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On Thermodynamic Consistency of Homogenization-Based Multiscale Theories

In this paper, the necessary and sufficient conditions for fulfilling the thermodynamic consistency of computational homogenization schemes in the framework of hierarchical multiscale theories are defined. The proposal is valid for arbitrary homogenization based multiscale procedures, including continuum and discontinuum methods in either scale. It is demonstrated that the well-known Hill–Mandel variational criterion for homogenization scheme is a necessary, but not a sufficient condition for the micro–macro thermodynamic consistency when dissipative material responses are involved at any scale. In this sense, the additional condition to be fulfilled considering that the multiscale thermodynamic consistency is established. The general case of temperature-dependent, higher order elastoplasticity is considered as theoretical framework to account for the material dissipation at micro and macro scales of observation. It is shown that the thermodynamic consistency enforces the homogenization of the nonlocal terms of the finer scale's free energy density; however, this does not lead to nonlocal gradient effects on the coarse scale. Then, the particular cases of local isothermal elastoplasticity and continuum damage are considered for the purpose of the proposed thermodynamically consistent approach for multiscale homogenizations. [DOI: 10.1115/1.4036243]

1 Introduction

The permanently increasing demand of high accuracy in predicting failure behavior of engineering solid materials, together with the recent rapid growth of parallel computing power, the experimental capabilities to characterize structure–property relationships down to atomistic level, and theories that admit multiple length scales, has led to an extensive use and, moreover, to the need of computational multiscale modeling methodologies. At present, multiscale modeling has broached different disciplines (solid mechanics, fluid mechanics, materials science, physics, mathematics, biological, and chemistry), and different length scales (from atoms to structure scale levels). Multiscale procedures have been applied in quite different forms since the very beginning of the scientific knowledge. One remarkable and very old application, although purely mathematical as it has no length involved on the smaller scale, is the Euclidean analytical procedure applied for the formulation of boundary value problems. They involve homogenization strategies to pass from the Eulerian differential equations of the smaller of infinitesimal scale to the final integral formulation of the larger or boundary value scale. Nowadays, modern multiscale procedures allow the fine scale to be explicitly modeled within really fine domains called representative volume element (RVE) where appropriated boundary conditions are introduced in order to obtain accurate representation of the involved physical problem. Multiscale schemes can be classified into hierarchical and concurrent methods. The latter involves strong coupling between coarse and fine scales. Concurrent multiscale procedures were followed, among others, by Guidault et al. [1], Hettich et al. [2], Eckardt and Könke [3], Lloberas-Valls et al. [4]. Hierarchical multiscale schemes and also the so-called semi-concurrent methods involve weak kinetic and kinematic coupling. So, in these multiscale procedures the fine-scale response obtained

from a fine-scale model solution is translated to the coarse-scale stresses using Hill's formulas (see Ref. [5]), or by the so-called Hill–Mandel equations [6] and incorporated to the coarse-scale model. Although many proposed concurrent methods involved very small length scales, e.g., Abraham et al. [7], Khare et al. [8], and Xiao and Belytschko [9] who considered concurrent atomistic/continuum multiscale approaches, the requirements of strong coupling between the involved scales and of domain decomposition techniques make the concurrent procedure of multiscale schemes less attractive and computationally more demanding than those multiscale schemes based on weak interface conditions. This is the main reason why the application of the hierarchical and semiconcurrent methods is growing much faster.

The weak interface conditions based approaches of multiscale material modeling can be subdivided into continuum–continuum, continuum–discontinuum, and discontinuum–discontinuum strategies regarding the continuity of the two involved scales. Among others, we may refer here to the continuum–continuum multiscale model proposed by Kouznetsova et al. [10] who used a second-order computational homogenization for both scales to enrich the macroscopic response; by de Souza Neto and Feijóo [6] and Peric et al. [11], where a variational foundation of the homogenization strategy for continuum–continuum multiscale approaches is proposed; and by Gitman et al. [12]. Regarding the continuum–discontinuum approach for multiscale models, the proposals by Nguyen et al. [13]; Coenen et al. [14]; Karamnejad et al. [15]; and Poh et al. [16] can be referred, among others. Particularly, Poh et al. proposed a homogenization theory which consistently translates a crystal plasticity model with one slip system into the macroscopic scale. Finally, and related to the discontinuum–discontinuum strategy, it was followed by Toro et al. [17]; Verhoosel et al. [18]; Oliver et al. [19], among others.

To avoid the intrinsic loss of ellipticity of the differential constitutive equations of softening materials in the fine scale, some proposals related to continuum–discontinuum and continuum–continuum multiscale material models did include nonlocal gradient formulations at the fine scale, see Refs. [16], [20], and [21]. It should be noted, however, that the consideration of nonlocal

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Contributed by the Materials Division of ASME for publication in the JOURNAL OF ENGINEERING MATERIALS AND TECHNOLOGY. Manuscript received November 1, 2016; final manuscript received February 22, 2017; published online May 12, 2017. Assoc. Editor: Peter W. Chung.

constitutive theories at the fine-scale does not prevent the possibility for discontinuous bifurcation on the coarse-scale.

A very important aspect to be considered in multiscale approaches is the thermodynamic consistency regarding all different scales involved. The strong coupling between the different scales of concurrent multiscale procedures allows a direct consideration of the thermodynamic consistency in the macroscopic models. However, the requirement of homogenization procedures in multiscale approaches based on weak interface conditions demands special considerations for fulfilling the thermodynamic consistency in all involved scales. This is a relevant aspect that, so far, was not explored in detail and systematically. In fact, some proposals in the literature, such as Refs. [6] and [22], did consider variational aspects involved in the homogenization process that establishes necessary and sufficient conditions for fulfilling the homogenization of thermodynamic consistency, provided nondissipative materials are considered on both scales. But such variation aspects are insufficient when dissipative materials are involved. Other relevant contributions did deal with multiscale homogenization strategies of thermodynamic variables, e.g., Pohl et al. [16] who proposed a consistent homogenization procedure to account for the grain size dependent behavior in crystalline materials, including the homogenization of the dissipation; Miehe et al. [23] who proposed a homogenization procedure involving microscopic, nonisothermal inelastic deformations at large strains, as well as the definitions of the macroscopic stresses and dissipation in terms of the volume averages of their microscopic counterparts; Maugin [24] who deeply discussed the homogenization theory for elastic and elastoplastic constituents, including the homogenization of both the plastic dissipation and macroscopic internal energy; and finally Suquet [25].

Despite the significant progress made in the formulation of homogenization procedures involving also the treatment of thermodynamic variables, there is still a need for formulating a unified and systematic procedure for thermodynamically consistent homogenizations. This formulation must allow straightforward extensions for any kind of dissipative constituents, under both isothermal and temperature-dependent conditions.

This paper is aimed at formulating this unified and systematic procedure for thermodynamically consistent multiscale homogenizations related to dissipative materials. Both elastoplastic and continue damage-based material theories are considered under isothermal and temperature dependent conditions. After summarizing the thermodynamic principles for general gradient thermoelastoplastic materials, the necessary and sufficient conditions for fulfilling the thermodynamic consistency of multiscale approaches based on weak interface conditions are deduced and systematically formulated. The thermodynamically consistent homogenization procedure in this work is valid for any type of homogenization based multiscale scheme involving continuum–continuum or continuum–discontinuum homogenization. It is deduced and demonstrated that the Hill–Mandel criterion for homogenization is only a necessary condition for the multiscale thermodynamic consistency when dissipative material responses are involved at the fine scale. When considering higher order or gradient plasticity, it is shown that the thermodynamic consistency imposes the homogenization of the nonlocal components of the fine scale’s free energy density which, however, does not lead to nonlocal gradient effects on the coarse scale counterpart.

2 Thermodynamic Principles

In order for any arbitrary constitutive theory to be thermodynamically consistent it must abide the first and second laws of thermodynamics. Both laws are generally condensed into the Clausius–Duhem inequality, which defines the dissipation and its condition of positiveness. Nonthermodynamically consistent material theories may lead to spurious dissipations, or to physically incorrect energy increases during loading cycles. A

summary of the thermodynamic principles is given in the following. Small strain kinematics is assumed.

The first law of thermodynamics for general thermomechanical systems states

$$\dot{E} + \dot{K} = P + Q \quad (1)$$

where E , K , P , and Q denote the internal energy, kinematic energy, mechanical source, and thermal source, respectively.

Not taking into account inertia forces, and considering the law of conservation of mass, the first law of thermodynamics can be rewritten as

$$\rho \dot{e} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + \rho r - \nabla \cdot \mathbf{h} \quad (2)$$

with e is the internal energy per unit mass, ρ is the material density, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{\varepsilon}$ is the strain tensor, r is the energy source, and \mathbf{h} is the heat flux vector

The second law of thermodynamics establishes

$$\dot{S} - Q_\theta \geq 0 \quad \text{or} \quad \rho s \dot{\theta} - \rho r + \nabla \cdot \mathbf{h} - \frac{\mathbf{h} \cdot \nabla \theta}{\theta} \geq 0 \quad (3)$$

with S and Q_θ are the entropy and entropy fluxes, respectively.

Combining Eqs. (2) with (3) and introducing Helmholtz’s free energy density $\psi = e - s\theta$, the Clausius–Duhem inequality can be deduced

$$D = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + \rho s \dot{\theta} - \dot{\psi} - \frac{\mathbf{h} \cdot \nabla \theta}{\theta} \geq 0 \quad (4)$$

where D is the dissipation and s is the entropy density.

Coleman’s equations can be deduced stating that the dissipation must be null for elastic cycles

$$s = -\frac{\partial \psi}{\partial \theta}, \quad \boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} \quad (5)$$

2.1 Thermodynamic Consistency for General Higher-Order Nonisothermal Elastoplasticity. Following Refs. [26–28], arbitrary thermodynamic states of nonisothermal gradient plasticity may be defined in terms of the elastic strain tensor $\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p$; the relative temperature $\theta = T - T_0$; and the internal variable κ which is the only one of nonlocal character. Under small strain kinematics, the free energy density can be expressed as

$$\psi(\boldsymbol{\varepsilon}^e, \theta, \kappa, \nabla \kappa) = \psi^e(\boldsymbol{\varepsilon}^e, \theta) + \psi^l(\kappa, \theta) + \psi^g(\nabla \kappa) \quad (6)$$

where ψ^e is the thermoelastic free energy density; ψ^l is the local thermoplastic free energy density, and ψ^g is the gradient plastic one, which take the following forms:

$$\begin{aligned} \psi^e &= \frac{1}{2} \boldsymbol{\varepsilon}^e : \mathbf{E}^e : \boldsymbol{\varepsilon}^e - \theta \mathbf{A} : \boldsymbol{\varepsilon}^e; & \psi^l &= \frac{H^l}{2} \kappa^2 - \theta s^\kappa; \\ \psi^g &= \frac{1}{2} l_c^2 \nabla \kappa \cdot \mathbf{H}^g \cdot \nabla \kappa \end{aligned} \quad (7)$$

where H^l is the local-plastic hardening/softening modulus, \mathbf{H}^g is the gradient softening tensor, l_c is the gradient characteristic length, and s^κ is the unrecovered entropy or frozen entropy.

The dissipations related to plastic processes, intrinsic dissipation due to heat variation, and heat transport result in

$$D^p = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p + Q_p \dot{\kappa}; \quad D^\theta = -s^k \dot{\theta}; \quad D^{\nabla\theta} = -\frac{\mathbf{h} \cdot \nabla\theta}{\theta} \quad (8)$$

where $Q_p = Q_p^l + Q_p^g$ with Q_p^l and Q_p^g the local and gradient dissipative stresses in the problem domain Ω

$$Q_p^l = -\frac{\delta\psi}{\delta\kappa}; \quad Q_p^g = \theta \nabla \cdot \left(\frac{1}{\theta} \frac{\partial\psi}{\partial\nabla\kappa} \right) \quad (9)$$

Additionally due to the existence of gradient terms, a dissipative term on the boundary appears

$$D^{(b)} = -\int_S Q_p^{(b)} \dot{\kappa} dS \quad (10)$$

being $Q_p^{(b)}$ the dissipative stress on the boundary S

$$Q_p^{(b)} = -\mathbf{n} \cdot \frac{\partial\psi}{\partial\nabla\kappa} \quad (11)$$

The general case of higher-order, temperature-dependent elastoplasticity involves the yield condition $\Phi = \Phi(\boldsymbol{\sigma}, \theta, Q_p^l, Q_p^g)$, and a plastic potential $\Phi^* = \Phi^*(\boldsymbol{\sigma}, \theta, Q_p^l, Q_p^g)$, being the rate form of the constitutive equations

$$\dot{\boldsymbol{\sigma}} = \mathbf{E}^e : \dot{\boldsymbol{\varepsilon}} - \mathbf{E}^e : \dot{\lambda} \frac{\partial\Phi^*}{\partial\boldsymbol{\sigma}} - \dot{\theta} \mathbf{A} \quad (12)$$

$$\dot{Q}_p^l = -H\dot{\kappa} + \frac{\partial s^k}{\partial\kappa} \dot{\theta} \quad (13)$$

$$\dot{Q}_p^g = \dot{Q}^g(\theta, \dot{\theta}, \nabla\kappa, \nabla\dot{\kappa}) \quad (14)$$

In the particular case of isothermal and local elastoplasticity, the terms related to $\theta, \nabla\theta, \dot{\theta}, \nabla\kappa, \nabla\dot{\kappa}$ should be neglected from previous equations.

3 Multiscale Homogenizations of Thermodynamical Variables

In this section, the procedures for multiscale homogenizations of different field variables are considered. The departing concept is the definition of free energy densities on the involved scales, expressed in terms of admissible and independent thermodynamic variables which are systematically considered for the purpose of the multiscale homogenizations in this section.

3.1 Free Energy Consistency (Helmholtz's Energy Homogenization). The volume average principle between the involved scales must be hold for the involved free energy densities through

$$\psi_M = \frac{1}{V} \int_V \psi_\mu dV \quad \text{or in rate form} \quad \dot{\psi}_M = \frac{1}{V} \int_V \dot{\psi}_\mu dV \quad (15)$$

using subindex $(\bullet)_M$ to refer to properties of the coarse scale and subindex $(\bullet)_\mu$ for the fine scale. Equation (15) implies that no additional energy can be generated or lost during the homogenization process.

The homogenization of the free energy (Eq. (15)) can be found in the literature, among others in Refs. [16], [19], [24], and [29]. However, the thermodynamic ramifications of this equation in a thermodynamically consistent framework are not clearly explored in the available literature.

In the particular case of a local, nonisothermal elastoplastic material on the fine scale $[\psi_\mu(\boldsymbol{\varepsilon}_\mu^e, \theta_\mu, \kappa_\mu)]$, using Eq. (8) the free energy consistency equation (15) can be reformulated as

$$\dot{\psi}_M = \frac{1}{V} \int_V \left(\boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu^e - s^k \dot{\theta} + \frac{\partial\dot{\psi}_\mu}{\partial\kappa} \dot{\kappa} \right) dV \quad (16)$$

3.2 Strain Homogenization. Without loss of generality the rate of the fine scale's strain tensor $\dot{\boldsymbol{\varepsilon}}_\mu$ can be additively decomposed into an average strain rate tensor (which is equal to the coarse scale's strain rate tensor) and a strain fluctuation rate tensor

$$\dot{\boldsymbol{\varepsilon}}_\mu = \dot{\boldsymbol{\varepsilon}}_M + \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu \quad (17)$$

with

$$\dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V} \int_V \dot{\boldsymbol{\varepsilon}}_\mu dV \quad \text{and} \quad 0 = \frac{1}{V} \int_V \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu dV \quad (18)$$

In regard to elastoplastic materials, the Prandtl–Reuss additive decomposition of the total strain rates into the elastic and plastic components is valid for each scale separately, so $\dot{\boldsymbol{\varepsilon}}_M = \dot{\boldsymbol{\varepsilon}}_M^e + \dot{\boldsymbol{\varepsilon}}_M^p$ and $\dot{\boldsymbol{\varepsilon}}_\mu = \dot{\boldsymbol{\varepsilon}}_\mu^e + \dot{\boldsymbol{\varepsilon}}_\mu^p$. In turn, the microscopic elastic and plastic strain rate tensors can be additively decomposed into the coarse scale's strain rate tensor and a strain fluctuation rate tensor, so $\dot{\boldsymbol{\varepsilon}}_\mu^e = \dot{\boldsymbol{\varepsilon}}_M^e + \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e$ and $\dot{\boldsymbol{\varepsilon}}_\mu^p = \dot{\boldsymbol{\varepsilon}}_M^p + \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^p$.

However, except for the particular case of a homogeneous strain field, the homogenization of the elastic and plastic strains is not the volume averages (see Ref. [30]). Then, in general,

$$\dot{\boldsymbol{\varepsilon}}_M^p \neq \frac{1}{V} \int_V \dot{\boldsymbol{\varepsilon}}_\mu^p dV \quad \text{and} \quad \dot{\boldsymbol{\varepsilon}}_M^e \neq \frac{1}{V} \int_V \dot{\boldsymbol{\varepsilon}}_\mu^e dV \quad (19)$$

as well as

$$0 \neq \frac{1}{V} \int_V \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^p dV \quad \text{and} \quad 0 \neq \frac{1}{V} \int_V \tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e dV \quad (20)$$

3.3 Stress Homogenization. From Coleman's equation (5), and using Eq. (17)

$$\begin{aligned} \dot{\boldsymbol{\sigma}}_M &= \frac{1}{V} \int_V \left(\frac{\partial\dot{\psi}_\mu}{\partial\boldsymbol{\varepsilon}_\mu^e} : \frac{\partial\boldsymbol{\varepsilon}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} + \frac{\partial\dot{\psi}_\mu}{\partial\boldsymbol{\varepsilon}_\mu^e} : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} \right) dV \\ &= \frac{1}{V} \int_V \dot{\boldsymbol{\sigma}}_\mu dV + \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} dV \end{aligned} \quad (21)$$

Under a general thermodynamic framework, the coarse scale stress is not necessarily a volume average of the fine scale stress.

3.4 Material Operator Homogenization. In order to calculate the elastic material operator the stress tensor is differentiated with respect to $\boldsymbol{\varepsilon}_M^e$

$$\begin{aligned} \mathbf{E}_M^e &= \frac{\partial\dot{\boldsymbol{\sigma}}_M}{\partial\boldsymbol{\varepsilon}_M^e} \\ &= \frac{1}{V} \int_V \frac{\partial\dot{\boldsymbol{\sigma}}_\mu}{\partial\boldsymbol{\varepsilon}_M^e} dV + \frac{1}{V} \int_V \frac{\partial\dot{\boldsymbol{\sigma}}_\mu}{\partial\boldsymbol{\varepsilon}_M^e} : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} dV + \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \frac{\partial^2\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e \partial\boldsymbol{\varepsilon}_M^e} dV \end{aligned} \quad (22)$$

$$\begin{aligned} \mathbf{E}_M^e &= \frac{1}{V} \int_V \mathbf{E}_\mu^e dV + \frac{1}{V} \int_V \mathbf{E}_\mu^e : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} dV + \frac{1}{V} \int_V \mathbf{E}_\mu^e : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} dV \\ &\quad + \frac{1}{V} \int_V \mathbf{E}_\mu^e : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} : \frac{\partial\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e} dV + \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \frac{\partial^2\tilde{\dot{\boldsymbol{\varepsilon}}}_\mu^e}{\partial\boldsymbol{\varepsilon}_M^e \partial\boldsymbol{\varepsilon}_M^e} dV \end{aligned} \quad (23)$$

As it can be seen, the coarse scale's material operator is not simply a volumetric average of the fine scale's material operators. The domains heterogeneity may generate variations in the kinematic field ($\tilde{\epsilon}_\mu$) of the fine scale, which in turn gives rise to very complex nonlinear material responses.

Repeating the procedure but calculating the derivative with respect to the total strain tensor, ϵ_M of the coarse scale, then the tangent material operator can be obtained as

$$\begin{aligned} E_M^t &= \frac{1}{V} \int_V E_\mu^t dV + \frac{1}{V} \int_V E_\mu^t : \frac{\partial \tilde{\epsilon}_\mu}{\partial \epsilon_M} dV + \frac{1}{V} \int_V E_\mu^t : \frac{\partial \tilde{\epsilon}_\mu^e}{\partial \epsilon_M^e} dV \\ &+ \frac{1}{V} \int_V E_\mu^t : \frac{\partial \tilde{\epsilon}_\mu}{\partial \epsilon_M} : \frac{\partial \tilde{\epsilon}_\mu^e}{\partial \epsilon_M^e} dV + \frac{1}{V} \int_V \sigma_\mu : \frac{\partial^2 \tilde{\epsilon}_\mu^e}{\partial \epsilon_M \partial \epsilon_M^e} dV \end{aligned} \quad (24)$$

Finally, given the relations

$$d\sigma_M = E^t : d\epsilon_M = E^e : d\epsilon_M^e \quad \text{and} \quad d\sigma_\mu = E^t : d\epsilon_\mu = E^e : d\epsilon_\mu^e \quad (25)$$

and considering a decoupled behavior of the elastic and plastic operators, then the plastic material operator can be calculated as $E_M^p = E_M^e - E_M^t$.

In the particular case of homogeneous kinematic field (Taylor boundary conditions) $\epsilon_\mu = \epsilon_M$, so $\tilde{\epsilon}_\mu = 0$ and the coarse scale's material operators result in

$$E_M^e = \frac{1}{V} \int_V E_\mu^e dV; \quad E_M^p = \frac{1}{V} \int_V E_\mu^p dV; \quad E_M^t = \frac{1}{V} \int_V E_\mu^t dV \quad (26)$$

Thus, they are defined as volume averages of the corresponding fine scale's material operators, which are weighted means that comply with the known rule of mixtures.

3.5 Temperature Homogenization. Without the loss of generality, the rate of the fine scale's temperature, $\dot{\theta}_\mu$, can be additively decomposed into an average temperature rate (which is equal to the coarse scale's temperature) and a temperature fluctuation rate

$$\dot{\theta}_\mu = \dot{\theta}_M + \dot{\tilde{\theta}}_\mu \quad (27)$$

Then,

$$\dot{\theta}_M = \frac{1}{V} \int_V \dot{\theta}_\mu dV \quad \text{and} \quad 0 = \frac{1}{V} \int_V \dot{\tilde{\theta}}_\mu dV \quad (28)$$

3.6 Entropy Homogenization. Analogous to the stress homogenization from Coleman's equation (5), and using Eq. (27)

$$\begin{aligned} s_M^t &= \frac{1}{V} \int_V \left(\frac{\partial \dot{\psi}_\mu}{\partial \theta_\mu} \frac{\partial \theta_\mu}{\partial \theta_M} + \frac{\partial \dot{\psi}_\mu}{\partial \tilde{\theta}_\mu} \frac{\partial \tilde{\theta}_\mu}{\partial \theta_M} \right) dV \\ &= \frac{1}{V} \int_V s_\mu^t dV + \frac{1}{V} \int_V s_\mu^t \frac{\partial \tilde{\theta}_\mu}{\partial \theta_M} dV \end{aligned} \quad (29)$$

Under a general thermodynamic framework, the coarse scale entropy is not necessarily a volume average of the fine scale entropy.

3.7 Dissipation Homogenization. From Eq. (4), under isothermal condition the free energy of each scale must satisfy, respectively,

$$\dot{\psi}_M = \sigma_M : \dot{\epsilon}_M - D_M \quad \text{and} \quad \dot{\psi}_\mu = \sigma_\mu : \dot{\epsilon}_\mu - D_\mu \quad (30)$$

Replacing Eqs. (30) and (21) into the free energy consistency equation (15)

$$D_M = \frac{1}{V} \int_V \sigma_\mu : \left(\frac{\partial \tilde{\epsilon}_\mu^e}{\partial \epsilon_M^e} : \dot{\epsilon}_M - \dot{\tilde{\epsilon}}_\mu^e \right) dV + \frac{1}{V} \int_V D_\mu dV \quad (31)$$

with

$$D_\mu = \sigma_\mu : \dot{\epsilon}_\mu - \dot{\psi}_\mu = \sigma_\mu : \dot{\epsilon}_\mu^p - \frac{\partial \dot{\psi}_\mu}{\partial \kappa_\mu} \dot{\kappa}_\mu \quad (32)$$

4 Reactive Forces Constrains

In this section, the consequences of reactive forces constrain are considered and analyzed.

Being $\dot{\tilde{\epsilon}}_\mu = \epsilon_\mu(\dot{\tilde{u}}_\mu) \nabla^s \dot{\tilde{u}}_\mu$, and using the divergence theorem results

$$\int_V \epsilon_\mu(\dot{\tilde{u}}_\mu) : \sigma_\mu dV = \int_S \dot{\tilde{u}}_\mu \cdot \mathbf{t}^e dS - \int_V \dot{\tilde{u}}_\mu \cdot \mathbf{b} dV \quad (33)$$

As stated in Ref. [6], Eq. (33) is equal to zero only if each integral vanish individually

$$0 = \int_S \dot{\tilde{u}}_\mu \cdot \mathbf{t}^e dS \quad \text{and} \quad 0 = \int_V \dot{\tilde{u}}_\mu \cdot \mathbf{b} dV \quad (34)$$

and each integral is zero if the forces on the RVE are purely reactive.

Concerning the surface force, only places where displacements are prescribed do work, as in any other point the traction force \mathbf{t}_e is zero. If it is purely reactive, it means that the work is zero in average, and this condition is verified by the boundary conditions. Trivially, under the absence of body forces \mathbf{b} , the second term vanishes as well. Furthermore, if the body force is constant in the volume it can be also seen that the integral vanishes, as if

$$\int_V \nabla^s \dot{\tilde{u}}_\mu dV = 0 \quad \text{then} \quad \int_V \dot{\tilde{u}}_\mu dV = 0 \quad (35)$$

In an analogous form

$$\int_V \sigma_\mu : \frac{\partial \tilde{\epsilon}_\mu^e}{\partial \epsilon_M^e} dV = \int_S \frac{\partial \dot{\tilde{u}}_\mu^e}{\partial \epsilon_M^e} \cdot \mathbf{t}^e dS - \int_V \frac{\partial \dot{\tilde{u}}_\mu^e}{\partial \epsilon_M^e} \cdot \mathbf{b} dV \quad (36)$$

As \tilde{u}_μ is equal to zero on all boundaries where $\mathbf{t}_e \neq 0$ for any value of ϵ_M^e , then the first integral of the last equation is also equal to zero under reactive surface forces. However, the same argument cannot be made for the body force term in case of elastoplastic materials. The integral vanishes only under the absence of body forces, as

$$\int_V \nabla^s \dot{\tilde{u}}_\mu^e dV \neq 0 \quad \text{then, generally} \quad \int_V \dot{\tilde{u}}_\mu^e dV \neq 0 \quad (37)$$

If Eqs. (36) and (33) are null then the homogenization equations (21), (23), (24), and (31) from the subsections of Sec. 3 can be rewritten as

$$\sigma_M = \frac{1}{V} \int_V \sigma_\mu dV \quad (38)$$

$$\mathbf{E}_M^e = \frac{1}{V} \int_V \mathbf{E}_\mu^e dV + \frac{1}{V} \int_V \mathbf{E}_\mu^e : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu^e}{\partial \boldsymbol{\varepsilon}_M^e} dV \quad (39)$$

$$\mathbf{E}_M^t = \frac{1}{V} \int_V \mathbf{E}_\mu^t dV + \frac{1}{V} \int_V \mathbf{E}_\mu^t : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu^t}{\partial \boldsymbol{\varepsilon}_M^t} dV \quad (40)$$

$$D_M = \frac{1}{V} \int_V D_\mu dV \quad (41)$$

The stress homogenization in Eq. (38), which is derived in this work within a complete thermodynamic framework, agrees with that used in the classical (not-necessarily thermodynamically consistent) stress homogenization generally used in the literature. Here, it is proven that this equation complies with the thermodynamic laws only when the RVE traction and body forces are purely reactive.

In regard to the dissipation, Eq. (41) is also commonly used in the literature. However in most cases, for example Ref. [23], it is assumed or proposed by the author. Here, this equation is deduced from the free energy homogenization equation (15) as a requirement for fulfilling thermodynamic consistency.

Finally, it is important to mention that in Ref. [6] it can be also seen that satisfying Eq. (34) is equivalent to satisfying the Hill–Mandel principle. The principle states an energy balance, see Ref. [5], among others, which establishes that the macroscopic energy density per unit volume must be equal to the average microscopic energy density per unit volume, i.e.,

$$\boldsymbol{\sigma}_M : \dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu dV \quad (42)$$

However, the power balance is only valid for total the total power and not valid for the decomposed elastic and plastic power in elastoplastic materials, i.e., in general

$$\boldsymbol{\sigma}_M : \dot{\boldsymbol{\varepsilon}}_M^e \neq \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu^e dV \quad \text{and} \quad \boldsymbol{\sigma}_M : \dot{\boldsymbol{\varepsilon}}_M^p \neq \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu^p dV \quad (43)$$

and instead, in order to calculate the elastic and plastic strain tensors the following relation must be used:

$$\dot{\boldsymbol{\varepsilon}}_M^e = (\mathbf{E}_M^e)^{-1} : \dot{\boldsymbol{\sigma}}_M \quad \text{and} \quad \dot{\boldsymbol{\varepsilon}}_M^p = \dot{\boldsymbol{\varepsilon}}_M - (\mathbf{E}_M^e)^{-1} : \dot{\boldsymbol{\sigma}}_M \quad (44)$$

5 Conditions for Thermodynamic Consistency in Multiscale Homogenization Schemes

In this section, the necessary and sufficient conditions for thermodynamically consistent multiscale homogenization procedures are established.

In order to maintain thermodynamic consistency between scales the only necessary conditions is

$$\psi_M = \frac{1}{V} \int_V \psi_\mu dV \quad (45)$$

Provided the forces on the RVE are purely reactive, the last equation leads to

$$D_M = \frac{1}{V} \int_V D_\mu dV \quad (46)$$

$$\boldsymbol{\sigma}_M : \dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu dV \quad (47)$$

Under the conditions stated in Sec. 4, the stress homogenization in Eq. (38) will automatically ensure the power balance of Eq. (42). This equation together with the dissipation in Eq. (41) will ensure

the free energy consistency. These are the necessary and sufficient conditions to ensure the consistency of the free energy between scales.

Hence, satisfying the Hill–Mandel principle (Eq. (47)) on its own is not enough to achieve a thermodynamically consistent homogenization between scales. Most of the proposed multiscale theories use homogenization procedures which abide this principle, e.g., see Ref. [31]. Therefore, an appropriate and simple procedure to turn these multiscale theories thermodynamically consistent is to include the additional constrain of Eq. (46) representing the dissipation homogenization.

It can be concluded that the Hill–Mandel principle is only a sufficient condition for the thermodynamic consistency of multiscale homogenization procedures when elastic materials are involved. However, when any dissipative material is considered, the Hill–Mandel principle is unable to provide a sufficient condition for thermodynamic consistency, as the homogenization of the additional dissipative terms is beyond the definitions involved in the Hill–Mandel principle.

Furthermore, as shown in Sec. 3, when working on a thermodynamically consistent framework additional constrains arises

$$0 = \int_S \mathbf{t}^e \cdot \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu^e}{\partial \boldsymbol{\varepsilon}_M^e} dS \quad \text{and} \quad 0 = \int_V \mathbf{b} \cdot \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu^e}{\partial \boldsymbol{\varepsilon}_M^e} dV \quad (48)$$

These equations also need to be fulfilled so that the resulting thermodynamically consistent stress tensor complies with Hill's formula.

6 Remarks on Continuum-to-Continuum Homogenization Schemes Related to Nonlocal Materials

If the nonlocal gradient elastoplastic material behavior is only assumed on the fine scale, then from Eq. (6) result

$$\psi_\mu = \psi_\mu^e + \psi_\mu^l + \psi_\mu^g \quad \text{and} \quad \psi_M = \psi_M^e + \psi_M^l \quad (49)$$

Thus, from the free energy homogenization follows:

$$\psi_M^e = \frac{1}{V} \int_V \psi_\mu^e dV \quad \text{and} \quad \psi_M^l = \frac{1}{V} \int_V \psi_\mu^l dV + \frac{1}{V} \int_V \psi_\mu^g dV \quad (50)$$

In Eq. (50), it can be observed that, although the dissipative component of the free energy density of the coarse scale is based on local or classical plasticity, it involves the nonlocal term of the fine scale's free energy density. In other words, being the characteristic length of the fine scale too small in relation to the coarse scale, the regularization capabilities of the fine scale's constitutive theory cannot be transferred to the coarse scale one. This is due to the principle of scale separation in which multiscale theories are based on the fundamental assumption that the characteristic length of the microscale is much smaller than the macroscale discretization.

The most general case of thermodynamically consistent approaches for multiscale homogenizations related to gradient-based constitutive laws correspond to the situation when both scales involve nonlocal materials. In this case, the coarse scale's free energy density is defined in the form

$$\psi_M = \frac{1}{V} \int_V \left(\psi_\mu^e + \psi_\mu^l + \psi_\mu^g \right) dV + \psi_M^g \quad (51)$$

being ψ_μ^g and ψ_M^g the nonlocal dissipative free energy densities of both the fine and the coarse scales which, in turn, are related to completely independent characteristic lengths.

7 Multiscale Homogenization Procedures Based on Discontinuous Materials

One of the most important current applications of multiscale homogenization schemes deals with discontinuous-to-discontinuous

or continuous-to-discontinuous scales transformations. Discontinuous materials are evaluated in the framework of the so-called discrete crack approach. In this case, cracks are represented by means of jumps in the velocity field, or displacement rate field, but not in terms of the velocity gradient jumps as in case of the smeared-crack approach. Several authors have proposed models based on the discrete crack approach to predict failure behavior of quasi-brittle materials.

Once the discontinuity is activated, a “tension–displacement” function is proposed, e.g., see Refs. [32] and [33]. The curve dictates the tension per surface area of the crack as a function of the crack opening displacement, with the total area under the curve being equal to the fracture energy of the involved material, also referred as toughness (see Fig. 1). An example of discontinuous approaches based on energy potentials can be seen in Refs. [16] and [34], among others.

Following Ref. [35], the joint displacement vector \mathbf{u} can be decomposed into elastic and plastically controlled fracture components, \mathbf{u}^e and \mathbf{u}^f , respectively. Being $\psi^c = \psi^c(\mathbf{u}^e, \kappa^f)$ the cohesive free energy, from Coleman and Noll’s method, the traction vector at the interface must be (Fig. 2)

$$\mathbf{t} = \frac{\partial \psi^c}{\partial \mathbf{u}^e} \quad (52)$$

And analogously to the inelastic dissipation in Eq. (8)

$$D^f = \mathbf{t} \cdot \dot{\mathbf{u}}^f - \frac{\partial \psi^c}{\partial \kappa^f} \dot{\kappa}^f \geq 0 \quad (53)$$

being $\dot{\mathbf{u}}^f = \dot{\mathbf{u}}^f(\dot{\kappa}^f)$ the crack opening rate in terms of the rate of the corresponding state variable and $Q^f = -(\partial \psi^c / \partial \kappa^f)$ the dissipative force due to the crack opening.

In the cases where one of the scales uses a discontinuous approach, this dissipation needs to be correctly associated with the other scale in order for the multiscale model to be thermodynamically consistent. In the most general case of homogenization schemes related to discontinuous-to-discontinuous scale transformations, the dissipation on the fine scale RVE may be decoupled into the dissipation in the discrete crack and the dissipation in the surrounding continuum, i.e.,

$$D_\mu = D_\mu^c + D_\mu^f \quad (54)$$

where D_μ^c is the dissipation of the continuous portion of the RVE as defined by Eq. (8), while D_μ^f represents the dissipation on the discrete cracks in the same RVE.

The dissipation on the coarse scale involves the dissipation in the injected discrete crack which can be expressed as

$$D_M = D_M^c + D_M^f = \frac{1}{V} \int_V D_\mu dV \quad \text{with} \quad D_M^f = \mathbf{t}_M \cdot \mathbf{u}_M^f + Q_M \kappa_M^f \quad (55)$$

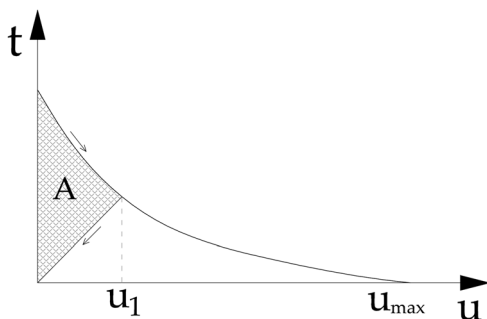


Fig. 1 Tension–displacement function for crack opening

where D_M^c is the contribution of the plastic dissipation of the continuum in the coarse scale, and D_M^f the dissipation associated to the discontinuous part.

In case of continuous-to-discontinuous homogenization schemes, the dissipation in the finer scale is defined solely by Eq. (8) which corresponds to the first term on the right-hand side of Eq. (54). The dissipation on the coarse scale is defined as in Eq. (55). Depending on the material model used for the coarse scale, the term D_M^c might vanish.

If a discontinuous-to-discontinuous scheme is used where an absolute decoupling between continuous and discontinuous terms is used the dissipation homogenization results

$$D_M^c = \frac{1}{V} \int_V D_\mu^c dV \quad \text{and} \quad D_M^f = \mathbf{t}_M \cdot \mathbf{u}_M^f + Q_M \kappa_M^f = \frac{1}{V} \int_V D_\mu^f dV \quad (56)$$

8 Final Remarks

8.1 Dissipation Homogenization. The homogenization of the dissipation is decidedly important when formulating multiscale constitutive theories. Particularly, the dissipation on the fine scale needs to be correctly taken into account for formulating that of the coarse scale due to the direct dependence of the last one on the fine scale dissipation. Nevertheless, as indicated in Sec. 6, additional degrading mechanisms may appear on the coarse scale, which do not depend on that of the fine scale. This means that the material of the coarse scale is characterized by multiple thermodynamic variables, some of them depend on the fine scale mechanical response by means of the homogenization process, while others are fully independent of the fine scale behavior.

8.2 Weak Thermodynamic Consistency in the Fine Scale. The Clausius–Duhem inequality for the coarse scale can be defined as

$$D_M = \frac{1}{V} \int_V D_\mu dV > 0 \quad (57)$$

This inequality on the coarse scale is automatically fulfilled if $D_\mu > 0$ is satisfied in a strong form on the fine scale, i.e., on each point of the RVE. However, the fulfilment in a weak form, i.e., $\int_V D_\mu dV > 0$, is also valid. In other words, material formulations on the fine scale which do not necessarily satisfy the Clausius–Duhem inequality at each point of the fine scale RVE are allowed as long as this inequality is fulfilled in an integral or weak form on the RVE.

9 Conclusions

The thermodynamic consistency of computational homogenization schemes related to hierarchical and semiconcurrent multiscale procedures was analyzed and defined in the framework of dissipative constitutive theories. It was demonstrated that the Hill–Mandel principle is only a sufficient condition for thermodynamic consistency of multiscale homogenization procedures when elastic or perfectly plastic materials theories are considered. When any other type of dissipative material is considered, an additional condition to the Hill–Mandel principle is required to fulfil the thermodynamic consistency of the involved multiscale homogenization scheme. In this work, it was also demonstrated that this additional condition is the homogenization of the dissipation which establishes that the coarse scale’s dissipation is the RVE volume average of that of the fine scale. A relevant consequence of imposing the thermodynamic consistency to multiscale homogenization schemes is that the fulfilment of the Clausius–Duhem inequality on the coarse scale requires only the satisfaction of this inequality in an integral or weak

form on the RVE domain. The conditions for thermodynamically consistent multiscale homogenizations were developed for general nonlocal and nonisothermal inelastic constitutive theories. Then the discontinuous-to-discontinuous multiscale transformations in the framework of the discrete crack procedure were also considered. Thereby, it was shown that the most general forms of the dissipations on both the fine and coarse scales were deduced when the dissipative energy takes place on both the discrete crack and the surrounding inelastic continuum. All together, the results and demonstrations in this paper clearly establish the substantial differences between classical and thermodynamically consistent homogenization schemes of multiscales material theories, and define the necessary conditions to be fulfilled regarding thermodynamic consistency.

Acknowledgment

The authors acknowledge the partial financial support for this work by CONICET (National Council of Scientific and Technical Research, Argentina) through the research Project No. PIP112-1079, and by the University of Buenos Aires through project UBACYT2011.

Appendix: Thermodynamically Consistent Constitutive Relations for Continuum-to-Continuum Multiscale Models

In this section, the constitutive equations for thermodynamically consistent continuum-to-continuum multiscale schemes based on homogenization are derived, for the conditions seen in Sec. 4. The particular cases of continuum damage and elastoplastic material theories are contemplated.

A.1 Continuum Damage Material

Material behavior based on the continuum damage is characterized by a progressive stiffness deterioration. In this case, the field variables which define any possible thermodynamic state of the material are the elastic strain field and the damage parameter d . Therefore, the Helmholtz free energy density of the material on the fine scale may be expressed as

$$\psi_\mu = \psi_\mu(\boldsymbol{\varepsilon}_\mu, d_\mu) \quad (\text{A1})$$

The secant material operator, \mathbf{E}_μ^s (see Fig. 2)

$$\mathbf{E}_\mu^s = (1 - d_\mu)\mathbf{E}_\mu^0 \quad (\text{A2})$$

Hence, the material operator of the coarse scale is

$$\mathbf{E}_M^s = \frac{1}{V} \int_V \mathbf{E}_\mu^s dV + \frac{1}{V} \int_V \mathbf{E}_\mu^s : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A3})$$

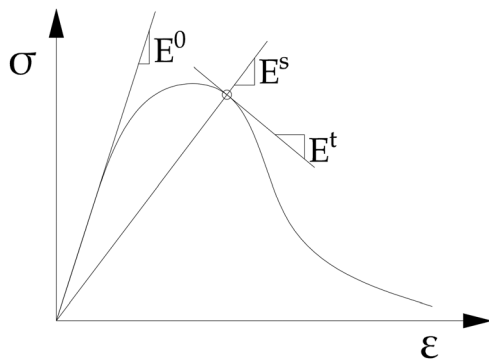


Fig. 2 One-dimensional representation of continuum damage-based material behavior

$$\mathbf{E}_M^s = \frac{1}{V} \int_V [(1 - d_\mu)\mathbf{E}_\mu^0] dV + \frac{1}{V} \int_V [(1 - d_\mu)\mathbf{E}_\mu^0] : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A4})$$

While the tangent material operator results

$$\mathbf{E}_M^t = \frac{1}{V} \int_V \frac{\partial \boldsymbol{\sigma}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A5})$$

$$\mathbf{E}_M^t = \frac{1}{V} \int_V \frac{\partial (\mathbf{E}_\mu^s : \boldsymbol{\varepsilon}_\mu)}{\partial \boldsymbol{\varepsilon}_\mu} : \frac{\partial \boldsymbol{\varepsilon}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A6})$$

$$\begin{aligned} \mathbf{E}_M^t &= \frac{1}{V} \int_V \left[\frac{\partial \mathbf{E}_\mu^s}{\partial \boldsymbol{\varepsilon}_\mu} : \boldsymbol{\varepsilon}_\mu : \frac{\partial \boldsymbol{\varepsilon}_M}{\partial \boldsymbol{\varepsilon}_M} + \mathbf{E}_\mu^s : \frac{\partial \boldsymbol{\varepsilon}_M}{\partial \boldsymbol{\varepsilon}_M} \right] dV \\ &+ \frac{1}{V} \int_V \left[\frac{\partial \mathbf{E}_\mu^s}{\partial \boldsymbol{\varepsilon}_\mu} : \boldsymbol{\varepsilon}_\mu : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} + \mathbf{E}_\mu^s : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} \right] dV \end{aligned} \quad (\text{A7})$$

$$\begin{aligned} \mathbf{E}_M^t &= \mathbf{E}_M^s + \frac{1}{V} \int_V \frac{\partial (\mathbf{E}_\mu^0 - d_\mu \mathbf{E}_\mu^0)}{\partial \boldsymbol{\varepsilon}_\mu} : \boldsymbol{\varepsilon}_\mu dV \\ &+ \frac{1}{V} \int_V \frac{\partial (\mathbf{E}_\mu^0 - d_\mu \mathbf{E}_\mu^0)}{\partial \boldsymbol{\varepsilon}_\mu} : \boldsymbol{\varepsilon}_\mu : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \end{aligned} \quad (\text{A8})$$

$$\begin{aligned} \mathbf{E}_M^t &= \mathbf{E}_M^s + \frac{1}{V} \int_V \frac{\partial (-d_\mu)}{\partial \boldsymbol{\varepsilon}_\mu} \mathbf{E}_\mu^0 : \boldsymbol{\varepsilon}_\mu dV \\ &+ \frac{1}{V} \int_V \frac{\partial (-d_\mu)}{\partial \boldsymbol{\varepsilon}_\mu} \mathbf{E}_\mu^0 : \boldsymbol{\varepsilon}_\mu : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \end{aligned} \quad (\text{A9})$$

and finally

$$\mathbf{E}_M^t = \mathbf{E}_M^s - \frac{1}{V} \int_V \frac{\partial d_\mu}{\partial \boldsymbol{\varepsilon}_\mu} \otimes \frac{\boldsymbol{\sigma}_\mu}{1 - d_\mu} dV - \frac{1}{V} \int_V \frac{\partial d_\mu}{\partial \boldsymbol{\varepsilon}_\mu} \otimes \frac{\boldsymbol{\sigma}_\mu}{1 - d_\mu} : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A10})$$

From Eq. (41), being $\boldsymbol{\varepsilon}_\mu^p = 0$, the dissipation results in this case

$$D_M = \frac{1}{V} \int_V - \frac{\partial \psi_\mu}{\partial d_\mu} \dot{d}_\mu dV \quad (\text{A11})$$

In the particular case of homogeneous damage, with the scalar damage $\alpha_\mu = \boldsymbol{\varepsilon}_\mu : \mathbf{E}_\mu^0 : \boldsymbol{\varepsilon}_\mu$, then Eq. (A10) results

$$\mathbf{E}_M^t = \mathbf{E}_M^s - \frac{1}{V} \int_V \frac{\partial d_\mu}{\partial \alpha_\mu} \frac{\boldsymbol{\sigma}_\mu \otimes \boldsymbol{\sigma}_\mu}{(1 - d_\mu)^2} dV - \frac{1}{V} \int_V \frac{\partial d_\mu}{\partial \alpha_\mu} \frac{\boldsymbol{\sigma}_\mu \otimes \boldsymbol{\sigma}_\mu}{(1 - d_\mu)^2} : \frac{\partial \tilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} dV \quad (\text{A12})$$

A.2 Elastoplastic Material

Under consideration of the flow theory of plasticity and in the framework of the Prandtl–Reuss additive decomposition of the total strain rate tensor, both the fine and coarse scales are as follows:

$$\dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V} \int_V (\dot{\boldsymbol{\varepsilon}}_\mu^e + \dot{\boldsymbol{\varepsilon}}_\mu^p) dV = \dot{\boldsymbol{\varepsilon}}_M^e + \dot{\boldsymbol{\varepsilon}}_M^p \quad (\text{A13})$$

consequently the tangent or continuum material operator of the fine scale takes the form

$$\mathbf{E}_\mu^t = \mathbf{E}_\mu^{ep} = \mathbf{E}_\mu^e - \frac{\mathbf{E}_\mu^e : \mathbf{n}_\mu \otimes \mathbf{m}_\mu : \mathbf{E}_\mu^e}{\mathbf{m}_\mu : \mathbf{E}_\mu^e : \mathbf{n}_\mu + \frac{\partial \Phi_\mu}{\partial Q_\mu^\kappa} \frac{\partial^2 \psi_\mu^p}{\partial \kappa^2} \frac{\partial \Phi_\mu^*}{\partial Q_\mu^\kappa}} \quad (\text{A14})$$

where Φ_μ^* is the plastic potential, $\mathbf{n}_\mu = (\partial\Phi_\mu^*/\partial\boldsymbol{\sigma}_\mu)$ is the flux tensor, Φ_μ is the yield function

$$\mathbf{m}_\mu = \frac{\partial\Phi_\mu}{\partial\boldsymbol{\sigma}_\mu}$$

$\mathbf{Q}_\mu^\kappa = -(\partial\psi_\mu^p/\partial\kappa_\mu)$ is the dissipative stress, $\mathbf{E}_\mu^p = \mathbf{E}_\mu^e - \mathbf{E}_\mu^{ep}$ is the plastic material operator.

Perfect Plasticity. In this case there is no hardening/softening parameter, so the fine scale's material operator results

$$\mathbf{E}_\mu^e = \mathbf{E}_\mu^p = \frac{\mathbf{E}_\mu^e : \mathbf{n}_\mu \otimes \mathbf{E}_\mu^e : \mathbf{m}_\mu}{\mathbf{m}_\mu : \mathbf{E}_\mu^e : \mathbf{n}_\mu} \rightarrow \mathbf{E}_\mu^{ep} = 0 \quad (\text{A15})$$

while the coarse scale's material operator

$$\mathbf{E}_M^{ep} = \frac{1}{V} \int_V \mathbf{E}_\mu^{ep} dV + \frac{1}{V} \int_V \mathbf{E}_\mu^{ep} : \frac{\partial\tilde{\boldsymbol{\varepsilon}}_\mu}{\partial\boldsymbol{\varepsilon}_M} dV = 0 \quad (\text{A16})$$

From Eq. (41), the dissipation results

$$D_M = \frac{1}{V} \int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu dV \quad (\text{A17})$$

Associated Plasticity ($\Phi_\mu = \Phi_\mu^*$) *With Isotropic Hardening/Softening.* The free energy density can be expressed as

$$\psi_\mu = \boldsymbol{\varepsilon}_\mu^e : \mathbf{E}_\mu^e : \boldsymbol{\varepsilon}_\mu^e + \int_\kappa \phi(\kappa_\mu) d\kappa_\mu \quad (\text{A18})$$

being the yield function

$$\Phi_\mu(\boldsymbol{\sigma}_\mu, \kappa_\mu) = \Phi_\mu^0(\boldsymbol{\sigma}_\mu) + \phi_\mu(\kappa_\mu) \quad (\text{A19})$$

and $\mathbf{n}_\mu = \mathbf{m}_\mu = \mathbf{v}_\mu$

$$\mathbf{Q}_\mu^\kappa = -\frac{\partial\psi_\mu^p}{\partial\kappa_\mu} = -\phi_\mu(\kappa_\mu)$$

$$\frac{\partial\Phi_\mu}{\partial\mathbf{Q}_\mu^\kappa} = \frac{\partial\Phi_\mu^*}{\partial\mathbf{Q}_\mu^\kappa} = -1$$

The fine scale's tangent material operator results

$$\mathbf{E}_\mu^{ep} = \mathbf{E}_\mu^e - \frac{\mathbf{E}_\mu^e : \mathbf{v}_\mu \otimes \mathbf{E}_\mu^e : \mathbf{v}_\mu}{\mathbf{v}_\mu : \mathbf{E}_\mu^e : \mathbf{v}_\mu + \frac{\partial\phi_\mu(\kappa_\mu)}{\partial\kappa_\mu}} \quad (\text{A20})$$

For the coarse scale $\mathbf{E}_M^{ep} = \mathbf{E}_M^e - \mathbf{E}_M^p$ with

$$\mathbf{E}_M^e = \frac{1}{V} \int_V \mathbf{E}_\mu^e dV + \frac{1}{V} \int_V \mathbf{E}_\mu^e : \frac{\partial\tilde{\boldsymbol{\varepsilon}}_\mu}{\partial\boldsymbol{\varepsilon}_M} dV \quad (\text{A21})$$

$$\begin{aligned} \mathbf{E}_M^p &= \frac{1}{V} \int_V \frac{\mathbf{E}_\mu^e : \mathbf{v}_\mu \otimes \mathbf{E}_\mu^e : \mathbf{v}_\mu}{\mathbf{v}_\mu : \mathbf{E}_\mu^e : \mathbf{v}_\mu + \frac{\partial\phi_\mu(\kappa_\mu)}{\partial\kappa_\mu}} dV \\ &+ \frac{1}{V} \int_V \frac{\mathbf{E}_\mu^e : \mathbf{v}_\mu \otimes \mathbf{E}_\mu^e : \mathbf{v}_\mu}{\mathbf{v}_\mu : \mathbf{E}_\mu^e : \mathbf{v}_\mu + \frac{\partial\phi_\mu(\kappa_\mu)}{\partial\kappa_\mu}} : \frac{\partial\tilde{\boldsymbol{\varepsilon}}_\mu}{\partial\boldsymbol{\varepsilon}_M} dV \end{aligned} \quad (\text{A22})$$

Using Eq. (41) the dissipation results

$$D_M = \frac{1}{V} \int_V \left(\boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu^p - \phi_\mu(\kappa_\mu) \dot{\kappa}_\mu \right) dV \quad (\text{A23})$$

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