composites are obtained by choosing $\mathbb{C}^0$ to be equal to the matrix stiffness $\mathbb{C}^s$ [5,6]. They are only conditionally symmetric [16]. As regards matrix-inclusion composites where all inclusions are pores with the same (vanishing) stiffness, symmetry of Mori–Tanaka stiffness estimates is ensured [16], which is noted for later reference. Self-consistent estimates for polycrystals representing highly disordered arrangements of material phases are obtained by choosing $\mathbb{C}^0$ to be equal to the homogenized stiffness $\mathbb{C}^{\text{hom}}$ [5,6], which raises the need for an iterative computation of $\mathbb{C}^{\text{hom}}$. Though there exists no rigorous proof for the symmetry of $\mathbb{C}^{\text{hom}}$, all numerical implementations of the self-consistent scheme used herein have so far yielded symmetric stiffness estimates.

3.2. Assessment of consistency with Levin's theorem

The consistency of the direct implementation of the stress average rule within the framework of the Mori–Tanaka scheme with the macrostress derived from Levin's theorem has already been investigated in the case of thermal loading applied to a two-phase material in [7]. We follow this line of consistency assessment, but our main focus lies on porous materials comprising not only *one* pore phase but *arbitrarily many* pore families with different pore stresses.

Inserting the average phase strains $\bar{\boldsymbol{\varepsilon}}^r$ and the strain concentration tensor $\mathbb{A}^r_{\text{esh}}$ from (7) into (4) and into (3), respectively, and defining $\delta\boldsymbol{\Sigma}$ as the difference between the two expressions for $\boldsymbol{\Sigma}$, yields the following consistency condition

$$\delta\boldsymbol{\Sigma} = \sum_{j=(n_s+1)}^{n_\alpha} \varphi_j \big(\boldsymbol{\pi}^j : (\mathbb{I} - \mathbb{A}^j_{\text{esh}}) + \mathbb{C}^{\text{hom}} : \mathbb{A}^j_\infty : \mathbb{P}^j : \boldsymbol{\pi}^j\big) = 0 \tag{8}$$

Considering the symmetries $C_{ijk\ell} = C_{jik\ell} = C_{ij\ell k} = C_{k\ell ij}$ of both $\mathbb{C}^{\text{hom}}$ and $\mathbb{C}^0$, as well as the symmetries $\pi_{k\ell} = \pi_{\ell k}$ of the prestress tensors $\boldsymbol{\pi}^j$, condition (8) can be re-arranged to take the form

$$\delta\boldsymbol{\Sigma} = \sum_{j=(n_s+1)}^{n_\alpha} \varphi_j \boldsymbol{\pi}^j : \big[\mathbb{I} - \mathbb{A}^j_\infty : \mathbb{L} + {}^t(\mathbb{C}^{\text{hom}} : \mathbb{A}^j_\infty : \mathbb{C}^{0-1}) - \mathbb{C}^{0-1} : \mathbb{C}^{\text{hom}}\big] = 0 \tag{9}$$

where ${}^t\mathbb{Q}$ stands for the transpose of the 4th order tensor $\mathbb{Q}$, reading in index notation: ${}^t(Q_{ijk\ell}) = (Q_{k\ell ij})$.

3.3. Frequently considered special case: Two-phase materials with one pore family

For a two-phase material comprising one solid phase (s) and one pore family (p) exhibiting an arbitrary (but symmetric) prestress $\boldsymbol{\pi}^p$, consistency equation (8) can be re-arranged into the form

$$\mathbb{A}^p_\infty : \big[(\mathbb{P}^s - \mathbb{P}^p) : (\mathbb{C}^0 : \mathbb{C}^{s-1} - \mathbb{I})\big] : \boldsymbol{\pi}^p = 0 \tag{10}$$

Eq. (10) is satisfied (i) if the elastic stiffness of the infinite matrix of the generalized Eshelby problem is equal to the one of the solid phase ($\mathbb{C}^0 = \mathbb{C}^s$), and/or (ii) if the Hill tensors of the solid and of the pores are identical ($\mathbb{P}^s = \mathbb{P}^p$). Condition (i) is satisfied when relying on the *Mori–Tanaka scheme* ($\mathbb{C}^0 = \mathbb{C}^s$). Accordingly, the Mori–Tanaka scheme is consistent with Levin's theorem when used for the description of a two-phase material with one pore family, no matter what Hill tensor is associated with the pores; see [7] for a similar consistency conclusion. When relying on the *self-consistent scheme* ($\mathbb{C}^0 = \mathbb{C}^{\text{hom}}$), condition (i) is violated since $\mathbb{C}^{\text{hom}} \neq \mathbb{C}^s$. Consequently, consistency of the self-consistent scheme requires condition (ii) to be satisfied, that is, the Hill tensors associated with the solid and with the pores, respectively, must be identical. Given $\mathbb{P}^s = \mathbb{P}^p$, it can be shown [12] that $\mathbb{L} = \mathbb{I}$, which is noted for later reference.

3.4. Matrix-inclusion composites with n_p pore families: consistency of the Mori–Tanaka scheme

Consider a material comprising *one* solid matrix and arbitrarily many prestressed pore families, and let us investigate the consistency of the Mori–Tanaka scheme by choosing $\mathbb{C}^0 = \mathbb{C}^s$ in (9). It is noteworthy that Mori–Tanaka stiffness estimates are symmetric for this class of composites, see Subsection 3.1 and [16]. Given n_p pore families with *different* average pore stresses, each summand in condition (9) must vanish, since the prestresses of the different pore families are independent from each other:

$$\boldsymbol{\pi}^j : \big[\mathbb{I} - \mathbb{A}^j_\infty : \mathbb{L} + {}^t(\mathbb{C}^{\text{hom}} : \mathbb{A}^j_\infty : \mathbb{C}^{s-1}) - \mathbb{C}^{s-1} : \mathbb{C}^{\text{hom}}\big] = 0 \quad \forall j = n_s + 1, \ldots, n_\alpha \tag{11}$$

All n_p conditions (11) can be shown to be satisfied, if all pore families are associated with the *same* Hill tensor, since this property brings (11) back to (10) specified for $\mathbb{C}^0 = \mathbb{C}^s$. Given that n_p pore families with *different* pore prestresses are associated with *different* Hill tensors, however, (11) is, in general, not satisfied. This highlights that the Mori–Tanaka scheme is only conditionally consistent with Levin's theorem, even if the related stiffness estimate exhibits diagonal symmetry ($C^{\text{hom}}_{ijk\ell} = C^{\text{hom}}_{k\ell ij}$).

3.5. Polycrystals with n_s solid phases and n_p pore families: consistency of the self-consistent scheme

The consistency of the self-consistent scheme is studied in the framework of a polycrystal comprising a highly disordered arrangement of n_s solid phases and n_p prestressed pore families. To this end, we specify (9) for $\mathbb{C}^0 = \mathbb{C}^{\text{hom}}$

and we consider that each summand in the obtained consistency equation must vanish, since the prestresses of the different pore families are independent from each other:

$$\boldsymbol{\pi}^j : \big[\mathbb{A}^j_\infty : \mathbb{L} - {}^t(\mathbb{C}^{\text{hom}} : \mathbb{A}^j_\infty : \mathbb{C}^{\text{hom}-1})\big] = 0 \quad \forall j = n_s+1, \dots, n_\alpha \tag{12}$$

Noting that ${}^t(\mathbb{C}^{\text{hom}} : \mathbb{A}^j_\infty : \mathbb{C}^{\text{hom}-1}) = \mathbb{A}^j_\infty$, all n_p conditions (12) are readily seen to be satisfied if

$$\mathbb{L} = \mathbb{I} \tag{13}$$

Remarkably, (13) was already obtained at the end of Subsection 3.3. Condition (13) is satisfied in the special cases where all phases are associated with the *same* Hill tensor [12]. As regards polycrystals built up by phases associated with different Hill tensors, Eq. (13) is, in general, not satisfied. Hence, the self-consistent scheme is only conditionally consistent with Levin's theorem.

4. Ponte Castañeda–Willis scheme: consistency of generalized Hashin–Shtrikman estimates

4.1. Extension of the PCW scheme towards consideration of phase-wise constant prestress

The Ponte Castañeda–Willis scheme [10] allows for a sound consideration of phase distribution statistics with ellipsoidal symmetry. In the following, we implement this approach with phase prestresses. The related strain-energy function of any point $\underline{x} \in \Omega$ takes the form $W(\underline{x}, \boldsymbol{\varepsilon}) = \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon} + \boldsymbol{\pi}(\underline{x}) : \boldsymbol{\varepsilon}$. Let W^0 denote the strain-energy function associated with a reference material with elastic stiffness $\mathbb{C}^0$ chosen such that $\boldsymbol{\varepsilon} : (\mathbb{C}^0 - \mathbb{C}^r) : \boldsymbol{\varepsilon} \geqslant 0$, for all $\boldsymbol{\varepsilon} \neq 0$ and for all material phases $r = 1, \dots, n_\alpha$. The Legendre transform gives

$$(W - W^0)^*(\underline{x}, \boldsymbol{\tau}) = \min_{\boldsymbol{\varepsilon}} \big\{\boldsymbol{\tau} : \boldsymbol{\varepsilon} - \big[W(\underline{x}, \boldsymbol{\varepsilon}) - W^0(\boldsymbol{\varepsilon})\big]\big\} = \frac{1}{2}(\boldsymbol{\tau} - \boldsymbol{\pi}) : (\mathbb{C} - \mathbb{C}^0)^{-1} : (\boldsymbol{\tau} - \boldsymbol{\pi}) \tag{14}$$

Assuming both the polarizations $\boldsymbol{\tau}$ and the prestresses $\boldsymbol{\pi}$ to be phase-wise constant and following the line of [10], the sought upper bound for the effective (RVE-related) strain energy can be expressed as

$$\begin{aligned} W^{\text{eff}} \leqslant \min_{\boldsymbol{\tau}} \Bigg[& \frac{1}{2}\boldsymbol{E} : \mathbb{C}^0 : \boldsymbol{E} + \boldsymbol{\tau} : \boldsymbol{E} - \frac{1}{2}\sum_{r=1}^{n_\alpha}\sum_{s=1}^{n_\alpha}(\boldsymbol{\tau}^r - \boldsymbol{\tau}^1) : \mathbb{G}^{rs} : (\boldsymbol{\tau}^s - \boldsymbol{\tau}^1) \\ & - \frac{1}{2}\sum_{r=1}^{n_\alpha}\varphi_r(\boldsymbol{\tau}^r - \boldsymbol{\pi}^r) : (\mathbb{C}^r - \mathbb{C}^0)^{-1} : (\boldsymbol{\tau}^r - \boldsymbol{\pi}^r)\Bigg] \end{aligned} \tag{15}$$

where $\mathbb{G}^{rs} = \int_\Omega\{\int_\Omega \chi^r(\underline{x})[\chi^s(\underline{x}') - \varphi_s]\mathbb{\Gamma}^0(\underline{x} - \underline{x}')\,\mathrm{d}\underline{x}'\}\,\mathrm{d}\underline{x}$ with $\chi^r(\underline{x} \in \Omega^s) = \delta_{rs}$ as the characteristic function of phase r, and with $\mathbb{\Gamma}^0$ as a linear integral operator whose kernel is linked to the Green's function [10]. Polarizations minimizing the r.h.s. of (15) read as

$$\begin{aligned} & \boldsymbol{\tau}^1 - \boldsymbol{\pi}^1 = \Bigg[\boldsymbol{E} + \frac{1}{\varphi_1}\sum_{r=2}^{n_\alpha}\sum_{s=2}^{n_\alpha}(\boldsymbol{\tau}^s - \boldsymbol{\tau}^1) : \mathbb{G}^{rs}\Bigg] : (\mathbb{C}^1 - \mathbb{C}^0) \\ & (\boldsymbol{\tau}^i - \boldsymbol{\pi}^i) : (\mathbb{C}^i - \mathbb{C}^0)^{-1} + \frac{1}{\varphi_i}\sum_{r=2}^{n_\alpha}(\boldsymbol{\tau}^r - \boldsymbol{\tau}^1) : \mathbb{G}^{ri} = \boldsymbol{E}, \quad i = 2, \dots, n_\alpha \end{aligned} \tag{16}$$

Re-inserting the optimal polarizations into (15) gives

$$W^{\text{eff}} \leqslant \frac{1}{2}\boldsymbol{E} : \mathbb{C}^0 : \boldsymbol{E} + \frac{1}{2}\bar{\boldsymbol{\tau}} : \boldsymbol{E} \tag{17}$$

Under the assumption of ellipsoidal statistical distribution of phases, the ensemble average of $\mathbb{G}^{rs}$ (denoted as $[\![\mathbb{G}^{rs}]\!]$) takes the form [10]

$$[\![\mathbb{G}^{ri}]\!] = \varphi_r(\delta_{ri}\mathbb{P}^r - \varphi_i\mathbb{P}^{ri}_d) = \varphi_i(\delta_{ir}\mathbb{P}^i - \varphi_r\mathbb{P}^{ir}_d) \tag{18}$$

where $\mathbb{P}^{ir}_d$ is a Hill tensor accounting for ellipsoidal symmetry of the distribution of the ellipsoidal inclusions constituting phase i and phase r [10]. Relatively simple closed-form bounds for W^{eff} are obtained when the distribution of all inclusion phases is the same for all inclusion pairs, so that $\mathbb{P}^{ir}_d = \mathbb{P}_d$ for i and $r = 1, \dots, n_\alpha$, which is considered throughout the following.

4.2. Application to matrix-inclusion composites—consistency proof

Estimates for matrix-inclusion composites can be obtained from Eqs. (16)–(17) by setting the stiffness of the reference medium equal to the one the matrix of the RVE (phase 1): $\mathbb{C}^0 = \mathbb{C}^m\ (= \mathbb{C}^1)$; throughout this Subsection, index m is equivalent to index 1. Inserting this choice into (16), it is readily seen that the optimal matrix polarization is equal to the matrix prestress: $\boldsymbol{\tau}^m = \boldsymbol{\pi}^m$. If the matrix stiffness $\mathbb{C}^m$ does not satisfy $\boldsymbol{\varepsilon} : (\mathbb{C}^m - \mathbb{C}^r) : \boldsymbol{\varepsilon} \geqslant 0$ for all $\boldsymbol{\varepsilon} \neq 0$ and for all $r = 1, \ldots, n_\alpha$, the r.h.s. of (17) does not represent an upper bound of W^{eff}, but can be used as an estimate of this quantity. Accordingly, we replace the sign "$\leqslant$" (17) in by "$\simeq$".

In order to assess the consistency of the Ponte Castañeda–Willis (PCW) scheme with Levin's theorem, it is noteworthy that the volume average over the optimal polarizations (16) can be written as

$$\bar{\boldsymbol{\tau}} = \boldsymbol{E} : \overline{(\mathbb{C} - \mathbb{C}^m) : \mathbb{A}_{\text{pcw}}}^{\text{inc}} + \overline{\boldsymbol{\pi} : \mathbb{A}_{\text{pcw}}}, \quad \overline{\mathbb{Q}}^{\text{inc}} := \sum_{r=2}^{n_\alpha} \varphi_r \mathbb{Q}^r \tag{19}$$

with

$$\mathbb{A}^r_{\text{pcw}} = \mathbb{A}^r_\infty : \left[\mathbb{I} - \mathbb{P}_d : \overline{(\mathbb{C} - \mathbb{C}^m) : \mathbb{A}_\infty}^{\text{inc}}\right]^{-1}, \quad r = 2, \ldots, n_\alpha, \quad \mathbb{A}^m_{\text{pcw}} = \frac{1}{\varphi_m}\left(\mathbb{I} - \overline{\mathbb{A}_{\text{pcw}}}^{\text{inc}}\right) \tag{20}$$

We have to show now that (20) contains the strain concentration tensors of the PCW scheme: Inserting $\bar{\boldsymbol{\tau}}$ from (19) into the r.h.s. of (17), specifying the resulting expression for a natural initial state of the RVE (no prestresses: $\boldsymbol{\pi} = 0$), and comparing the result with $W^{\text{eff}} = \frac{1}{2}\boldsymbol{E} : \mathbb{C}^{\text{hom}} : \boldsymbol{E}$, allows for extracting the unconditionally symmetric PCW estimate of the homogenized stiffness tensor, see, e.g., Eq. (3.20) of [10]. Comparing this estimate with the classical Hill–Laws [17,9] expression $\mathbb{C}^{\text{hom}} = \mathbb{C}^m + \sum_{r=2}^{n_\alpha} \varphi_r (\mathbb{C}^r - \mathbb{C}^m) : \mathbb{A}^r$ proves (20) to contain the strain concentration tensors of the PCW scheme. In the presence of prestresses ($\boldsymbol{\pi} \neq 0$), insertion of $\bar{\boldsymbol{\tau}}$ from (19) into $\boldsymbol{\Sigma}_{\text{pcw}} = \bar{\boldsymbol{\sigma}} = \mathbb{C}^m : \boldsymbol{E} + \bar{\boldsymbol{\tau}}$ yields $\boldsymbol{\Sigma}_{\text{pcw}} = \overline{\mathbb{C} : \mathbb{A}_{\text{pcw}}} : \boldsymbol{E} + \overline{\boldsymbol{\pi} : \mathbb{A}_{\text{pcw}}}$. Comparison of this result with (3) proves the PCW scheme to be unconditionally consistent with Levin's theorem.

4.3. Application to polycrystals

PCW-type self-consistent estimates for polycrystals are obtained by choosing $\mathbb{C}^0$ to be equal to the homogenized stiffness $\mathbb{C}^{\text{hom}}$, and by setting the $\boldsymbol{E}$-proportional part of $\bar{\boldsymbol{\tau}}$ in (19) equal to zero [10]. Consistency of this approach with the strain average rule, $\overline{\mathbb{A}_{\text{pcw}}} = \mathbb{I}$, can be shown to require $\mathbb{C}^{\text{hom}}$ to satisfy

$$\sum_{r=1}^{N_\alpha} \varphi_r (\mathbb{P}^r - \mathbb{P}_d) : (\mathbb{C}^r - \mathbb{C}^{\text{hom}}) : \mathbb{A}^r_\infty = 0 \tag{21}$$

Considering condition (21) in $(20)_1$ specified for $\mathbb{C}^m = \mathbb{C}^{\text{hom}}$, lets the strain concentration tensor of the PCW scheme degenerate to the one of the Eshelby problem-based self-consistent scheme of Section 3. Consistency of the latter scheme with Levin's theorem requires condition (13) to be satisfied, which results in $\mathbb{A}^r_{\text{pcw}} = \mathbb{A}^r_{\text{esh}} = \mathbb{A}^r_\infty$, and further in

$$\mathbb{C}^{\text{hom}} = \sum_{r=1}^{N_\alpha} \varphi_r\, \mathbb{C}^r : \mathbb{A}^r_\infty \quad \Rightarrow \quad \sum_{r=1}^{N_\alpha} \varphi_r (\mathbb{C}^r - \mathbb{C}^{\text{hom}}) : \mathbb{A}^r_\infty = 0 \tag{22}$$

Comparing $(22)_2$ with (21), it is readily seen that all phase shape-related Hill tensors must be the same such that the Hill tensor difference $(\mathbb{P}^r - \mathbb{P}_d)$ can be taken out of the sum in (21), which, in turn, highlights that the distribution-related Hill tensor $\mathbb{P}_d$ has no influence on $\mathbb{C}^{\text{hom}}$. This indicates that taking the distribution statistics of all inclusion phases to be the same for all inclusion pairs ($\mathbb{P}^{ir}_d = \mathbb{P}_d$ for i and $r = 1, \ldots, n_\alpha$) is a very strong assumption when dealing with polycrystals. We conclude that in the framework of a polycrystal comprising phases with *different* shapes, the Ponte Castañeda–Willis approach is to be based on *different* Hill tensors $\mathbb{P}^{ir}_d$ accounting for *different* ellipsoidal symmetries of phase distribution statistics. Preferentially, the $\mathbb{P}^{ir}_d$ tensors should be identified from experimental observations. This way, the Ponte Castañeda–Willis scheme will be consistent with Levin's theorem, also for polycrystals with arbitrarily many prestressed pore families.

5. Conclusions

Levin's theorem requires both a kinematically admissible displacement field and a statically admissible stress field. From this property we conclude that consistency of a homogenization scheme with Levin's theorem reflects that the predicted average phase strains are kinematically admissible, and that the predicted average phase stresses are statically admissible. Both situations are very desirable, particularly when performing drying analyses of porous materials.

Regarding schemes based on Eshelby problems (the Mori–Tanaka scheme and the self-consistent scheme), diagonal symmetry of obtained stiffness tensor estimates does not represent a sufficient condition for their consistency with Levin's theorem. Nonetheless, these schemes have a certain potential for modeling drying of porous materials, including the special case of a medium comprising one solid phase and several pore families (exhibiting different average pore stresses) if the *same* Hill tensor is associated with all phases. Hence, Eshelby-based schemes can be used, e.g., for drying analyses of materials whose pore space is built up by spherical pores, with radii which are different, but on the same order of magnitude [14].

Different pore shapes and different pore pressures—such as those encountered when considering spherical pores *and* cracks on the same level of observation, in order to study the cracking risk during drying—should be modeled in the framework of the Ponte Castañeda–Willis scheme. Regarding matrix-inclusion composites, this approach can be based on the simple assumption of one identical distribution Hill tensor ($\mathbb{P}_d^{ir} = \mathbb{P}_d$). As for polycrystals, phase distribution statistics have to be accounted for in more detail, by identifying different distribution Hill tensors, preferentially from experimental observations. This way, the Ponte Castañeda–Willis scheme will be consistent with Levin's theorem, when analyzing microheterogeneous porous materials comprising arbitrarily many prestressed pore families.

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