Constitutive relations involving internal variables based on a micromechanical analysis

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Abstract: The exact description of the overall behavior of composites with nonlinear dissipative phases requires an infinity of internal variables. Approximate models involving only a finite number of those can be obtained by considering a decomposition of the microscopic anelastic strain field on a finite set of shape functions. The Transformation Field Analysis of [Dvorak, 1992] is obtained as a special case of the proposed theory by considering shape functions which are uniform within a given subdomain. The interest of considering nonuniform shape functions is shown.
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1. INTRODUCTION

Among all Paul Germain's scientific achievements, his contribution to the formulation of constitutive relations in the coherent framework of Continuum Thermodynamics has a prominent place. His book on "Mécanique des Milieux Continus" [Germain, 1973], contemporary of the seminal work of [Halphen et al, 1975] on "Generalized Standard Materials" (GSM), opened a way which was further pursued, developed and illustrated by many authors inside and outside France (see [Germain et al, 1983, Lemaître et al, 1988, Lubliner, 1990, Maugin, 1992] for a review).

This theory relies on two fundamental concepts, the notion of internal variables often denoted α, and the notion of thermodynamic potentials, the free energy ρw and the dissipation potential φ, endowed with specific mathematical properties.

The internal variables α at time t are supposed to contain all the relevant information about the material history for times $\tau \leq t$. The choice of these variables depend obviously on the constitutive relations under consideration. Some of these variables have a purely macroscopic interpretation. Other variables are sometimes *interpreted* as microstructural variables but most often the equations governing their evolution are not really derived from micromechanical considerations.

The aim of this paper is to give an example of an approximate micromechanical scheme in which internal variables at the macroscopic level have a well understood micromechanical interpretation. More specifically, we consider a nonhomogeneous material with elementary constituents which are standard is the simplest possible form. The only internal variable is the anelastic strain. It is well known that the overall behavior of such a composite has a GSM structure but with infinitely many internal variables which are the fields of local internal variables. This result will be recalled in section 2 following the presentation of [Suquet, 1985]. Similar ideas were already present in different forms in the works of [Rice, 1970] and [Mandel, 1972] among others.

In practice it is necessary to reduce the number of internal variables by considering that the local fields of anelastic strains depend only on a finite number of "shape functions" describing the variations of the local plastic fields. This reduction is done in section 3. It is remarked that the proposed method reduces to the "Transformation Field Analysis" of [Dvorak et al, 1994], when the plastic strain fields are assumed to be uniform within each individual phase. This corresponds to the case where the shape functions are the characteristic functions of the phases. The proposed theory is more general in that the shape functions are not required to be uniform within a given domain. The method is illustrated in section 4 and its merits are assessed by comparison with the TFA.

2. STABILITY OF THE STANDARD STRUCTURE BY CHANGE OF SCALE

Consider a "representative volume element" (r.v.e) V of the nonhomogeneous material composed of N different phases or subdomains. This r.v.e is subjected to an average loading characterized by a given path in the space of overall strain or stress. Attention is limited to isothermal evolutions and infinitesimal deformations. The overall Cauchy stress $\overline{\sigma}$ and the overall infinitesimal deformation $\overline{\varepsilon}$ are the averages of their local counterparts σ and ε

$$\overline{\sigma} = \langle \sigma \rangle, \quad \overline{\varepsilon} = \langle \varepsilon \rangle, \quad \text{where } \langle f \rangle = \frac{1}{|V|} \int_V f(\boldsymbol{x}) \, d\boldsymbol{x}. \tag{1}$$

The local stress and strain fields are determined through the resolution of the "local" evolution problem posed for the r.v.e. and consisting of equilibrium equations, boundary conditions and constitutive relations. The boundary conditions are assumed to be such that Hill's micro-macro localization condition is satisfied: for any compatible strain field ε and any stress field σ in equilibrium, both meeting the boundary conditions imposed on the boundary of the r.v.e., the following equality holds

$$\langle \sigma : \varepsilon \rangle = \langle \sigma \rangle : \langle \varepsilon \rangle = \overline{\sigma} : \overline{\varepsilon}. \tag{2}$$

Examples of boundary conditions meeting (2) include uniform strains, uniform stresses, periodicity conditions (see [Suquet, 1987] for more details). Periodicity boundary conditions will be assumed in the following.

2.1 Standard constitutive relations

The behavior of the individual constituent at point $\boldsymbol{x}$ is defined by a "standard" model, *i.e.* by two thermodynamic potentials. The free energy ρw defines (through the state laws) the forces available in the system at rest to drive the dissipative mechanisms, and the dissipation potential φ relates the rate of the dissipative mechanisms (complementary laws) with the associated forces. For simplicity we shall consider that the only dissipative mechanism comes through an anelastic strain (plastic or viscoplastic strain) $\boldsymbol{\varepsilon}^{\mathrm{an}}$ and that the free energy is a quadratic function of the elastic strain

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathrm{e}} + \boldsymbol{\varepsilon}^{\mathrm{an}}, \quad \rho w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{an}}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{an}}) : \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{an}}). \tag{3}$$

Then the state laws and the complementary laws read respectively:

$$\text{State laws:} \quad \boldsymbol{\sigma}(\boldsymbol{x}) = \rho \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{x}), \boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})) = \boldsymbol{L}(\boldsymbol{x}) : (\boldsymbol{\varepsilon}(\boldsymbol{x}) - \boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})), \tag{4}$$

$$\text{Complementary laws:} \quad \boldsymbol{\sigma} = \frac{\partial \varphi}{\partial \dot{\boldsymbol{\varepsilon}}^{\mathrm{an}}}(\boldsymbol{x}, \dot{\boldsymbol{\varepsilon}}^{\mathrm{an}}(\boldsymbol{x})). \tag{5}$$

The potentials ρw and φ may depend on $\boldsymbol{x}$ (nonhomogeneity of the volume element) and are assumed to be convex with respect to their other arguments.

2.2 Generalized standard structure of the overall constitutive relations

The free energy is an additive quantity or in other words the overall free energy of the r.v.e. V is the average of the local free energy. As shown in [Suquet, 1987], the state variables at the macroscopic level consist of the average strain $\overline{\boldsymbol{\varepsilon}}$ and of an infinite number of internal variables which are the values of the anelastic strain field at every microscopic point $\boldsymbol{x} \in V$:

$$\boldsymbol{\alpha} = \{\boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}. \tag{6}$$

The overall free energy reads

$$\widetilde{\rho w}\left(\overline{\boldsymbol{\varepsilon}}, \{\boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}\right) = \langle \rho w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{an}}) \rangle, \quad \text{with} \quad \widetilde{\rho} = \langle \rho \rangle. \tag{7}$$

The forces associated with the state variables are

$$\widetilde{\rho} \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{\varepsilon}}}\left(\overline{\boldsymbol{\varepsilon}}, \{\boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}\right), \quad \mathcal{A} = \{\mathcal{A}_{\boldsymbol{x}}\}_{\boldsymbol{x} \in V}, \quad \mathcal{A}_{\boldsymbol{x}} = -\widetilde{\rho} \frac{\partial \widetilde{w}}{\partial \boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})}\left(\overline{\boldsymbol{\varepsilon}}, \{\boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}\right). \tag{8}$$

The first force can be computed using Hill's lemma

$$\widetilde{\rho} \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{\varepsilon}}}\left(\overline{\boldsymbol{\varepsilon}}, \{\boldsymbol{\varepsilon}^{\mathrm{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}\right) = \left\langle \rho \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{an}}) : \frac{\partial \boldsymbol{\varepsilon}}{\partial \overline{\boldsymbol{\varepsilon}}} \right\rangle = \left\langle \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}}{\partial \overline{\boldsymbol{\varepsilon}}} \right\rangle = \langle \boldsymbol{\sigma} \rangle : \left\langle \frac{\partial \boldsymbol{\varepsilon}}{\partial \overline{\boldsymbol{\varepsilon}}} \right\rangle = \overline{\boldsymbol{\sigma}},$$

since $\left\langle \dfrac{\partial \varepsilon}{\partial \overline{\varepsilon}} \right\rangle = \boldsymbol{I}$. Similarly, the set of forces $\{\mathcal{A}_{\boldsymbol{x}}\}_{\boldsymbol{x} \in V}$ coincides with the local stress field $\{\boldsymbol{\sigma}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}$. The effective dissipation potential reads

$$\widetilde{\varphi}(\{\dot{\boldsymbol{\varepsilon}}^{\mathsf{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}) = \langle \varphi(\dot{\boldsymbol{\varepsilon}}^{\mathsf{an}}) \rangle. \tag{9}$$

With the choices (6) (7) (9), the effective constitutive relations of the composite have a generalized standard structure:

$$\text{State variables:} \quad \overline{\varepsilon}, \quad \boldsymbol{\alpha} = \{\boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x})\}_{\boldsymbol{x} \in V}, \tag{10}$$

$$\text{State laws:} \quad \overline{\boldsymbol{\sigma}} = \widetilde{\rho} \frac{\partial \widetilde{w}}{\partial \overline{\varepsilon}}(\overline{\varepsilon}, \boldsymbol{\alpha}), \quad \mathcal{A} = -\widetilde{\rho} \frac{\partial \widetilde{w}}{\partial \boldsymbol{\alpha}}(\overline{\varepsilon}, \boldsymbol{\alpha}), \tag{11}$$

$$\text{Complementary laws:} \quad \mathcal{A} = \frac{\partial \widetilde{\varphi}}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}). \tag{12}$$

2.3 Green operator Γ

At rest (no evolution of the system) the stress and strain field in the r.v.e. solve the following linear elastic problem, with appropriate boundary conditions

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : (\boldsymbol{\varepsilon}(\boldsymbol{x}) - \boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x})), \quad \operatorname{div}(\boldsymbol{\sigma}(\boldsymbol{x})) = 0, \quad \langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}. \tag{13}$$

The strain field $\boldsymbol{\varepsilon}(\boldsymbol{x})$ solution of this problem is a nonlocal function of the anelastic strain field and can be expressed as:

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x}) : \overline{\boldsymbol{\varepsilon}} + \frac{1}{|V|} \int_V \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}') : \boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x}') \, d\boldsymbol{x}' = \boldsymbol{A}(\boldsymbol{x}) : \overline{\boldsymbol{\varepsilon}} + \boldsymbol{D} * \boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x}), \tag{14}$$

where

$$\boldsymbol{D} * \boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x}) \overset{def}{=} \frac{1}{|V|} \int_V \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}') : \boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x}') \, d\boldsymbol{x}'. \tag{15}$$

In this relation $\boldsymbol{A}(\boldsymbol{x})$ denotes the elastic strain-localization tensor, and $\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}') : \boldsymbol{L}(\boldsymbol{x}')$ gives the strain at point $\boldsymbol{x}$ created by an eigenstrain $\boldsymbol{\varepsilon}^{\mathsf{an}}(\boldsymbol{x}')$ at point $\boldsymbol{x}'$. $\boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}')$ denotes the elastic Green operator which can be expressed in terms of the derivatives of the Green function for the Navier equations with elastic coefficients $\boldsymbol{L}$. More specifically, given a field of eigenstress $\boldsymbol{\tau}(\boldsymbol{x})$, the solution of the elasticity problem:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{x}) + \boldsymbol{\tau}(\boldsymbol{x}), \quad \operatorname{div}(\boldsymbol{\sigma}(\boldsymbol{x})) = 0, \quad \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{0}, \tag{16}$$

can be expressed as:

$$\varepsilon(\boldsymbol{x}) = -\langle \boldsymbol{\Gamma} * \boldsymbol{\tau} \rangle (\boldsymbol{x}). \tag{17}$$

$\boldsymbol{\Gamma}$ has simple properties which will be useful in the sequel

$$\int_V \boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}') \, d\boldsymbol{x}' = \boldsymbol{0}, \quad \int_V \boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}') \, d\boldsymbol{x} = \boldsymbol{0}, \quad \boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}') = {}^{\mathrm{T}}\boldsymbol{\Gamma}(\boldsymbol{x}', \boldsymbol{x}). \tag{18}$$

3. REDUCTION OF THE NUMBER OF INTERNAL VARIABLES

3.1 State variables

In order to reduce the number of internal variables, we assume throughout the following that the field of anelastic strains can be expressed as a function of a finite number of "shape functions" θ_α:

$$\varepsilon^{\mathsf{an}}(\boldsymbol{x}) = \sum_{\alpha=1}^{A} \varepsilon_\alpha^{\mathsf{an}} \, \theta_\alpha(\boldsymbol{x}). \tag{19}$$

The "reduced" state variables of the model are the overall strain and the component of the anelastic strain field on the shape functions:

$$\overline{\varepsilon} \quad \text{and} \quad \boldsymbol{\alpha} = \{\varepsilon_\alpha^{\mathsf{an}}\}_{\alpha=1,..,A}. \tag{20}$$

A typical example of such shape functions is provided by the characteristic functions of phases or subdomains within the same phase (we shall consider the subdomains as separate phases even though a single mechanical phase can be divided into several subdomains):

$$\chi_r(\boldsymbol{x}) = 1 \text{ if } x \in V_r, \quad \chi_r(\boldsymbol{x}) = 0 \text{ otherwise.} \tag{21}$$

This specific choice leads to the "Transformation Field Analysis" of [Dvorak, 1992] where the plastic strain field is assumed to be uniform over each individual subdomain V_r. However it may be interesting in certain circumstances to consider shape functions which are richer than the characteristic functions to account for spatial nonuniformity of the (anelastic) strain field within one phase or subdomain. The resulting theory will be called the "Nonuniform Transformation Field Analysis" (NTFA).

It is assumed that the shape functions have their support entirely contained in a single phase. In more mathematical terms it is assumed that

$$\theta_\alpha(\boldsymbol{x})\chi_r(\boldsymbol{x}) = 0 \text{ or } \theta_\alpha(\boldsymbol{x}) \quad \forall r = 1, ..., N. \tag{22}$$

Therefore one can define $\boldsymbol{L}_\alpha$ and φ_α as the stiffness tensor and the dissipation potential of the phase r in which the shape function θ_α has its support.

3.2 State laws

With the decomposition (19), the effective free-energy (7) and the thermodynamic forces associated with the state variables $(\overline{\varepsilon}, \{\varepsilon_\alpha^{an}\}_{\alpha=1,\dots,A})$ read as

$$
\left.
\begin{aligned}
\widetilde{\rho}\widetilde{w}\left(\overline{\varepsilon}, \{\varepsilon_\alpha^{an}\}_{\alpha=1,\dots,A}\right) &= \frac{1}{2}\left\langle (\varepsilon - \sum_{\alpha=1}^{A}\varepsilon_\alpha^{an}\theta_\alpha) : L : (\varepsilon - \sum_{\beta=1}^{A}\varepsilon_\beta^{an}\theta_\beta)\right\rangle, \\[2mm]
\overline{\sigma} &= \widetilde{\rho}\frac{\partial \widetilde{w}}{\partial \overline{\varepsilon}}\left(\overline{\varepsilon}, \{\varepsilon_\alpha^{an}\}_{\alpha=1,\dots,A}\right) = \left\langle L : (\varepsilon - \sum_{\alpha=1}^{A}\varepsilon_\alpha^{an}\theta_\alpha)\right\rangle, \\[2mm]
\mathcal{A}_\alpha &= -\widetilde{\rho}\frac{\partial \widetilde{w}}{\partial \varepsilon_\alpha^{an}}\left(\overline{\varepsilon}, \{\varepsilon_\alpha^{an}\}_{\alpha=1,\dots,A}\right) = \langle L : (\varepsilon - \varepsilon^{an})\theta_\alpha\rangle = \langle \sigma\theta_\alpha\rangle.
\end{aligned}
\right\}
\tag{23}
$$

The state laws can be more easily expressed in terms of the following generalized stresses and strains

$$
a_\alpha = \frac{\langle \sigma\theta_\alpha\rangle}{\langle \theta_\alpha\rangle}, \quad e_\alpha = \frac{\langle \varepsilon\theta_\alpha\rangle}{\langle \theta_\alpha\rangle}, \quad e_\alpha^{an} = \frac{\langle \varepsilon^{an}\theta_\alpha\rangle}{\langle \theta_\alpha\rangle}.
\tag{24}
$$

Note that

$$
\mathcal{A}_\alpha = a_\alpha\langle \theta_\alpha\rangle, \quad \varepsilon_\alpha^{an} = \sum_{\beta=1}^{A}(g)_{\alpha\beta}^{-1}\langle \theta_\beta\rangle e_\beta^{an}, \quad \text{where} \quad g_{\alpha\beta} = \langle \theta_\alpha\theta_\beta\rangle.
\tag{25}
$$

Multiplying the local state law (4) by θ_α and averaging over V yields

$$
a_\alpha = L_\alpha : (e_\alpha - e_\alpha^{an}), \quad \alpha = 1, \dots, A.
\tag{26}
$$

Under the approximation (19), (14) becomes

$$
\varepsilon(x) = A(x) : \overline{\varepsilon} + \sum_{\beta=1}^{A}(D * \theta_\beta)(x) : \varepsilon_\beta^{an}.
\tag{27}
$$

Upon multiplication of equation (27) by θ_α and averaging over V, one obtains

$$
e_\alpha = A_\alpha : \overline{\varepsilon} + \sum_{\beta=1}^{A}D_{\alpha\beta} : \varepsilon_\beta^{an},
\tag{28}
$$

where

$$
A_\alpha = \frac{\langle A\theta_\alpha\rangle}{\langle \theta_\alpha\rangle}, \quad D_{\alpha\beta} = \frac{\langle \theta_\alpha D * \theta_\beta\rangle}{\langle \theta_\alpha\rangle}.
\tag{29}
$$

Similarly, incorporating (27) into (23b) yields

$$\overline{\sigma} = \langle L : A \rangle : \overline{\varepsilon} + \sum_{\alpha=1}^{A} (\langle L : D * \theta_\alpha \rangle - L_\alpha \langle \theta_\alpha \rangle) : \varepsilon_\alpha^{\mathrm{an}}. \tag{30}$$

The state laws, expressing the forces $\overline{\sigma}$ and $\mathcal{A}_\alpha$ in terms of the state variables $\overline{\varepsilon}$ and $\varepsilon_\alpha^{\mathrm{an}}$ consist of (30), (26) with (28) and (25).

3.3 Complementary laws

Under the approximation (19), the dissipation potential (9) can be expressed in terms of the rates of the internal variables $\{\varepsilon_\alpha^{\mathrm{an}}\}_{\alpha=1,\ldots,A}$:

$$\widetilde{\varphi}(\dot{\alpha}) = \langle \varphi(\dot{\varepsilon}^{\mathrm{an}}) \rangle, \quad \text{where} \quad \dot{\varepsilon}^{\mathrm{an}}(x) = \sum_{\alpha=1}^{A} \dot{\varepsilon}_\alpha^{\mathrm{an}} \theta_\alpha(x). \tag{31}$$

Then

$$\frac{\partial \widetilde{\varphi}}{\partial \dot{\varepsilon}_\alpha^{\mathrm{an}}} (\{\dot{\varepsilon}_\alpha^{\mathrm{an}}\}_{\alpha=1,\ldots,A}) = \left\langle \frac{\partial \varphi}{\partial \dot{\varepsilon}^{\mathrm{an}}} (\dot{\varepsilon}^{\mathrm{an}}) \theta_\alpha \right\rangle = \langle \sigma \theta_\alpha \rangle = \mathcal{A}_\alpha. \tag{32}$$

Therefore the constitutive relations of the composite (in reduced form) have a generalized standard structure defined by the state variables (20), the free energy (23) and the dissipation potential (31).

There is however a difficulty in applying the complementary law (32) in *exact form*. This would require the knowledge of $\langle \varphi(\dot{\varepsilon}^{\mathrm{an}}) \rangle$ which cannot be expressed simply in terms of the $\dot{\varepsilon}_\alpha^{\mathrm{an}}$'s. Another approximation has to be introduced. Note that thanks to the convexity of φ_α one has:

$$\frac{\langle \theta_\alpha \varphi_\alpha(\dot{\varepsilon}^{\mathrm{an}}) \rangle}{\langle \theta_\alpha \rangle} \geq \varphi_\alpha \left(\frac{\langle \dot{\varepsilon}^{\mathrm{an}} \theta_\alpha \rangle}{\langle \theta_\alpha \rangle} \right) \tag{33}$$

The right-hand-side of (33) can be considered as an approximation of its left-hand-side. Then

$$\langle \theta_\alpha \sigma \rangle = \left\langle \theta_\alpha \frac{\partial \varphi_\alpha}{\partial \dot{\varepsilon}^{\mathrm{an}}} (\dot{\varepsilon}^{\mathrm{an}}) \right\rangle \simeq \left\langle \theta_\alpha \frac{\partial \varphi_\alpha}{\partial \dot{\varepsilon}^{\mathrm{an}}} \left(\frac{\langle \dot{\varepsilon}^{\mathrm{an}} \theta_\alpha \rangle}{\langle \theta_\alpha \rangle} \right) \right\rangle = \langle \theta_\alpha \rangle \frac{\partial \varphi_\alpha}{\partial \dot{\varepsilon}^{\mathrm{an}}} \left(\frac{\langle \dot{\varepsilon}^{\mathrm{an}} \theta_\alpha \rangle}{\langle \theta_\alpha \rangle} \right).$$

Therefore the complementary equations (32) can be expressed (in approximate form) as:

$$a_\alpha = \frac{\partial \varphi_\alpha}{\partial \dot{\varepsilon}^{\mathrm{an}}} (\dot{e}_\alpha^{\mathrm{an}}). \tag{34}$$

3.4 Link with the Transformation Field Analysis

The link with the Transformation Field Analysis of [Dvorak, 1992] can be made by choosing the shape functions to coincide with the characteristic functions (21) of the phases or subdomains:

$$\theta_\alpha(\boldsymbol{x}) = \chi_r(\boldsymbol{x}), \quad \langle \theta_\alpha \rangle = c_r, \quad \langle \theta_\alpha \theta_\beta \rangle = c_r \delta_{rs}, \quad r, s = 1, ..., N,$$

where c_r is the volume fraction of phase r and δ_{rs} is the Kronecker symbol. The anelastic strain is assumed to be uniform within each subdomain V_r. The generalized stress and strains $\boldsymbol{a}_\alpha$ and $\boldsymbol{e}_\alpha$ reduce to the average stress and strain over the subdomain V_r.

The state laws (26) and the complementary laws (34) read:

$$\overline{\boldsymbol{\sigma}} = \sum_{r=1}^{N} c_r \boldsymbol{\sigma}_r, \quad \boldsymbol{\sigma}_r = \boldsymbol{L}_r : (\boldsymbol{\varepsilon}_r - \boldsymbol{\varepsilon}_r^{\text{an}}), \quad \boldsymbol{\sigma}_r = \frac{\partial \varphi_r}{\partial \dot{\boldsymbol{\varepsilon}}^{\text{an}}} (\dot{\boldsymbol{\varepsilon}}_r^{\text{an}}), \quad r = 1, ..., N, \tag{35}$$

where the average strains $\boldsymbol{\varepsilon}_r$ in the different subdomains are given by:

$$\boldsymbol{\varepsilon}_r = \boldsymbol{A}_r : \overline{\boldsymbol{\varepsilon}} + \sum_{s=1}^{N} \boldsymbol{D}_{rs} : \boldsymbol{\varepsilon}_s^{\text{an}}, \quad r = 1, ..., N. \tag{36}$$

The fourth-order tensors $\boldsymbol{A}_\alpha$ and $\boldsymbol{D}_{\alpha\beta}$ are the average strain localization tensors $\boldsymbol{A}_r$ and the influence tensors $\boldsymbol{D}_{rs}$ which are the basic ingredients of the TFA ([Dvorak, 1992]):

$$\boldsymbol{A}_r = \frac{1}{c_r} \frac{1}{|V|} \int_V \boldsymbol{A}(\boldsymbol{x}) \chi_r(\boldsymbol{x}) \, d\boldsymbol{x},$$

and

$$\boldsymbol{D}_{rs} = \frac{1}{c_r} \frac{1}{|V|} \frac{1}{|V|} \int_V \int_V \chi_r(\boldsymbol{x}) \boldsymbol{\Gamma}(\boldsymbol{x}, \boldsymbol{x}') : \boldsymbol{L}(\boldsymbol{x}') \chi_s(\boldsymbol{x}') \, d\boldsymbol{x}' d\boldsymbol{x}.$$

A few well known algebraic properties of these tensors are useful in their computations

$$\sum_{r=1}^{N} \boldsymbol{D}_{sr} = \boldsymbol{I} - \boldsymbol{A}_s, \quad \sum_{r=1}^{N} \boldsymbol{D}_{sr} \boldsymbol{L}_r^{-1} = 0, \quad c_s \boldsymbol{L}_s \boldsymbol{D}_{sr} = c_r^{\mathsf{T}} \boldsymbol{D}_{rs} \boldsymbol{L}_r.$$

4. EXAMPLES

The relative merits of the above models are assessed by means of the following two-dimensional example. The r.v.e. consists of a square unit cell containing a square inclusion (phase 1) located at its center (with volume fraction $c_1 = 0.25$). The unit cell is subjected to periodic boundary conditions. The inclusion is linear elastic. The surrounding matrix is elastic perfectly plastic (von Mises criterion with yield stress $\sigma_0 = 100$ MPa). The inclusion and the matrix have the same elastic moduli $E = 100$ GPa, $\nu = 0.25$.
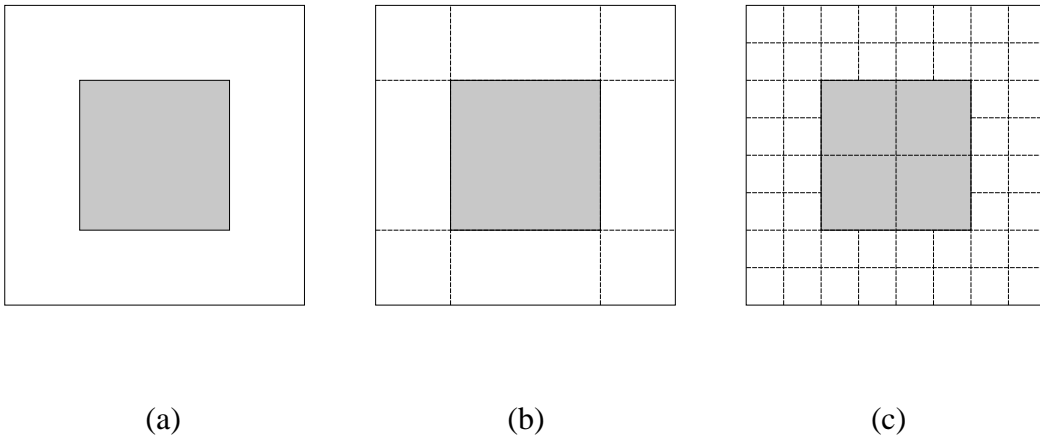
Figure 1: *Unit cell. Subdivisions used for the implementation of the TFA. (a): 2 subdomains, matrix and inclusion. (b): 8 subdomains in the matrix. (c): 48 subdomains in the matrix, 4 subdomains in the inclusion.*
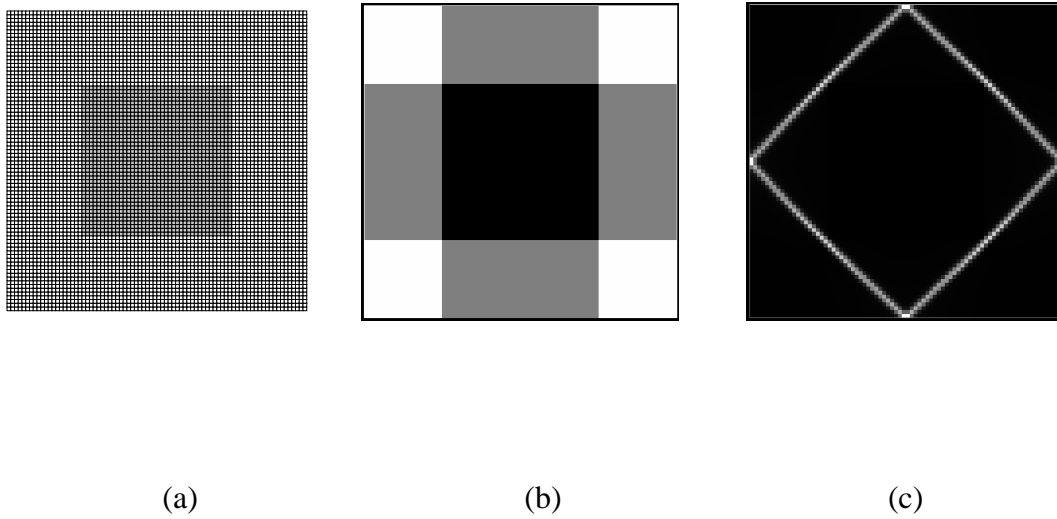

Figure 2: *(a) Mesh used in the FEM calculations. (b) Shape function 1 (flow mode in simple shear). (c) Shape function 2 (flow mode in uniaxial tension).*
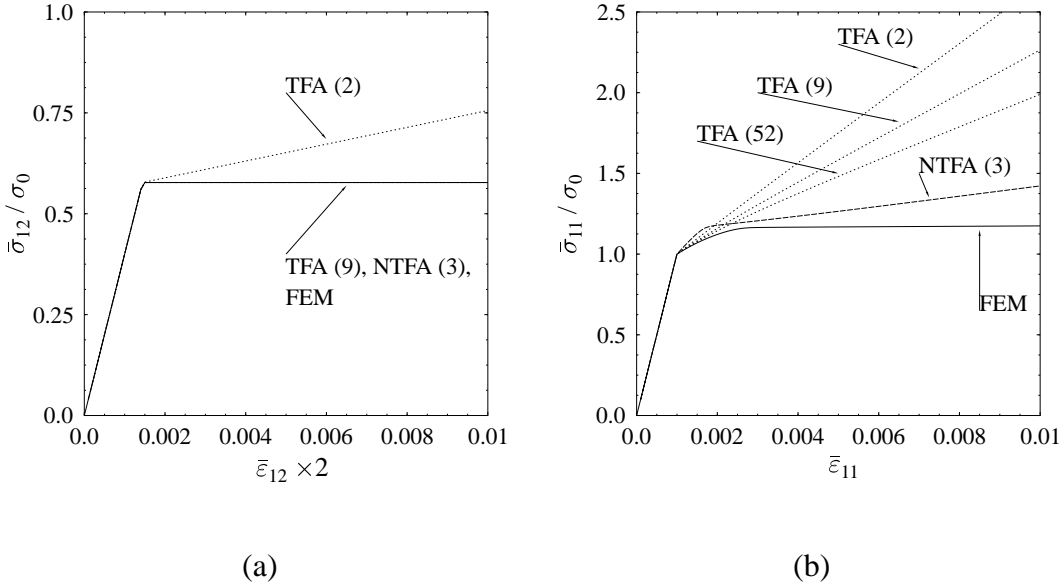
Figure 3: *Effective stress strain curves. (a) Pure shear. (b) Uniaxial tension. The number in parentheses denotes the number of subdomains or shape functions used in the implementation of the TFA or NTFA.*

The unit cell is subjected to an in-plane overall stress

$$\overline{\boldsymbol{\sigma}} = \overline{\sigma}_{11}\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 + \overline{\sigma}_{22}\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 + 2\overline{\sigma}_{12}\boldsymbol{e}_1 \otimes_s \boldsymbol{e}_2. \tag{37}$$

Attention has been paid to two specific cases, simple shear ($\overline{\sigma}_{11} = \overline{\sigma}_{22} = 0$) and uniaxial tension ($\overline{\sigma}_{12} = \overline{\sigma}_{22} = 0$). The exact responses (up to numerical errors) of the unit cell under the simple shear and uniaxial tension has been computed by the FEM. The TFA and the NTFA have also been implemented.

Several subdivisions of the unit cell have been considered in the implementation of the TFA. The cruder subdivision considers the plastic strain to be uniform in the matrix (Figure 1a). Finer subdivisions were also investigated in which the matrix was divided into 8 and 48 subdomains respectively, as shown in Figure 1b and 1c. The elastic properties of the inclusion and of the matrix being identical, the elastic strain localization is trivial $\boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{I}$. The influence matrices $\boldsymbol{D}_{rs}$ are computed numerically by the Finite Element Method using a regular mesh of 80×80 quadrilateral 8 nodes elements shown in Figure 2a. A uniform eigenstrain $\boldsymbol{\varepsilon}^{\text{an}}$ is prescribed to the subdomain V_s and the average strain in subdomain V_r caused by this perturbation is computed. The corresponding relation yields the influence tensor $\boldsymbol{D}_{rs}$.

Only three shape functions were used in the NTFA (more shape functions could have been used but it is worth noting that satisfactory results can be obtained with relatively few

shape functions). The first shape function θ_1 is the characteristic function of the inclusion. The second shape function θ_2 is the flow mode in pure shear. The third shape function θ_3 is the flow mode under uniaxial tension. These modes and the corresponding influence matrices $\boldsymbol{D}_{\alpha\beta}$ were computed numerically by the FEM using the mesh shown in Figure 2a. Snapshots are shown in Figure 2b (pure shear) and 2c (uniaxial tension). Whiter zones denote higher strains. Remarkably enough, the pattern flow mode under pure shear shows zones with uniform strains. An exact solution for this problem can be constructed in closed form. The strain field, solution of the elasto-plastic evolution problem, is a pure slip solution which can be expressed in terms of $\varepsilon^{\mathbf{e}} = \dfrac{\sigma_0}{2\sqrt{3}\mu}$ as

$$\varepsilon_{12} = \varepsilon^{\mathbf{e}} \text{ in } A, \quad \varepsilon_{12} = \frac{\overline{\varepsilon}_{12} - \varepsilon^{\mathbf{e}}}{1 - \sqrt{c_1}} + \varepsilon^{\mathbf{e}} \text{ in } B, \quad \varepsilon_{12} = \frac{\overline{\varepsilon}_{12} - \varepsilon^{\mathbf{e}}}{2(1 - \sqrt{c_1})} + \varepsilon^{\mathbf{e}} \text{ in } C, \qquad (38)$$

where A denotes the inclusion, B denotes the subdomains located at the top right, top left, bottom right, bottom left in Figure 1b, and C denotes the remaining subdomains in Figure 1b.

The responses of the unit cell to the imposed loadings as predicted by the TFA and NTFA models are shown in Figure 3. The predictions of the TFA with the cruder discretization *i.e.* with one subdomain for the inclusion and one subdomain for the matrix are unrealistically stiff (this is well known [Suquet, 1997], [Chaboche et al, 1999]). When the discretization is refined (the number of subdomains is increased), the predictions of the TFA become more realistic. In simple shear, the exact solution is recovered by the discretization with 8 subdomains as follows straightforwardly from the exact solution (38). But in general the convergence towards the exact solution can be slow as the number of subdomains is increased. This is shown in Figure 3b where it is seen that, even with 48 subdomains in the matrix, the prediction of the TFA is not very accurate. The prediction of the NTFA with only 3 modes is as accurate as the prediction of the TFA with many more subdomains. This is due to the fact that the solution is nonuniform and that this nonuniformity is built-in into the shape functions.

In conclusion, we have shown that the reduction of the number of internal variables achieved by the TFA can be improved. We have considered a decomposition of the microscopic anelastic field on shape functions which are nonuniform and which capture the expected nonuniformity of the exact fields.

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