Asociación Argentina
de Mecánica Computacional

Mecánica Computacional Vol XXXV, págs. 1281-1290 (artículo completo)
Martín I. Idiart, Ana E. Scarabino y Mario A. Storti (Eds.)
La Plata, 7-10 Noviembre 2017

# THERMODYNAMIC FRAMEWORK OF MULTISCALE HOMOGENIZATION SCHEMES FOR DISSIPATIVE MATERIALS

**Felipe Lopez Rivarola**[a], **Guillermo J. Etse**[a,b] **and Paula C. Folino**[a]

[a]*Universidad de Buenos Aires. Facultad de Ingeniería. LMNI-INTECIN (UBA-CONICET).*
*felipelr@gmail.com;*

[b]*CONICET - Universidad Nacional de Tucumán, Facultad de Ciencias Exactas y Tecnología.*
*getse@herrera.unt.edu.ar;*

**Keywords:** Multiscale, RVE, Thermodynamic Consistency, Computational homogenisation.

**Abstract.** The prediction of failure processes in composite, heterogeneous materials require multiscale analysis to account for the complex mechanisms and features taking place. Between the different multiscale schemes the more commonly used are those based on homogenization procedures, due to their versatility. In this work a thermodynamically consistent homogenisation based multiscale approach is formulated for modelling thermo-plastic materials. The proposal is valid for arbitrary multiscale procedures, including local or nonlocal methods, and continuum or discontinuum methods in either scale. The necessary and sufficient conditions for fulfilling the thermodynamic consistency are defined. It is demonstrated that the Hill-Mandel variational criterion for homogenization scheme is a necessary, but not a sufficient condition when dissipative material responses are involved at any scale. On this point, the additional condition that needs to be fulfilled 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. Additionally, it is shown that the thermodynamic consistency enforces the homogenization of the nonlocal terms of the micro scale's free energy density; however, this does not necessarily lead to nonlocal effects on the macro scale. Finally, the particular cases of local isothermal elastoplasticity and continuum damage are considered for the purpose of the proposed approach for multiscale homogenizations.

## 1 INTRODUCTION

Despite the advances made in the theoretical frameworks of homogenisation procedures, an unified and systematic procedure for thermodynamically consistent homogenisations is still needed. This formulation must allow straightforward extensions for any kind of dissipative constituents, under any condition. In order to have a consistent framework, multiscale approaches must consider the thermodynamic consistency regarding all different scales involved. Concurrent multiscale procedures take into account the thermodynamic consistency in a direct way, due to the strong coupling between scales. However, weak interface multiscale models demands special considerations for fulfilling the thermodynamic consistency between the involved scales. This topic has, so far, not been explored in a detailed and systematical way. Particularly when dissipative materials are involved.

This work is aimed at formulating this unified and systematic procedure for thermodynamically consistent multiscale homogenisations 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 thermo-elastoplastic 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 homogenisation procedure in this work is valid for any type of homogenisation based multiscale scheme. It is deduced and demonstrated that the Hill-Mandel criterion for homogenisation is only a necessary condition for the multiscale thermodynamic consistency when dissipative material responses are involved at the fine scale.

The work is organized as follows: A thermodynamic background for thermo-plastic materials is described in Section 2, detailing the energetically complementary variables involved in the problem, the derivation of Coleman's equations and the dissipation of each physical process. A semi-concurrent multiscale setting introducing a new concept for the energetic consistency between the scales using a thermodynamically consistent framework, is proposed in Section 3. The dissipation consistency between the scales is studied in Section 4. The proposed theoretical framework is particularized in Section 5. The necessary conditions for satisfying the thermodynamic consistency are discussed in Section 6. Finally, some conclusions are compiled in Section 7.

## 2 THERMODYNAMICS OF DISSIPATIVE MEDIA

Thermodynamically consistent formulations of constitutive equations for dissipative materials departure from the fundamental laws of thermodynamics. This leads to the well-known Clausius-Duhem inequality which establishes the positiveness of the dissipations. In this section, the thermodynamic framework of the constitutive equations under non-isothermal conditions are summarized. The particular case of small kinematics (strains and displacements) and neglectable inertial forces is considered.

### 2.1 First law of thermodynamics

The first law of thermodynamics for general thermomechanical systems states

$$\dot{E} + \dot{K} = P + Q \tag{1}$$

with: $E$, $K$, $P$, and $Q$, the internal energy, kinematic energy, mechanical source, and thermal source respectively.

Considering the conservation of mass, and not taking into account inertia forces, it can be re-written as

$$\rho \dot{e} = \boldsymbol{\sigma} : \boldsymbol{\nabla}^s \dot{\boldsymbol{u}} + \rho r - \boldsymbol{\nabla} \cdot \boldsymbol{h} \tag{2}$$

being $\rho$ the density of the solid, $e$ the internal energy density, $\boldsymbol{\sigma}$ the Cauchy stress tensor, $u$ the displacement field, $r$ the energy source, $\boldsymbol{h}$ the heat flux vector, and $\boldsymbol{\varepsilon}$ the strain tensor.

### 2.2 Second law of thermodynamics

The entropy inequality of a thermodynamic system can be expressed as

$$\dot{S} - Q_\theta \geq 0 \qquad \text{or} \qquad \rho \dot{s} \theta - \rho r + \boldsymbol{\nabla} \cdot \boldsymbol{h} - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla} \theta}{\theta} \geq 0 \tag{3}$$

with $S$ and $Q_\theta$ the entropy and entropy flux respectively; and $s$ the entropy density, $\theta$ the absolute temperature, and $s^{fl}$ the entropy density of the fluid.

### 2.3 Clausius-Duhem inequality

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

$$-\rho \dot{\psi} - \rho s \dot{\theta} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla} \theta}{\theta} \geq 0 \tag{4}$$

### 2.4 Coleman's equations

Assuming that arbitrary thermodynamic states of non-isothermal processes are completely determined by the elastic strain $\boldsymbol{\varepsilon}^e$, the temperature, and the internal variable $\kappa$, the Helmholtz's free energy density can then be expressed as $\psi = \psi(\boldsymbol{\varepsilon}^e, \theta, \kappa)$. In this work it is assumed that the free energy of the whole system can be additively decomposed into an elastic free energy, and a plastic free energy.

$$\psi = \psi^e + \psi^p \tag{5}$$

Moreover, if the general framework of the flow theory of plasticity is assumed, the rates of the total strain tensor and of the total entropy can be additively decomposed into their elastic and plastic components.

Coleman's equations can be deduced stating that Eq. (4) must be null for elastic cycles

$$s = -\frac{\partial \psi}{\partial \theta} \quad , \quad \boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} \tag{6}$$

### 2.5 Dissipation

By making use of Coleman's equation the dissipation can be expressed as

$$D = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla} \theta}{\theta} - \rho \frac{\partial \psi}{\partial \kappa} \dot{\kappa} \geq 0 \tag{7}$$

and it can be decoupled into

$$\begin{aligned} &\text{Intrinsic Dissipation: } D^s = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \rho \frac{\partial \psi}{\partial \kappa} \dot{\kappa} \geq 0 \\ &\text{Heat transport Dissipation: } D^{th} = -\frac{\boldsymbol{h} \cdot \boldsymbol{\nabla} \theta}{\theta} \geq 0 \end{aligned} \tag{8}$$

Using Eqs. (7) and (4), Helmholtz's free energy density can be re-written as

$$\rho\dot{\psi} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^e + \rho\frac{\partial\psi}{\partial\kappa}\dot{\kappa} - \rho s\dot{\theta} \tag{9}$$

Additionally, the eventual dissipation in discrete cracks must be taken into account. Being $\psi^c = \psi^c(\boldsymbol{u}^e, \kappa^f)$ the cohesive free energy density, from Coleman and Noll's method, the traction vector at the interface must be

$$\boldsymbol{t} = \frac{\partial\psi^c}{\partial\boldsymbol{u}^e} \tag{10}$$

And, analogously, the energy dissipated due to crack opening is

$$D^f = \boldsymbol{t}\cdot\dot{\boldsymbol{u}}^f - \frac{\partial\psi^c}{\partial\kappa^f}\dot{\kappa}^f \geq 0 \tag{11}$$

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

## 2.6 Extension to non-local thermodynamics

As can be seen in Nguyen and Andrieux (2005), due to the introduction of the gradient terms of independent variables as state variables there is need of an extended thermodynamic framework. If the free energy does not only depend on $\theta$ but also on $\boldsymbol{\nabla}\theta$ then

$$\psi = e - s\theta - \boldsymbol{s'}\cdot\boldsymbol{\nabla}\theta \tag{12}$$

Where the entropy definition remains unchanged $\left(s = -\dfrac{\partial\psi}{\partial\theta}\right)$. The vector $s'$, called the entropy vector, can be deduced from analogous Coleman's equations and is defined as

$$\boldsymbol{s'} = -\frac{\partial\psi}{\partial\boldsymbol{\nabla}\theta} \tag{13}$$

Concerning the involved dissipations, these are not modified by this enhancement.

As explained in Blanco and Giusti (2014) this modification is needed because if the macroscopic temperature gradient is a variable in the microscopic temperature field problem, the microscopic stress field and the macroscopic stress field also depends on the macroscopic temperature gradient. Hence, the macroscopic stress itself depends on the macroscopic temperature gradient, which under a classic thermodynamic framework cannot occur.

# 3 THERMODYNAMICALLY CONSISTENT MULTISCALE HOMOGENIZATION METHOD

In this section, the work done in Lopez Rivarola et al. (2017) will be generalized and restructured. The proposed framework in based on the fundamental idea of stating the consistency between the Helmholtz's free energy densities of the involved scales, which implies not only the elastic energy density, but also the dissipations associated to all inelastic mechanisms. Additionally, an assumption regarding the primal variables insertion from the macroscale to the microscale is stated. The dual variables, as well as the material operatros, are then deduced as a thermodynamic consequence.

Using sub-index $(\bullet)_M$ for the properties of the coarse scale, and sub-index $(\bullet)_\mu$ for the fine scale. The multiscale procedure will be:

- 1) Propose an energy consistency between scales. A Helmholtz free energy density consistency is chosen for the microscale, and the macroscopic relations will be deduced from the framework.

- 2) Propose a homogenization procedure for the primal variables. In this work the primal variables are the displacement, and the temperature. The microscopic variables can then be additively decomposed in the classical sense into three parts: a constant value (equal to the macroscale value), a linear function (related to the macroscale value's gradient), and a fluctuation. The gradient operator is not the same for all scales, as it's calculated using a different coordinate system ($\boldsymbol{\nabla}_M \neq \boldsymbol{\nabla}_\mu$). In order to simplify the nomenclature, $\boldsymbol{\nabla}_M(\bullet)_M = [\boldsymbol{\nabla}(\bullet)]_M$ and $\boldsymbol{\nabla}_\mu(\bullet)_\mu = [\boldsymbol{\nabla}(\bullet)]_\mu$.

- 3) Deduce the dual variables homogenization from the thermodynamic relations. Given the energetic consistency between the scales and Coleman's equations, the homogenization of the dual variables can be deduced. In this work these variables are: stress, entropy, and entropy vector.

- 4) Deduce the macroscopic operators from the thermodynamic relations. Using the differential equations that relates the free energy with the utilized variables the homogenization of the operators can be deduced.

### 3.1 Axiom 1 - Energy consistency

The energetic consistency is enforced by means of the homogenization of microscopic Helmholtz free energy density. In multiphysics and multiscale problems the formulation of a virtual power principle is not a trivial fact. This proposal aims to formulate a rational procedure for general multiscale homogenizations.

The consistency is then postulated through the volume average

$$\psi_M = \frac{1}{V}\int_V \psi_\mu \, dV \tag{14}$$

In this work the following expression for the elastic Helmholtz free energy density is adopted

$$\psi_\mu^e = \frac{1}{2}\,\boldsymbol{\varepsilon}_\mu^e : \boldsymbol{E}_\mu^e : \boldsymbol{\varepsilon}_\mu^e \; - \; \frac{1}{2}\frac{\mathscr{C}_\mu}{T_0}\theta_\mu^2 \; - \; \theta_\mu \boldsymbol{A}_\mu : \boldsymbol{\varepsilon}_\mu^e \tag{15}$$

being: $\mathscr{C}$ the volumetric heat capacity; $T_0$ the reference temperature; $\boldsymbol{A} = \boldsymbol{E} : \boldsymbol{I}\alpha$, with $\alpha$ the thermal dilation coefficient, $\boldsymbol{E}^e$ the elastic constitutive tensor, and $\boldsymbol{I}$ the second order identity tensor.

With respect to the plastic behavior, the following expression of Helmholtz free energy density is adopted

$$\psi_\mu^p = \frac{1}{2}\kappa_\mu H_\mu \kappa_\mu \tag{16}$$

being $H$ the plastic hardening-softening modulus. Considering a decoupled behavior of the elastic and plastic energy, $\psi_\mu^p$ is independent of the elastic variables $\boldsymbol{\varepsilon}_\mu^e$, and $\theta_\mu$.

So, from Coleman's equations, i.e. Eq. (6)

$$\boldsymbol{\sigma}_\mu = \frac{\partial \psi_\mu}{\partial \boldsymbol{\varepsilon}_\mu^e} = \boldsymbol{E}_\mu^e : \boldsymbol{\varepsilon}_\mu^e \; - \; \theta_\mu \boldsymbol{A}_\mu \tag{17}$$

$$s_\mu = -\frac{\partial \psi_\mu}{\partial \theta_\mu} = \; \boldsymbol{A}_\mu : \boldsymbol{\varepsilon}_\mu^e \; + \; \frac{\mathscr{C}_\mu}{T_0}\theta_\mu \tag{18}$$

$$\tag{19}$$

### 3.2 Axiom 2 - Physical primal variables

*Displacement and strain homogenization*

Without loss of generality the microscale's displacement rate $\dot{\boldsymbol{u}}$ can be decomposed into an average displacement rate (which is equal to the macrocale's displacement rate), a linear function of $\boldsymbol{x}$ (associated to the macroscale's displacement rate gradient) and a displacement fluctuation rate

$$\dot{\boldsymbol{u}}_\mu(\boldsymbol{x}) = \dot{\boldsymbol{u}}_M \; + \; [\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_M \cdot (\boldsymbol{x} - \boldsymbol{x_0}) \; + \; \widetilde{\dot{\boldsymbol{u}}}_\mu \tag{20}$$

being $\boldsymbol{x_0} = \dfrac{1}{V}\int_V \boldsymbol{x}\, dV$. It is assumed that

$$\dot{\boldsymbol{u}}_M = \frac{1}{V}\int_V \dot{\boldsymbol{u}}_\mu(\boldsymbol{x})\, dV \quad \text{and, hence} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\boldsymbol{u}}}_\mu\, dV \tag{21}$$

As a consequence

$$[\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_\mu = [\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_M + [\boldsymbol{\nabla}\widetilde{\dot{\boldsymbol{u}}}]_\mu \quad \text{or} \quad \dot{\boldsymbol{\varepsilon}}_\mu = \dot{\boldsymbol{\varepsilon}}_M + \widetilde{\dot{\boldsymbol{\varepsilon}}}_\mu \tag{22}$$

so

$$\dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}_\mu\, dV \quad \text{and} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\boldsymbol{\varepsilon}}}_\mu\, dV \tag{23}$$

It is important to remark that this Axiom is postulated for total strains, and is not valid for elastic and plastic strains individually as can be seen in Maugin (1992). Under general models

$$\dot{\boldsymbol{\varepsilon}}^e_M \neq \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}^e_\mu\, dV \quad \text{and} \quad \dot{\boldsymbol{\varepsilon}}^p_M \neq \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}^p_\mu\, dV \tag{24}$$

*Temperature and temperature gradient homogenization*

Proceeding analogously

$$\dot{\theta}_\mu(\boldsymbol{x}) = \dot{\theta}_M \; + \; \left[\boldsymbol{\nabla}\dot{\theta}\right]_M \cdot (\boldsymbol{x} - \boldsymbol{x_0}) \; + \; \widetilde{\dot{\theta}}_\mu \tag{25}$$

Assuming

$$\dot{\theta}_M = \frac{1}{V}\int_V \dot{\theta}_\mu(\boldsymbol{x})\, dV \quad \text{and, hence} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\theta}}_\mu\, dV \tag{26}$$

Then, as a consequence

$$\left[\boldsymbol{\nabla}\dot{\theta}\right]_\mu = \left[\boldsymbol{\nabla}\dot{\theta}\right]_M + \left[\boldsymbol{\nabla}\widetilde{\dot{\theta}}\right]_\mu \tag{27}$$

and

$$\left[\boldsymbol{\nabla}\dot{\theta}\right]_M = \frac{1}{V}\int_V \left[\boldsymbol{\nabla}\dot{\theta}\right]_\mu dV \quad \text{and} \quad 0 = \frac{1}{V}\int_V \left[\boldsymbol{\nabla}\widetilde{\dot{\theta}}\right]_\mu dV \tag{28}$$

### 3.3 Corollary 1 - Dual Variables

*Macroscopic Stress Tensor*: From Eqs. (6) and (14)

$$\boldsymbol{\sigma}_M = \frac{1}{V}\int_V \frac{\partial \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M} dV = \frac{1}{V}\int_V \left(\boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}^e_\mu}{\partial \boldsymbol{\varepsilon}^e_M} \; - \; s_\mu \frac{\partial \theta_\mu}{\partial \boldsymbol{\varepsilon}^e_M} \; + \; H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \boldsymbol{\varepsilon}^e_M}\right) dV \tag{29}$$

*Macroscopic Entropy*: From Eqs. (6) and (14)

$$s_M = \frac{1}{V}\int_V -\frac{\partial \psi_\mu}{\partial \theta_M} dV = -\frac{1}{V}\int_V \left( \boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}^e_\mu}{\partial \theta_M} - s_\mu \frac{\partial \theta_\mu}{\partial \theta_M} + H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \theta_M} \right) dV \tag{30}$$

*Macroscopic Entropy vector*: From Eqs. (13) and (14)

$$\boldsymbol{s}' = \frac{1}{V}\int_V -\frac{\partial \psi_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} dV = -\frac{1}{V}\int_V \left( \boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}^e_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} - s_\mu \frac{\partial \theta_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} + H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} \right) dV \tag{31}$$

It can be seen that the macroscale stress, entropy and entropy vector are not necessarily a volume average of the microscale values.

### 3.4 Corollary 2 - Macroscopic operators

Proposing a macroscopic free energy function analogous to Eq. (15) and the free energy consistency in Eq. (14) homogenization expressions for the operators are deduced.

*Macroscopic tangent constitutive tensor*

$$\boldsymbol{E}_M = \frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}_M \partial \boldsymbol{\varepsilon}^e_M} = \frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\varepsilon}_M} = \frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}_M \partial \boldsymbol{\varepsilon}^e_M} dV \tag{32}$$

*Macroscopic tensor of thermomechanical expansion*

$$\boldsymbol{A}_M = -\frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}^e_M \partial \theta_M} = \frac{\partial s_M}{\partial \boldsymbol{\varepsilon}^e_M} = -\frac{\partial \boldsymbol{\sigma}_M}{\partial \theta_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M \partial \theta_M} dV \tag{33}$$

*Macroscopic volume heat capacity*

$$\frac{\mathscr{C}_M}{T_0} = -\frac{\partial^2 \psi_M}{\partial \theta_M \partial \theta_M} = \frac{\partial s_M}{\partial \theta_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \theta_M \partial \theta_M} dV \tag{34}$$

As the behavior of microscopic domain depends on the macroscopic temperature gradient, the macroscopic free energy needs to be enhanced as seen in Section 2.6. This leads to the existence of operators that do not present a counterpart in the microscale, which are

$$\boldsymbol{A}'_M = -\frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}^e_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \boldsymbol{\varepsilon}^e_M} = -\frac{\partial \boldsymbol{\sigma}_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \tag{35}$$

$$\mathscr{C}'_M = -\frac{\partial^2 \psi_M}{\partial \theta_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \theta_M} = \frac{\partial s_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \theta_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \tag{36}$$

$$\mathscr{G}'_M = -\frac{\partial^2 \psi_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \tag{37}$$

## 4 ENERGY BALANCE - DISSIPATION CONSISTENCY

Besides the relations previously stated an energy balance condition is necessary. Classic homogenization theory uses the Hill-Mandel principle to this end. In this proposal, in order to have a fully consistent homogenization procedure, the energy balance is obtained from the dissipation and not from arbitrary potentials. The following expressions of the macroscopic dissipation terms can be obtained for the corresponding homogenization processes

$$D^s_M = \frac{1}{V}\int D^s_\mu \, dV \quad , \quad D^{th}_M = \frac{1}{V}\int D^{th}_\mu \, dV \tag{38}$$

Hence, the energy balance formula for the heat flow is

$$\frac{h_M \, [\boldsymbol{\nabla}\theta]_M}{\theta_M} = \frac{1}{V}\int \frac{\boldsymbol{h_\mu} \cdot [\boldsymbol{\nabla}\theta]_\mu}{\theta_\mu} \, dV \tag{39}$$

In regards to the intrinsic dissipation a general homogenization equation of inelastic variables is not trivial. As it depends on the inelastic variables of every point of the RVE, the homogenisation depends on as many variables as the discretization of the RVE domain. A single dissipative variable (damage, plastic, or other) on the microscale can originate more than one macroscopic dissipative variable.

Thus, in the proposed approach the energy balance is naturally derived from the considered thermodynamic framework, without the need to assume or, moreover, impose arbitrary potentials.

## 5 REACTIVE FORCES CONSTRAINS

It is reasonable to assume that the microscopic plastic variable is independent of the macroscopic elastic strain. Additionally it will be assumed that the microscopic temperature does no depend on the macroscopic elastic strain. Under these conditions only the first tem in the right side of Eq. (29) survives, and we can rewrite the equation as

$$\boldsymbol{\sigma}_M = \frac{1}{V}\int_V \frac{\partial \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M} dV = \frac{1}{V}\int_V \left( \boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}^e_M}{\partial \boldsymbol{\varepsilon}^e_M} + \boldsymbol{\sigma}_\mu : \frac{\partial \widetilde{\boldsymbol{\varepsilon}^e_\mu}}{\partial \boldsymbol{\varepsilon}^e_M} \right) dV \tag{40}$$

Being $\dot{\widetilde{\boldsymbol{\varepsilon}}}_\mu = \dot{\widetilde{\nabla^s \boldsymbol{u}_\mu}}$, and using the divergence theorem then

$$\int_V \dot{\widetilde{\boldsymbol{\varepsilon}_\mu(\widetilde{\boldsymbol{u}}_\mu)}} : \boldsymbol{\sigma}_\mu \, dV = \int_S \dot{\widetilde{\boldsymbol{u}}}_\mu \cdot \boldsymbol{t}^e \, dS - \int_V \dot{\widetilde{\boldsymbol{u}}}_\mu \cdot \boldsymbol{b} \, dV \tag{41}$$

As it can be seen in de Souza Neto and Feijóo (2006), for Eq. (41) to be equal to zero each integral vanish individually

$$0 = \int_S \dot{\widetilde{\boldsymbol{u}}}_\mu \cdot \boldsymbol{t}^e \, dS \quad \text{and} \quad 0 = \int_V \dot{\widetilde{\boldsymbol{u}}}_\mu \cdot \boldsymbol{b} \, dV \tag{42}$$

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

In an analogous form

$$\int_V \boldsymbol{\sigma}_\mu : \frac{\partial \widetilde{\boldsymbol{\varepsilon}^e_\mu}}{\partial \boldsymbol{\varepsilon}^e_M} \, dV = \int_S \frac{\partial \widetilde{\boldsymbol{u}^e_\mu}}{\partial \boldsymbol{\varepsilon}^e_M} \cdot \boldsymbol{t}^e \, dS - \int \frac{\partial \widetilde{\boldsymbol{u}^e_\mu}}{\partial \boldsymbol{\varepsilon}^e_M} \cdot b \, dV \tag{43}$$

As $\widetilde{\boldsymbol{u}}_\mu$ is equal to zero on all boundaries where $\boldsymbol{t}_e \neq 0$ for any value of $\boldsymbol{\varepsilon}_M^e$, then the first integral of the last equation is also equal to zero under reactive surface forces. For the body force term, the integral vanishes only under the absence of body forces.

If Eqs. (43) and (41) are null then the homogenisation Eqs. (40) can be re-written as

$$\boldsymbol{\sigma}_M = \frac{1}{V}\int_V \boldsymbol{\sigma}_\mu \, dV \tag{44}$$

The same procedure can be used to deduce that under these conditions

$$\boldsymbol{E}_M^e = \frac{1}{V}\int_V \boldsymbol{E}_\mu^e \, dV + \frac{1}{V}\int_V \boldsymbol{E}_\mu^e : \frac{\partial \widetilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M^e} \, dV \tag{45}$$

$$\boldsymbol{E}_M^t = \frac{1}{V}\int_V \boldsymbol{E}_\mu^t \, dV + \frac{1}{V}\int_V \boldsymbol{E}_\mu^t : \frac{\partial \widetilde{\boldsymbol{\varepsilon}}_\mu}{\partial \boldsymbol{\varepsilon}_M} \, dV \tag{46}$$

$$D_M = \frac{1}{V}\int_V D_\mu \, dV \tag{47}$$

The stress homogenisation equation, which has been derived from a thermodynamic framework, is the same used in the classical homogenisation. Hence, this equation satisfies the thermodynamic consistency only under purely reactive forces.

In regard to the dissipation, Eq. (47), can also be found used in the literature. However, here this equation has been deduced as a requirement for fulfilling thermodynamic consistency.

## 6 CONDITIONS FOR THE THERMODINAMIC CONSISTENCY OF MULTISCALE HOMOGENISATION SCHEMES

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

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

$$\psi_M = \frac{1}{V}\int_V \psi_\mu \, dV \tag{48}$$

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

$$D_M = \frac{1}{V}\int_V D_\mu \, dV \tag{49}$$

$$\boldsymbol{\sigma}_M : \dot{\boldsymbol{\varepsilon}_M} = \frac{1}{V}\int_V \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}_\mu} \, dV \tag{50}$$

Under reactive forces the stress homogenisation Eq. (44) automatically ensure the power balance of Eq. (50). This equation, together with the dissipation homogenisation in Eq. (49) ensures the free energy consistency. These are the necessary and sufficient conditions to ensure the consistency of the free energy between scales.

Hence the Hill-Mandel principle alone is not enough to procure a thermodynamically consistent homogenisation between scales. As most of the utilized multiscale theories abide this principle, an appropriate and simple procedure to turn these multiscale procedures into thermodynamically consistent is to include the additional constrain of Eq. (49) representing the dissipation homogenisation.

## 7 CONCLUSIONS

The thermodynamic consistency of homogenisation base multiscale schemes was analysed and defined in the framework of dissipative constitutive theories. It was demonstrated that the Hill-Mandel principle is only a sufficient condition for the thermodynamic consistency of multiscale homogenisation procedures when elastic or perfectly plastic materials theories are considered. However, when any dissipative material is considered, an additional condition to the Hill-Mandel Principle is required. This condition is the homogenisation of the dissipation which establishes that the macroscale's dissipation is the RVE volume average of that of the fine scale. The conditions for thermodynamically consistent multiscale homogenisations were developed for general inelastic constitutive theories. All together, the results and demonstrations in this work clearly establish the substantial differences between classical and thermodynamically consistent homogenisation schemes of multiscales material theories.

## REFERENCES

Blanco P. and Giusti S. Thermomechanical multiscale constitutive modeling: accounting for microstructural thermal effects. *J Elast*, 115:27–46, 2014.

de Souza Neto E.A. and Feijóo R.A. Variational foundations of multi-scale constitutive models of solid: Small and large strain kinematical formulation. *LNCC (National Laboratory for Scientific Computing) R and D Report*, 16, 2006.

Lopez Rivarola F., Etse J., and Folino P. On thermodynamic consistency of homogenization-based multiscale theories. *ASME. J. Eng. Mater. Technol.*, 139(3):031011–031011–9, 2017. doi:10.1115/1.4036243.

Maugin G.A. *The thermomechanics of plasticity and fracture*. Press Syndicate of the University of Cambridge, The Pitt Building, Trumpington Street, Cambridge CB2 1RP, 1992.

Nguyen Q.S. and Andrieux S. The non-local generalized standard approach: a consistent gradient theory. *Comptes Rendus Mécanique*, 333(2):139 – 145, 2005. ISSN 1631-0721. doi: http://dx.doi.org/10.1016/j.crme.2004.09.010.