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SAINT-VENANT'S PRINCIPLE, MACROHOMOGENEITY AND VARIATIONAL FORMULATIONS FOR ELASTIC RANDOM MEDIA

PRINCIPE DE SAINT-VENANT, MACROHOMOGÉNÉITÉ ET FORMULATIONS VARIATIONNELLES POUR LES MILIEUX ÉLASTIQUES ALÉATOIRES

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ABSTRACT: The problem of the determination of the effective behaviour of a linear elastic random heterogeneous material is considered anew in the more general situation of the analysis of a structure made of such a material. Macrohomogeneous conditions make the scale transition possible. The connection between both scales operates through a representative volume element with finite extension and with well-known shape. A global Hashin and Shtrikman variational formulation leads to rigorous formal bounds on the effective moduli, which can be made explicit for a composite exhibiting an ellipsoidal distribution of the phases.

RÉSUMÉ : Le problème de la détermination du comportement homogène équivalent d'un matériau élastique linéaire à microstructure aléatoire est replacé dans le cadre plus général du calcul d'une structure constituée d'un tel matériau. Des conditions de macrohomogénéité rendent possibles la transition d'échelle, qui s'effectue au travers d'un volume élémentaire représentatif d'extension finie et de forme bien définie. Une formulation variationnelle globale de type Hashin et Shtrikman permet de construire des encadrements formels rigoureux pour le comportement homogène équivalent, que l'on peut expliciter pour un composite présentant une distribution ellipsoïdale des phases.

1. INTRODUCTION

When analyzing the mechanical response of a structure S it is usually not appropriate to describe all the details of the heterogeneous microstructure of the constitutive material, first because the required computational power would be too large and second, because of lack of information about the microstructure, which generally cannot be described in a completely deterministic way. When the length scale L of the applied loads is much larger than the characteristic length l of a typical inhomogeneity, it is more efficient to consider an identically shaped and loaded structure, but made of a homogeneous material. If the behaviour of the latter is chosen in an appropriate way, the stress and

strain fields that can be computed in this second problem are exactly equal to some averages of the fields in the initial structural problem, taken over some representative volume element (RVE). The determination of this equivalent homogeneous behaviour as a function of the behaviour of the constitutive phases and the geometrical parameters of the microstructure, which is independent of the loads applied to the structure, has been the goal of numerous works in the past forty years. But many open questions remain.

Here we address this problem once again, but in a way that differs slightly from many other more usual approaches. The difference relies mainly on the presentation of the homogenization procedure. Usually one separates clearly

the local scale transition problem from the structural analysis and considers a particular isolated RVE, often subjected to homogeneous boundary conditions or periodic ones. Furthermore, the size of such a volume element is supposed to be very large, or even infinite, and its particular shape is not specified. Here we deal with RVEs with well defined shape and large, with respect to l , but finite extension. We will also keep in mind that the load to which each representative volume element in the structure is subjected is the result of some macroscopic boundary conditions on the structure and that it is usually not homogeneous but varies on both macroscopic and microscopic length scales: we will assume that it can be split into its average and the deviation from this average, the characteristic length of the latter being l or smaller. We will also focus on some more technical aspects which could be considered as minor but which have their importance especially for anisotropic composite materials. Some slight mishandling of the governing equations may lead to inconsistent results and another purpose of this paper is to emphasize some of them and to describe on a physical basis the significance of these not-to-be-mishandled details.

This discussion is limited to materials with linear elastic but anisotropic behaviour and to small strains. Let $C(\underline{x}) = S^{-1}(\underline{x})$ be the tensor of elastic moduli at point \underline{x} in the heterogeneous structure \mathcal{S} and C^{eff} be the tensor of effective moduli to be determined. The fields $\underline{\sigma}(\underline{x})$ and $\underline{\epsilon}(\underline{x})$ are the stress and strain fields which solve the initial problem; $\underline{\Sigma}(\underline{x})$ and $\underline{E}(\underline{x})$ are the fields that are computed when $C(\underline{x})$ is replaced by C^{eff} , with identical boundary conditions. The latter might be of several types, either traction or displacement conditions; we will not specify them more precisely, but they are required to vary on a length scale L . Even if macroscopically distributed body forces could also be considered provided that their magnitude is small so as to generate only small stress and strain gradients, we will assume that there are none.

2. MICROSTRUCTURE AND RVE

As already mentioned, the spatial distribution of moduli and the applied load that are under consideration are such that the characteristic length L of the variations of $\underline{\Sigma}$ and \underline{E} is much larger than the typical length l of the fluctuations of the moduli of the heterogeneous material.

It is then possible to define some "moving domains" $\Omega_{\underline{x}}$, characterized by $\underline{y} \in \Omega_{\underline{x}} \Leftrightarrow \underline{y} - \underline{x} \in \Omega_0$, such that the fields $\underline{\Sigma}$ and \underline{E} can be considered to be uniform over each of them, and that each domain $\Omega_{\underline{x}}$ contains the whole "microstructural information" that characterizes the heterogeneous material at point \underline{x} . The domain Ω_0 is supposed to contain the origin, the latter being far away from the boundary $\partial\Omega_0$. For the sake of simplicity, it is assumed convex and with regular boundary, so that an outer normal \underline{n} can be defined. Let ρ characterize its finite extension; it is required that $L \gg \rho \gg l$.

Let $\langle f \rangle_{\Omega}$ denote the average of any quantity f on any subdomain Ω of \mathcal{S} . The averaging process $\langle \cdot \rangle_{\Omega_{\underline{x}}}$ serves to characterize the statistical information available on the microstructure at point \underline{x} . This is the so-called "ergodic" condition. The simplest type of such possible available information is the number of times a particular event can be observed at a point \underline{y} in $\Omega_{\underline{x}}$. This is the first-order information on the microstructure. The volume fraction c_r of the constitutive phases r is the most standard first-order information. It can be written as $c_r(\underline{x}) = \langle \kappa_r \rangle_{\Omega_{\underline{x}}}$, where κ_r is the characteristic function of phase r in \mathcal{S} . Second-order information gives, as a function of \underline{h} , the number of occurrences of a particular event at a point \underline{y} in $\Omega_{\underline{x}}$ and, simultaneously, of another particular event at point $\underline{y} + \underline{h}$. In classical approaches, one uses correlation functions $\phi_{rs}(\underline{x}, \underline{h}) = \langle \kappa_r(\cdot) \kappa_s(\cdot + \underline{h}) \rangle_{\Omega_{\underline{x}}}$, which give the probability that $C(\underline{y}) = C_r$ and $C(\underline{y} + \underline{h}) = C_s$, C_r being the moduli of constitutive phase r . Information of higher orders can also be defined but will not be referred to in the present paper.

The domain $\Omega_{\underline{x}}$ is the RVE at point \underline{x} . All microstructures that will be considered here are statistically homogeneous. This means that the quantities described above, and more generally the average over $\Omega_{\underline{x}}$ of any quantity depending

on the phase distribution, do not depend on \underline{x} . Another consequence is the property $\phi_{rs}(\underline{h}) = \phi_{sr}(-\underline{h})$, the dependence on \underline{x} of these functions being now omitted. The microstructures under consideration are also without any order at long distances : two events observed at points separated by a large distance are independent. That means in particular that the second order correlation functions have well known limits for large $\|\underline{h}\|$: $\phi_{rs}(\underline{h}) \rightarrow c_r c_s$. These limits are reached when $\|\underline{h}\|$ is of order ρ or less. Thus periodic microstructures are out of the scope of this work. Since there can only be one phase at a particular point, one also has $\phi_{rs}(0) = \delta_{rs} c_r$.

3. SCALE TRANSITION

The classical theorem of potential energy ensures that:

$$W = \Phi(C, \underline{\epsilon}) = \text{Min}_{\underline{\epsilon}^*} \Phi(C, \underline{\epsilon}^*), \quad (1)$$

where $\Phi(C, \underline{\epsilon}^*)$ is the potential energy of any trial strain field $\underline{\epsilon}^*$ compatible with the displacement boundary conditions, associated with the structural analysis on the heterogeneous structure, given by the sum of the integral $\frac{1}{2} \int_S \underline{\epsilon}^* : C : \underline{\epsilon}^* d\omega$ and integrals over ∂S related to the boundary conditions.

When the loads and the microstructure are such that the strain field $\underline{\epsilon}$ has two scales of variation, $L \gg l$, it is possible to limit the search for optimal strain fields within the set of trial fields that have such separate scales of variations. The optimization problem then reads:

$$W = \text{Min}_{\underline{\underline{\epsilon}}^*, \underline{\epsilon}'^*} \Phi(C, \underline{\underline{\epsilon}}^* + \underline{\epsilon}'^*), \quad (2)$$

where the fields $\underline{\underline{\epsilon}}^*$ vary on a length scale L and are thus homogeneous on all the domains $\Omega_{\underline{x}}$ and the fields $\underline{\epsilon}'^*$ fluctuate with a length scale l and have a null average on all the domains $\Omega_{\underline{x}}$. The trial fields $\underline{\underline{\epsilon}}^*$ have also to be compatible with the (macroscopic) boundary conditions whereas the fields $\underline{\epsilon}'^*$ have to be compatible with null displacements on the sub-boundary of S where displacements are prescribed. The

optimization can then be performed in two steps:

$$W = \text{Min}_{\underline{\underline{\epsilon}}^*} \text{Min}_{\underline{\epsilon}'^*} \Phi(C, \underline{\underline{\epsilon}}^* + \underline{\epsilon}'^*). \quad (3)$$

This new formulation is equivalent to the first one and does not simplify the problem : the first optimization step has to be done for all macroscopic compatible trial strain fields $\underline{\underline{\epsilon}}^*$.

The field $\underline{\epsilon}'^o$ associated to a particular macroscopic trial field $\underline{\underline{\epsilon}}^*$ within the RVE $\Omega_{\underline{x}}$ at any point \underline{x} can be considered as the solution of a local structural problem - a microstructural problem - with some non-uniform boundary conditions applied on $\partial\Omega_{\underline{x}}$, compatible with the requirement that the average of $\underline{\epsilon}'^o$ over $\Omega_{\underline{x}}$ vanishes and with variations with length scale l . These local problems may be solved for all the RVEs in S , but in order to use their solution for the minimization problem on S , some complex conditions relating the boundary conditions on these local problem should be imposed, in order that the juxtaposed local fields generate a compatible field on the whole structure. A minimization with respect to this set of boundary conditions should also be performed in order to reach the required minimum over all possible fields in S .

The fundamental assumption which simplifies this problem and which indeed makes the scale transition possible is the fact that the result of these microstructural problems do not actually depend on their particular local boundary conditions, but depend only on the average strain $\underline{\underline{\epsilon}}^*$, except in some thin layer close to the boundary. This hypothesis, which will be referred to as the "*macrohomogeneity condition*", might be considered as a particular application of Saint-Venant's principle : the boundary conditions that fluctuate around 0 on a length scale l generate fields that are non negligible only at a distance from the boundary less than a few times l . The values of the fields "inside" the RVE do not depend on these fluctuations. Note that this concept of macrohomogeneity refers not only to the spatial phase distribution in the heterogeneous material, but also to the applied loads : a given material subjected to different loads might or might not be macrohomogeneous. This concept has been first proposed by Hill (1).

The global fields over the whole structure can

be constructed by juxtaposing the optimal "internal" fields $\underline{\epsilon}'^o$, which lead to compatible fields since the above assumption ensures that they are equal to the fields that would have been obtained if the optimization had been performed directly on the whole structure. Furthermore, no optimization on the set of local boundary conditions on the RVEs needs to be performed, since all of them lead to the same value.

The volume of the domain of $\Omega_{\underline{x}}$ where the local fields depend on the particular boundary conditions is of order $\rho^2 \times l$, whereas the volume of $\Omega_{\underline{x}}$ is of order ρ^3 . The average $2\bar{\phi}(\underline{x}, \underline{E}^*)$ over $\Omega_{\underline{x}}$ of the strain energy density $(\underline{E}^* + \underline{\epsilon}'^o) : C : (\underline{E}^* + \underline{\epsilon}'^o)$ computed in the microstructural problem with some particular boundary conditions is thus equal, in the limit $\rho \gg l$, to the same average that would have been computed when the optimization had been performed on \mathcal{S} . It is also equal to the average that would have been obtained if homogeneous strain conditions had been applied, i.e. displacements equal to $\underline{E}^* \cdot \underline{y}$ on $\underline{y} \in \partial\Omega_{\underline{x}}$. In this latter case, Hill's lemma (1) can be applied so that $2\bar{\phi}(\underline{x}, \underline{E}^*) = \underline{E}^* : \langle C : (\underline{E}^* + \underline{\epsilon}'^o) \rangle_{\Omega_{\underline{x}}}$, which because of the linearity of the local problem with homogeneous boundary conditions, can be written $\underline{E}^* : C^{\text{eff}} : \underline{E}^*$, where C^{eff} can be shown to be symmetric and positive definite.

The second step of problem (3) can then be performed and is shown to be equivalent to the structural analysis on a homogeneous structure with moduli C^{eff} with boundary conditions equal to those applied on the heterogeneous structure. Furthermore, the macroscopic fields $\underline{\Sigma}$ and \underline{E} that solve it are the averages of the local fields $\underline{\sigma}$ and $\underline{\epsilon}$ over the RVEs:

$$\underline{\Sigma}(\underline{x}) = \langle \underline{\sigma} \rangle_{\Omega_{\underline{x}}} \quad \text{and} \quad \underline{E}(\underline{x}) = \langle \underline{\epsilon} \rangle_{\Omega_{\underline{x}}} \quad (4)$$

The resolution of the microstructural problem on $\Omega_{\underline{x}}$ for this effective value of $\underline{E}^*(\underline{x})$ and for a particular set of local boundary conditions, for instance homogeneous conditions, leads to the effective local field $\underline{\epsilon}$ and $\underline{\sigma}$ at point \underline{x} . This can be done for any point \underline{x} such that $\Omega_{\underline{x}}$ belongs to \mathcal{S} . Points close to $\partial\Omega_{\underline{x}}$ would need some special treatment which is out of the scope of this paper.

4. EFFECTIVE MODULI

Classically the tensor C^{eff} is computed by solving this microstructural problem for any \underline{E}^* :

$$\underline{E}^* : C^{\text{eff}} : \underline{E}^* = \text{Min}_{\langle \underline{\epsilon}^* \rangle_{\Omega_{\underline{x}}} = \underline{E}^*} \langle \underline{\epsilon}^* : C : \underline{\epsilon}^* \rangle_{\Omega_{\underline{x}}} \quad (5)$$

The variations of the fields $\underline{\epsilon}^*$ are required to have a length scale l much smaller than the size of $\Omega_{\underline{x}}$. From a structural point of view, this is a non-standard problem, since the boundary conditions are not precisely given. In a macro-homogeneous situation, the obtained minimum is well defined and the corresponding local fields are unique, except in some small layer close to $\partial\Omega_{\underline{x}}$. Generally one solves this problem for homogeneous strain or stress boundary conditions or periodic conditions. Such arbitrary choices add some non-physical constraints which may lead to difficulties which need to be addressed with some additional assumptions and sometimes non-rigorous approximations.

Another way to deal with the determination of C^{eff} is to come back to the global structural problem. If an effective behaviour can be defined as described above, then the first step of global optimization can be rewritten as :

$$\bar{\Phi}(C^{\text{eff}}, \underline{E}^*) = \text{Min}_{\underline{\epsilon}'^*} \bar{\Phi}(C, \underline{E}^* + \underline{\epsilon}'^*) \quad (6)$$

This minimization has to be done for all admissible macroscopic strain fields \underline{E}^* . The fields $\underline{\epsilon}'^*$, which need to be compatible with the null boundary conditions on \mathcal{S} , are assumed to fluctuate with length scale l or less and to have null averages on all RVEs. This problem seems more complicated but has well-defined boundary conditions. It is the formulation we are going to deal with in this paper. It is shown in what follows that the procedures which have been applied to the classical "local" formulation (5) can also be applied to this "global" formulation and lead to the same kind of results. The advantage of the characterization (6) is that some aspects of these procedures can be treated in a easier and probably more physical way since it allows to get rid of the non-natural homogeneous stress or strain boundary conditions applied on all RVEs in the classical approach and to avoid the difficulties they induce.

The simplest choice for $\underline{\underline{\epsilon}}^*$ in the problem (6) is $\underline{\underline{\epsilon}}'^* = 0$. It leads to $\langle \underline{\underline{E}}^* : [C^{\text{eff}} - C] : \underline{\underline{E}}^* \rangle_S \leq 0$, since the terms related to the boundary conditions single out. The field $\underline{\underline{E}}^*$ being homogeneous over all RVEs, one gets:

$$\langle \underline{\underline{E}}^* : [C^{\text{eff}} - \langle C \rangle_{\Omega_{\underline{\underline{x}}}}] : \underline{\underline{E}}^* \rangle_S \leq 0. \quad (7)$$

This relation has to be satisfied for all compatible fields $\underline{\underline{E}}^*$ and can be interpreted as a weak form of the local inequality $C^{\text{eff}} \leq \langle C \rangle_{\Omega_{\underline{\underline{x}}}}$. One could deduce this local result from the global one, for instance by constructing two macroscopic trial fields that are homogeneous over some RVE and differ only by their value in a neighbourhood of this RVE. We do not go into such details here and shall consider such weak inequalities as a sufficient characterization of C^{eff} .

The average $\langle C \rangle_{\Omega_{\underline{\underline{x}}}}$ is the well-known Voigt bound for C^{eff} , which makes only use of the first order statistical information and thus is valid for any microstructure with prescribed phase volume fractions. More restrictive bounds can be obtained when using fluctuating trial fields, generated by a procedure first proposed by Hashin and Shtrikman (2) for the local formulation.

5. HIGHER-ORDER FORMAL BOUNDS

The idea is to make use of the solution of an auxiliary problem with same geometry and boundary conditions as the problem on S , but with homogeneous constitutive material C^0 - the reference material - and subjected to an additional polarization field $\underline{\underline{p}}^* = [C - C^0] : \underline{\underline{\eta}}^*$, where $\underline{\underline{\eta}}^*$ belongs to the space $T_2^s(S)$ of symmetric second-order tensor fields over S . The solution of this problem is a field $\underline{\underline{\xi}}$ which is kinematically admissible with the overall conditions on S and such that $C^0 : \underline{\underline{\xi}} + [C - C^0] : \underline{\underline{\eta}}^*$ is statically admissible with the overall loads. We will limit the set of "trial field generators" $\underline{\underline{\eta}}^*$ in such a way that these generated fields can be split into macroscopic and microscopic parts my means of the averaging procedure $\langle \cdot \rangle_{\Omega_{\underline{\underline{x}}}}$. So $\langle \underline{\underline{\xi}} \rangle_{\Omega_{\underline{\underline{x}}}}$ and $C^0 : \langle \underline{\underline{\xi}} \rangle_{\Omega_{\underline{\underline{x}}}} + \langle [C - C^0] : \underline{\underline{\eta}}^* \rangle_{\Omega_{\underline{\underline{x}}}}$ are macroscopic admissible strain and stress fields, compatible with the overall loads. In the mean-

while, the fields $\underline{\underline{\epsilon}}'^* = \underline{\underline{\xi}} - \langle \underline{\underline{\xi}} \rangle_{\Omega_{\underline{\underline{x}}}}$ and $C^0 : \underline{\underline{\epsilon}}'^* + [C - C^0] : \underline{\underline{\eta}}^* - \langle [C - C^0] : \underline{\underline{\eta}}^* \rangle_{\Omega_{\underline{\underline{x}}}}$ are microscopic admissible fields, compatible with null boundary conditions. The field that will be used in formulation (6) is not $\underline{\underline{\xi}}$ but $\underline{\underline{\epsilon}}^* = \underline{\underline{E}}^* + \underline{\underline{\epsilon}}'^*$, which has the required macroscopic value.

Some straightforward calculations, using the above properties of these fields, allow us to write the potential energy in the following manner :

$$\Phi(C, \underline{\underline{E}}^* + \underline{\underline{\epsilon}}'^*) = \text{HS}^0(\underline{\underline{\eta}}^*) + \Delta_\phi^0(\underline{\underline{\eta}}^*), \quad (8)$$

where HS is the Hashin and Shtrikman functional, given by:

$$2\text{HS}^0(\underline{\underline{\eta}}^*) = 2\Phi(C^0, \underline{\underline{E}}^*) + \int_S \underline{\underline{\eta}}^* : [C - C^0] : [\underline{\underline{E}}^* + \underline{\underline{\epsilon}}'^* - \underline{\underline{\eta}}^*] d\omega, \quad (9)$$

and $\Delta_\phi^0(\underline{\underline{\eta}}^*)$ is the quadratic integral:

$$2\Delta_\phi^0(\underline{\underline{\eta}}^*) = \int_S [\underline{\underline{\eta}}^* - \underline{\underline{\epsilon}}'^*] : [C - C^0] : [\underline{\underline{\eta}}^* - \underline{\underline{\epsilon}}'^*] d\omega. \quad (10)$$

This result differs from the more classical one in three aspects. First, the above quantities are given as functions of $\underline{\underline{E}}^*$ which is *not* the field computed in the auxiliary problem with a null polarization. Second, the integrals are computed over the whole structure S , consistently with the "global" formulation. Third, the use of $\underline{\underline{\eta}}^*$ in place of the polarization tensor $\underline{\underline{p}}^*$ as a trial field generator avoids the use of quantities like $[C - C^0]^{-1}$ which might be singular for some particular - and often opted for - choices of C^0 . Note that all the effects of the boundary conditions in $\text{HS}(C^0, \underline{\underline{\eta}}^*)$ are included in $\Phi(C^0, \underline{\underline{E}}^*)$. The corresponding terms single out with their homologous terms in the effective potential energy $\Phi(C^{\text{eff}}, \underline{\underline{E}}^*)$, so that one no longer has to be concerned with particular macroscopic boundary conditions.

If the reference medium is stiffer than all the constitutive phases, the difference $\Delta_\phi^0(\underline{\underline{\eta}}^*)$ is negative and can be removed from relation (6), the functional HS providing an upper bound for the effective potential energy of the structure S . The second step in the Hashin and Shtrikman procedure consists in selecting polarization tensor

fields that make $\text{HS}^0(\underline{\eta}^*)$ stationary, so as to get the best upper bound, with respect to $\underline{\eta}^*$. This optimization has to be performed in some subset of $\mathbb{T}_2^s(\mathcal{S})$. If this subset is the whole space, one gets the effective potential energy associated to \underline{E}^* , but this result can usually not be reached for the reasons mentioned in the introduction. That is why the optimization has to be limited to some subspace, suited to the available information and computational power. Let $\mathcal{P}(\mathbb{T}_2^s(\mathcal{S}))$ be such a subspace, image of $\mathbb{T}_2^s(\mathcal{S})$ by some orthogonal projection operator \mathcal{P} , which is assumed to be *local*: the value of $\mathcal{P}(f)(\underline{x})$ depends only on the values f takes in $\Omega_{\underline{x}}$.

Let $\underline{\eta}_{\mathcal{P}}^{\circ}$ be the field that makes $\text{HS}(C^0, \underline{\eta}^*)$ stationary in $\mathcal{P}(\mathbb{T}_2^s(\mathcal{S}))$. It can be shown (3) that it is characterized by the relation

$$\mathcal{P} \left([C - C^0] : \left[\underline{\underline{\epsilon}}^*(\underline{\eta}_{\mathcal{P}}^{\circ}) - \underline{\eta}_{\mathcal{P}}^{\circ} \right] \right) = 0 \quad (11)$$

and that the optimal value of the functional reads:

$$2\text{HS}^0(\underline{\eta}_{\mathcal{P}}^{\circ}) = 2\Phi(C^0, \underline{E}^*) + \int_{\mathcal{S}} \underline{E}^* : \left\langle [C - C^0] : \underline{\eta}_{\mathcal{P}}^{\circ} \right\rangle_{\Omega_{\underline{x}}} d\omega. \quad (12)$$

In the next section, it will be shown that $\underline{\underline{\epsilon}}^{*'} is a local function of $\underline{\eta}^*$: its value on \underline{x} depends only on the values of the polarization field in $\Omega_{\underline{x}}$. Thus the global optimality condition (11) splits into local and independent conditions : it can be shown *in fine* that the optimal polarization field and thus the optimal trial field in $\Omega_{\underline{x}}$ depend only on the value of \underline{E}^* at \underline{x} . So one is led to local problems, as is expected in the framework of homogenization, but without having to restrict *a priori* the analysis to a local problem with particular boundary conditions.$

Since condition (11) is linear, the optimal field in $\Omega_{\underline{x}}$ is a linear function of $\underline{E}^*(\underline{x})$ and the macroscopic value of the optimal polarization $\underline{\eta}_{\mathcal{P}}^{\circ}$ required to compute the optimal value of HS can be written as $[C^{\text{HS}_0}_{\mathcal{P}} - C^0] : \underline{E}^*(\underline{x})$, so that:

$$2\text{HS}^0(\underline{\eta}_{\mathcal{P}}^{\circ}) = 2\Phi(C^{\text{HS}_0}_{\mathcal{P}}, \underline{E}^*), \quad (13)$$

for all macroscopic strain fields \underline{E}^* . The tensor $C^{\text{HS}_0}_{\mathcal{P}}$ is the Hashin and Shtrikman estimate, associated to the reference medium C^0 and the

projector \mathcal{P} . It is uniform since the microstructure is assumed statistically homogeneous. Within this general framework, it can be shown to be symmetric and non singular. If C^0 is chosen according to the rules given previously, it is an upper bound for C^{eff} since the characterization (6) provides a weak form of the inequality:

$$C^{\text{eff}} \leq C^{\text{HS}_0}_{\mathcal{P}}. \quad (14)$$

In that case $C^{\text{HS}_0}_{\mathcal{P}}$ is also shown to be positive.

Due to space restrictions, the discussion has been limited to the potential energy but it can also be extended to the complementary energy. One then gets lower bounds if the reference medium is chosen appropriately and a Hashin and Shtrikman compliance tensor $S^{\text{HS}_0}_{\mathcal{P}}$ can be defined. It is the exact inverse of $C^{\text{HS}_0}_{\mathcal{P}}$.

Note finally that if \mathcal{P} is the identity, $C^{\text{HS}_0}_{\mathcal{P}}$ and $S^{\text{HS}_0}_{\mathcal{P}}$ are equal to the effective tensors C^{eff} and S^{eff} . Thus the above analysis allows us to establish their existence without having to split *a priori* the global problem into independent local microstructural problems, and without any explicit use of the macrohomogeneity condition as defined in section 3. The latter is anyway a required assumption, since it will be assumed in the next section that $\underline{\underline{\epsilon}}^{*}'$ has two scales of variations when the polarization fields itself admits such a decomposition. This hypothesis can as well be seen as a variant of Saint-Venant's principle: fluctuations with length scale Λ of the polarization field generate fields that can be neglected at a distance larger than a few times Λ .

6. STRAIN DUE TO POLARIZATION

Let us consider the solution $(\underline{\underline{\xi}}, \underline{\underline{\sigma}})$ of the auxiliary problem, generated by the polarization \underline{p}^* and the macroscopic boundary conditions, and define a set of homothetic domains $\mathcal{D}_{\underline{x}}^{\lambda}$ centered on point \underline{x} , such that $\underline{y} \in \mathcal{D}_{\underline{x}}^{\lambda} \Leftrightarrow \underline{x} + \lambda(\underline{y} - \underline{x}) \in \mathcal{D}_{\underline{x}}^{\lambda}$. The strain $\underline{\underline{\xi}}(\underline{x})$ can be written, without any approximation, in terms of the polarization field within $\mathcal{D}_{\underline{x}}^{\lambda}$ and of the values on the boundary $\partial\mathcal{D}_{\underline{x}}^{\lambda}$ of the displacement and traction field solution of the auxiliary problem, by means of the Green's function $\underline{\underline{G}}^0$ associated with the *infinite* medium with moduli C^0 and its symmetrized

first and second-order derivatives $\underline{\underline{E}}^0$ and Γ^0 :

$$\begin{aligned} \underline{\underline{\tilde{\varepsilon}}}(\underline{x}) &= \langle \underline{\underline{\tilde{\varepsilon}}} \rangle_{\Omega_{\underline{x}}} + \int_{\partial \mathcal{D}_{\underline{x}}^\lambda} [\cdots] ds_{\underline{y}} - \\ \int_{\mathcal{D}_{\underline{x}}^\lambda} \Gamma^0(\underline{x} - \underline{y}) : \left[\underline{\underline{p}}^*(\underline{y}) - \langle \underline{\underline{p}}^* \rangle_{\Omega_{\underline{x}}} \right] d\omega_{\underline{y}} \end{aligned} \quad (15)$$

where the terms in the integral over $\partial \mathcal{D}_{\underline{x}}^\lambda$ involve the fluctuating part of the stress vector $\underline{\underline{f}}'(\underline{y}) = \left[\underline{\underline{\tilde{\sigma}}}(\underline{y}) - \langle \underline{\underline{\tilde{\sigma}}} \rangle_{\Omega_{\underline{x}}} \right] \cdot \underline{n}$ as well as the fluctuating part of the displacement. By means of an appropriate change of variables, the integral involving $\underline{\underline{f}}'(\underline{y})$ can be written as $\int_{\partial \mathcal{D}_{\underline{x}}^\lambda} \underline{\underline{E}}^0(\underline{x} - \underline{u}) \cdot \underline{\underline{f}}'(\underline{x} + \lambda(\underline{u} - \underline{x})) ds_{\underline{u}}$, where the homogeneity of degree -2 of $\underline{\underline{E}}^0$ has been used.

Assuming now that $\underline{\underline{\tilde{\varepsilon}}}$ fluctuates on a length scale l around its average, the force $\underline{\underline{f}}'$ fluctuates with respects to \underline{u} on a length scale l/λ , whereas $\underline{\underline{E}}^0$ fluctuates on a fixed length scale. For large values of λ , $\underline{\underline{f}}'$ can then be replaced by its local average. If this situation is reached for λ such that $\lambda \|\underline{u} - \underline{x}\| \ll L$, then this local average vanishes and so does the integral. This limit is reached more quickly if $\mathcal{D}_{\underline{x}}^\lambda$ is centered on \underline{x} , since the variation of $\underline{\underline{E}}^0$ with respect to \underline{u} is then smoother. The integral term involving the fluctuating part of the displacement can be shown to vanish in the same limit.

An alternative way of defining a macrohomogeneous situation is then to say that this limit is reached when $\mathcal{D}_{\underline{x}}^\lambda$ is replaced by the RVE $\Omega_{\underline{x}}$, so that one has the relation:

$$\begin{aligned} \underline{\underline{\tilde{\varepsilon}}}(\underline{x}) &= \langle \underline{\underline{\tilde{\varepsilon}}} \rangle_{\Omega_{\underline{x}}} + \underline{\underline{E}}_{\Omega_0}^0 : \langle \underline{\underline{p}}^* \rangle_{\Omega_{\underline{x}}} \\ &- \int_{\Omega_{\underline{x}}} \Gamma^0(\underline{x} - \underline{y}) : \underline{\underline{p}}^*(\underline{y}) d\omega_{\underline{y}}, \end{aligned} \quad (16)$$

with $\underline{\underline{E}}_{\Omega_0}^0 = \int_{\Omega_0} \Gamma^0(\underline{y}) d\omega_{\underline{y}}$. The trial tensor field $\underline{\underline{\varepsilon}}^*$ used in the variational formulation is obtained using the same relation : one simply has to replace $\langle \underline{\underline{\tilde{\varepsilon}}} \rangle_{\Omega_{\underline{x}}}$ by $\underline{\underline{E}}^*$.

From a more physical point of view, this relation means that local fluctuations of the strain are only due to local sources and macroscopic loads do only affect the macroscopic value of the field. This result differs slightly from those used by other authors (4, 5, 6, 7) by the facts that the integral is limited to a finite domain which prevents convergence problems, that the value of the macroscopic part is explicitly given and

that the integral is computed on a moving domain centered on \underline{x} , so that no approximation is made for points close to the boundary of a RVE, as would be the case in a local formulation with imposed boundary conditions. This relation can be used for any point \underline{x} such that $\Omega_{\underline{x}}$ belongs to \mathcal{S} . Points close to $\partial \mathcal{S}$ would need special treatment, but since Ω_0 is much smaller than \mathcal{S} , their contribution to the global response of the structure can be neglected.

7. ELLIPSOIDAL DISTRIBUTIONS

The formal bounds can be made explicit for several types of projections \mathcal{P} . Classically, one uses polarization fields that are uniform over each constitutive phase: $\underline{\underline{\eta}}^* = \sum_r \underline{\underline{\eta}}_r \kappa_r$. In a local formulation, the tensors $\underline{\underline{\eta}}_r$ would be constant. For the present global approach, they are supposed to be macroscopic functions of \underline{x} . The corresponding projection transforms any field \underline{f} into the field $\sum_r \langle \underline{f} \kappa_r \rangle_{\Omega_{\underline{x}}} \kappa_r$. When the optimality condition (11) is made explicit for this projection and the generated trial strain field is computed according to (16), one gets a local problem at any point \underline{x} , which, when solved, gives the optimal values of the tensors $\underline{\underline{\eta}}_r$ at this point as a linear function of $\underline{\underline{E}}^*(\underline{x})$. This problem is governed by the tensors

$$\hat{\Gamma}_{rs}^0 = \int_{\Omega_0} \phi_{rs}(\underline{h}) \Gamma^0(\underline{h}) d\omega_{\underline{h}} \quad (17)$$

which have a closed form expression when the phase distribution satisfies ellipsoidal symmetry conditions:

$$\phi_{rs}(\underline{h}) = \tilde{\phi}_{rs}(\|\underline{\underline{A}}_{rs} \cdot \underline{h}\|), \quad (18)$$

where the $\tilde{\phi}_{rs}$ are scalar functions and $\underline{\underline{A}}_{rs}$ are symmetric second-order tensors. Note that these tensors and functions are not independent but linked by some relations induced by the condition $\sum_r \kappa_r(\underline{x}) = 1$, which expresses that there is one and only one phase at each point \underline{x} . The integration (17) can then be performed by discretizing the domain Ω_0 into concentric ellipsoidal layers, with orientation and aspect ratio given by $\underline{\underline{A}}_{rs}$. The contribution of these layers

all vanish since the integral of Γ^0 on a domain delimited by two homothetic ellipsoids centered at the origin vanishes. The integrals $\hat{\Gamma}_{r,s}^0$ then reduce to the local part of Γ^0 and to the integration on the domain delimited by Ω_0 and the largest of the above ellipsoids Ω_0 contains. In this domain, \underline{h} is larger than the decorrelation distance so that $\phi_{r,s}$ reaches its limit. Thus:

$$\hat{\Gamma}_{r,s}^0 = \delta_{r,s} c_r \mathbf{E}_{\mathcal{E}_{r,s}}^0 + c_r c_s [\mathbf{E}_{\Omega_0}^0 - \mathbf{E}_{\mathcal{E}_{r,s}}^0], \quad (19)$$

where $\mathbf{E}_{\mathcal{E}_{r,s}}^0 = \int_{\mathcal{E}_{r,s}} \Gamma^0(\underline{y}) d\omega_y$, $\mathcal{E}_{r,s}$ being an ellipsoid centered at the origin and with shape given by $\underline{A}_{r,s}$. The optimal tensors $\underline{\eta}_{r,s}$ then satisfy the equations:

$$\underline{\eta}_{r,s} + \mathbf{E}_{\mathcal{E}_{r,s}}^0 : [\mathbf{C}^r - \mathbf{C}^0] : \underline{\eta}_{r,s} = \underline{\mathbf{E}}_r^0, \quad (20)$$

with $\underline{\mathbf{E}}_r^0 = \underline{\mathbf{E}}_r^* + \sum_s c_s \mathbf{E}_{\mathcal{E}_{r,s}}^0 : \underline{p}_s$. They are thus formally equal to the strains in ellipsoidal inclusions $\mathcal{E}_{r,s}$ embedded in an infinite medium \mathbf{C}^0 and subjected to the load $\underline{\mathbf{E}}_r^0$ at infinity.

If the $\underline{A}_{r,s}$ are all identical, so are the tensors $\underline{\mathbf{E}}_r^0$. The bounds thus obtained are the anisotropic Hashin and Shtrikman bounds first given by Willis (5). They can also be considered as estimates, in the sense of Mori and Tanaka (8), for the effective moduli of a composite with aligned ellipsoidal inclusions in a matrix \mathbf{C}^0 , even if, according to the present analysis, the matrix/inclusion morphology is not explicitly taken into account. The resulting tensors are symmetric and positive definite, as they should be. If the $\underline{A}_{r,s}$ are not identical, but consistent with the condition $\sum_r \kappa_r(\underline{x}) = 1$, one can show that the resulting tensors are still symmetric. Some extensions of the Mori and Tanaka model to ellipsoidal but non aligned inclusions suggest to consider this set of inclusion problems but with an identical applied strain at infinity and the obtained tensors are not symmetric. Such a situation would have been obtained in the present analysis if one had neglected the contribution of large \underline{h} in integrals (17). This suggests that these extensions of the Mori and Tanaka model do not accurately model all the local interactions that govern the behaviour of such materials.

Alternative approaches, such as the heterogeneous pattern-based one (6, 9) and its simplified version for homogeneous patterns (7) are

able to deal correctly with situations where inclusions are not aligned. The present analysis can be applied to these situations; in particular specific projection operators \mathcal{P} adapted to the considered microstructure can be defined. The resulting bounds take into account the whole set of interactions that govern such materials and, as a consequence, they exhibit all the required properties for tensors of elastic moduli (3).

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