Variational Formulation for Multi-Scale Constitutive Models in Steady-State Heat Conduction Problem on Rigid Solids

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Abstract. *Based on the volume averaging of the microscopic temperature and heat flux fields over a local representative volume element (RVE), in this work we present a general variational formulation for multi-scale constitutive models in steady-state heat conduction problem on rigid solids. In order to describe the RVE material behaviour, we use local continuum constitutive theories. This formulation provides an axiomatic framework within which each class of models is completely defined by a specific choice of kinematical constraints over the RVE. As a consequence of the Hill-Mandel Principle of Macro-Homogeneity, the system of external heat sources (RVE boundary flux and heat source fields) can be viewed as a reaction to such constraints and is automatically characterized once the set of kinematically admissible temperature associated to the RVE is specified. Finally, we derive a class of RVE constitutive models considering different physical choice for the kinematical constraints.*

Keywords: *multi-scale constitutive models, heat conduction problem, kinematical variational formulation.*

1. Introduction

The constitutive modelling of solids by means on so-called multi-scale theories has become the subject of intensive research in applied and computational mechanics. Probably the growing interest in the modelling of solids by multi-scale techniques has two important cases, the first is the current need for more accurate constitutive models, and the second is related to the limit of the descriptive/predictive capability of conventional phenomenological continuum models. One important example of these facts is the mathematical modelling of biological tissue. The typical microstructure of biological material can be extremely elaborate, resulting in a macroscopic constitutive response of difficult representation by means of conventional phenomenological constitutive models. Often, the modelling of such phenomena by purely macroscopic theories results in important discrepancies between the predicted and observed constitutive response.

In the last years, many contributions have been made to the modelling of constitutive response by means of multi-scale techniques (see, for instance, Nemat-Nasser, 1999; Michel *et al.*, 1999; Hori & Nemat-Nasser, 1999; Miehe & Koch, 2002; Matsui *et al.*, 2004; Yang & Becker, 2004; Bilger *et al.*, 2005; Owen & Oñate, 2005; and references therein). However, this multi-scale models are often presented in a rather *ad-hoc* manner, making it difficult to distinguish between the basic assumptions and their consequences. Recently, was proposed a methodology to derive a family of multi-scale constitutive models based on variational arguments (de Souza Neto & Feijóo, 2006). The formulation presented there, and applied to small and large strain problem, provides a clearly structured axiomatic framework to derive any class of constitutive multi-scale models.

Based on the theory proposed in de Souza Neto & Feijóo,2006; the objective of the present work is to develop a general kinematic variational framework for infinitesimal multi-scale models in steady-state heat conduction problem on rigid solids. The most important multi-scale techniques used in this work are: the Hill-Mandel principle of Macro-Homogeneity and homogenization by volume averaging of vector fields (temperature gradient and heat flux).

This work is organized in the following way. In section 2 is presented the general kinematic variational framework for infinitesimal multi-scale models, based on the volume averaging over the domain. Using the variational framework given in the previous sections, four well-known classes of multi-scale models are developed in section 3. Ending this article, in section 4 some final remarks are presented.

2. Infinitesimal multi-scale models

In this section is presented the variational formulation of a family of infinitesimal continuum constitutive models. The main assumption is that the heat flux and the gradient of temperature at any material point $\boldsymbol{x}$ of the continuum Ω are the volume average of the heat flux and the gradient of temperature over a local microscopic cell (see Figure 1).

In the next sections a microscopic cell, denoted by Ω_μ (with boundary $\partial\Omega_\mu$), is referred to as the *Representative*

Volume Element (RVE). Thus, to assure that this type of multi-scale models are well described is necessary that the characteristic length of the RVE, l_μ, is much smaller than the characteristic length, l, of the macro-continuum. The RVE domain consist in two parts, one called matrix and denoted with Ω_μ^e and the another denominated inclusion and denoted Ω_μ^i, as can see in Figure 1. In addition,

$$\Omega_\mu = \Omega_\mu^e \cup \Omega_\mu^i; \quad \partial\Omega_\mu^e = \partial\Omega_\mu \cup \partial\Omega_\mu^i.$$

For simplicity, we shall consider only RVEs whose inclusion does not intersect the RVE boundary, i.e., it is assumed that

$$\partial\Omega_\mu \cap \bar{\Omega}_\mu^i = \emptyset,$$

where $\bar{\Omega}_\mu^i$ denotes the closure of the set Ω_μ^i.

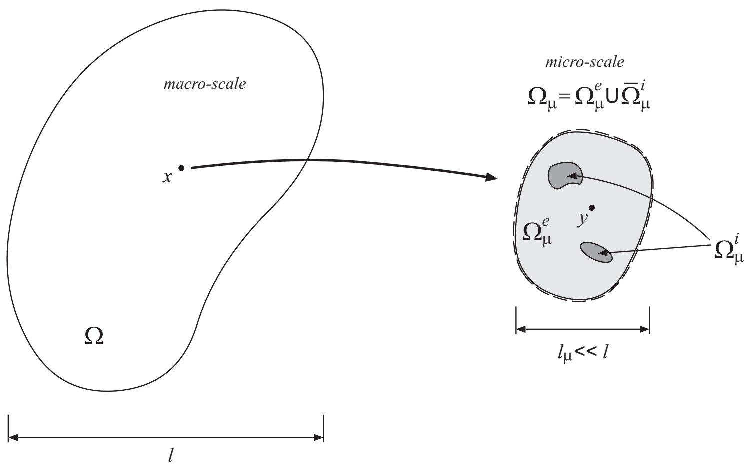

Figure 1. Macro-continuum with a local micro-structure.

2.1 The homogenized temperature gradient and the RVE kinematics

According to mentioned at the beginning of this section, we start the variational formulation of the multi-scale constitutive theories assuming that the gradient of temperature in a point $\boldsymbol{x}$ of the macro-continuum, $\nabla u\left(\boldsymbol{x}\right)$, is the volume average of the microscopic temperature gradient, ∇u_μ, over the RVE associated with the point $\boldsymbol{x}$. Then,

$$\nabla u\left(\boldsymbol{x}\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla u_\mu\left(\boldsymbol{y}\right) dV, \tag{1}$$

where V_μ is a total volume of the RVE, i.e., $V_\mu = V_\mu^e + V_\mu^i$, and $u_\mu\left(\boldsymbol{y}\right)$ is a temperature field in the micro-scale corresponding to each point $\boldsymbol{y}$ of the RVE. The procedure given by eq. (1), called *homogenization*, maps a field over the RVE ($\nabla u_\mu\left(\boldsymbol{y}\right)$ in this case) into a corresponding quantity defined in the macro-continuum ($\nabla u\left(\boldsymbol{x}\right)$ in this case).

2.1.1 Minimum RVE kinematical constraints

Due to the used homogenization process defined by eq. (1), all kinematically admissible field for this problem must satisfy eq. (1). Formally, a necessary condition for a temperature field $u_\mu\left(\boldsymbol{y}\right)$ to be kinematically admissible is that

$$u_\mu \in \mathcal{K}_\mu,$$

where $\mathcal{K}_\mu$ is the minimally constrained set of kinematically admissible microscopic temperatures, that is

$$\mathcal{K}_\mu \equiv \left\{ v \in \mathcal{W} : \int_{\Omega_\mu} \nabla v dV = V_\mu \nabla u \right\}, \tag{2}$$

where $\mathcal{W}$ is an adequate Sobolev's space for this problem.

Alternatively, the above expression can be written in terms of an integral over the RVE boundary in the following manner,

$$\mathcal{K}_\mu \equiv \left\{ v \in \mathcal{W} : \int_{\partial\Omega_\mu} v\mathbf{n} dA = V_\mu \nabla u \right\}, \tag{3}$$

where the outward unit vector $\mathbf{n}$ is normal to the boundary $\partial\Omega_\mu$. In order to obtain the previous definition eq. (3), is only necessary to use the tensor relation $\text{div}(\varphi\mathbf{S}) = \varphi\text{div}(\mathbf{S}) + \mathbf{S}\nabla\varphi$ (taking into account that $\mathbf{S} = \mathbf{I}$ and $\varphi = v$) and the divergence theorem in the definition of the space $\mathcal{K}_\mu$ given by eq. (2).

2.1.2 Additive split of the microscopic temperature

Without loss of generality, any microscopic temperature field u_μ, can be split into a sum of the following way

$$u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} + \tilde{u}_\mu(\boldsymbol{y}), \tag{4}$$

where the term $\nabla u(\boldsymbol{x}) \cdot \boldsymbol{y}$ varies linearly in $\boldsymbol{y}$, and $\tilde{u}_\mu(\boldsymbol{y})$ is a fluctuation of the temperature field. Based on the decomposition shown in eq. (4), the microscopic temperature gradient can be written as,

$$\nabla u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) + \nabla\tilde{u}_\mu(\boldsymbol{y}), \tag{5}$$

where we have a homogenous part (constant in $\boldsymbol{y}$) that coincides with the macroscopic temperature gradient at point $\boldsymbol{x}$, and a gradient of microscopic fluctuation temperature, that generally varies in $\boldsymbol{y}$.

Introducing the previous decomposition (eq. 5) in the definition of space $\mathcal{K}_\mu$, we observe that

$$V_\mu \nabla u = \int_{\Omega_\mu} \nabla u_\mu dV = \int_{\Omega_\mu} (\nabla u + \nabla\tilde{u}_\mu)\, dV = V_\mu\nabla u + \int_{\Omega_\mu} \nabla\tilde{u}_\mu dV \quad \Rightarrow \quad \int_{\Omega_\mu} \nabla\tilde{u}_\mu dV = 0,$$

then, the microscopic fluctuation temperature $\tilde{u}_\mu$, satisfies

$$\tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu,$$

where the minimally constrained vector space of kinematically admissible temperature fluctuations of the RVE is defined as

$$\tilde{\mathcal{K}}_\mu \equiv \left\{ v \in \mathcal{W} : \int_{\Omega_\mu} \nabla v dV = 0 \right\}; \tag{6}$$

or in terms of a boundary integral over $\partial\Omega_\mu$, as

$$\tilde{\mathcal{K}}_\mu \equiv \left\{ v \in \mathcal{W} : \int_{\partial\Omega_\mu} v\mathbf{n} dA = 0 \right\}. \tag{7}$$

Thus, according to the definition of vector space $\tilde{\mathcal{K}}_\mu$, the minimally constrained set of kinematically admissible temperature in the micro-scale, can alternatively be written as

$$\mathcal{K}_\mu \equiv \left\{ v_\mu \in \mathcal{W} : v_\mu = \nabla u \cdot \boldsymbol{y} + \tilde{v}_\mu, \tilde{v}_\mu \in \tilde{\mathcal{K}}_\mu \right\}. \tag{8}$$

Then, for a given macroscopic gradient of temperature, ∇u, the set $\mathcal{K}_\mu$ is a translation of the space $\tilde{\mathcal{K}}_\mu$ (Oden, 1979). The set of kinematically admissible temperature over the RVE, $\mathcal{K}_\mu$, and the associated space of virtual kinematically admissible temperature of the RVE, denoted by $\mathcal{V}_\mu$, have a fundamental role in the definition of the equilibrium of the RVE. In particular, the space of virtual admissible variation $\mathcal{V}_\mu$ can be defined as

$$\mathcal{V}_\mu \equiv \left\{ \eta \in \tilde{\mathcal{K}}_\mu : \eta = v_1 - v_2; v_1, v_2 \in \mathcal{K}_\mu \right\}. \tag{9}$$

From the previous definition and eq. (8), it is straightforward to see that in general $\mathcal{V}_\mu \subset \tilde{\mathcal{K}}_\mu$.

Now, placing eq. 4 in terms of virtual temperatures it is possible to write the additive form of microscopic virtual temperature in the following way,

$$\delta u_\mu = \nabla(\delta u) \cdot \boldsymbol{y} + \delta\tilde{u}_\mu, \tag{10}$$

in the same manner, it is possible to establish that any fluctuation of kinematically admissible virtual temperature, $\delta\tilde{u}_\mu$, satisfies

$$\delta\tilde{u}_\mu \in \mathcal{V}_\mu.$$

2.2 Equilibrium of the RVE

Restricted to the purely local constitutive theory, the axioms of *Constitutive Determinism and Local Action* (Truesdell, 1999) establish that, in general form, a heat flux $\boldsymbol{q}$ at any point $\boldsymbol{x}$ of he continuum is uniquely determined by the gradient of temperature at this point $\boldsymbol{x}$. That is, there exists a constitutive functional $\mathcal{F}$ such that,

$$\boldsymbol{q}(\boldsymbol{x}) = \mathcal{F}(\nabla u(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Omega. \tag{11}$$

In the same way that the macroscopic case, the microscopic heat flux in the RVE, $\boldsymbol{q}_\mu$, satisfies the following relation

$$\boldsymbol{q}_\mu(\boldsymbol{y}) = \mathcal{F}_y(\nabla u_\mu(\boldsymbol{y})), \quad \forall \boldsymbol{y} \in \Omega_\mu. \tag{12}$$

For the particular case of an isotropic, homogenous and linear material, the functional $\mathcal{F}_y$ assumes the classical form

$$\mathcal{F}_y(\nabla u_\mu(\boldsymbol{y})) = -k\nabla u_\mu(\boldsymbol{y}) \quad \forall \boldsymbol{y} \in \Omega_\mu, \tag{13}$$

where $k = k(\boldsymbol{y})$ is a thermal conductivity of the RVE represented by Ω_μ.

Assuming that the RVE is subjected, in general, to a internal heat sources $b^e = b^e(\boldsymbol{y})$ in Ω_μ^e, $b^i = b^i(\boldsymbol{y})$ in Ω_μ^i, and a external heat flux $t = t(\boldsymbol{y})$ acting over the exterior boundary $\partial\Omega_\mu$, the *Principle of Virtual Work* establishes that the RVE is in equilibrium if and only if the following variational equation holds,

$$\int_{\Omega_\mu^e} \boldsymbol{q}_\mu \cdot \nabla\eta dV + \int_{\Omega_\mu^i} \boldsymbol{q}_\mu \cdot \nabla\eta dV + \int_{\Omega_\mu^e} b^e\eta dV + \int_{\Omega_\mu^i} b^i\eta dV - \int_{\partial\Omega_\mu} t\eta dA = 0 \qquad \forall \eta \in \mathcal{V}_\mu, \tag{14}$$

where $\mathcal{V}_\mu$ is an appropriate space of kinematically admissible variations over the RVE.

For sufficiently regular vector field $\boldsymbol{q}_\mu(\boldsymbol{y})$ in the domain Ω_μ, the Euler-Lagrange equation, associated to the variational equilibrium given by eq. (14), may be written in the differential form as,

$$\begin{cases} \mathrm{div}\boldsymbol{q}_\mu = b^e & in\ \Omega_\mu^e \\ \mathrm{div}\boldsymbol{q}_\mu = b^i & in\ \Omega_\mu^i \\ \boldsymbol{q}_\mu \cdot \mathbf{n} = t & on\ \partial\Omega_\mu \\ [\![\boldsymbol{q}_\mu \cdot \mathbf{n}]\!] = 0 & on\ \partial\Omega_\mu^i \end{cases}, \tag{15}$$

where the outward unit vector **n** is normal to the boundary $\partial\Omega_\mu$ and the symbol $[\![\bullet]\!]$ is used to denote a jump condition over the boundary of the inclusion, i.e.,

$$[\![\bullet]\!] := (\bullet)|_e - (\bullet)|_i,$$

being $(\bullet)|_e$ associated to the matrix, represented by Ω_μ^e, and $(\bullet)|_i$ associated to the inclusion, represented by Ω_μ^i.

Particularizing equation (15) for the case given by eq. (13) and considering that $k(\boldsymbol{y})$ is piecewise constant, we have the classical form of the heat conduction on rigid solid based on laplacian operator,

$$\begin{cases} -\tilde{k}^e\Delta u_\mu = b^e & in\ \Omega_\mu^e \\ -\tilde{k}^i\Delta u_\mu = b^i & in\ \Omega_\mu^i \\ -\tilde{k}^e\frac{\partial u_\mu}{\partial n} = t & on\ \partial\Omega_\mu \\ [\![\tilde{k}\frac{\partial u_\mu}{\partial n}]\!] = 0 & on\ \partial\Omega_\mu^i \end{cases},$$

where $\tilde{k}^e$ and $\tilde{k}^i$ are the (constant) thermal conductivity in each part of the domain Ω_μ, i.e.,

$$k(\boldsymbol{y}) = \begin{cases} \tilde{k}^e, \ \forall \boldsymbol{y} \in \Omega_\mu^e \\ \tilde{k}^i, \ \forall \boldsymbol{y} \in \Omega_\mu^i \end{cases}.$$

2.3 The homogenized heat flux

In the same manner to the shown early in this section, it is necessary establish a relation between the microscopic heat flux, $\boldsymbol{q}_\mu(\boldsymbol{y})$, and the macroscopic heat flux associated to material point $\boldsymbol{x}$, $\boldsymbol{q}(\boldsymbol{x})$. This association is made with the same principle shown in section 2.1, called *homogenization*. Thus, the homogenized heat flux is obtained through the following expression,

$$\boldsymbol{q}(\boldsymbol{x}) = \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu(\boldsymbol{y})\, dV, \tag{16}$$

or in terms of integrals over RVE decomposition (matrix and inclusion),

$$\boldsymbol{q}(\boldsymbol{x}) = \frac{1}{V_\mu}\left[\int_{\Omega_\mu^e} \boldsymbol{q}_\mu(\boldsymbol{y})\,dV + \int_{\Omega_\mu^i} \boldsymbol{q}_\mu(\boldsymbol{y})\,dV\right]. \tag{17}$$

It is important to note that, from previously expression, the RVE is described as a continuum, then it is necessary that the RVE must be sufficiently large for its continuum representation to make sense.

Now, using the following tensorial relationship

$$\int_\Omega (\nabla \mathbf{v})\,\mathbf{w}dV = \int_{\partial\Omega} \mathbf{v}(\mathbf{w}\cdot\mathbf{n})\,dA - \int_\Omega \mathbf{v}\mathrm{div}(\mathbf{w})\,dV,$$

in eq. (17), with $\mathbf{w} = \boldsymbol{q}_\mu$, $\mathbf{v} = \boldsymbol{y} \Rightarrow \nabla\mathbf{v} = \mathbf{I}$, we get

$$\begin{aligned} \boldsymbol{q}(\boldsymbol{x}) &= \frac{1}{V_\mu}\left[\int_{\partial\Omega_\mu^e} (\boldsymbol{q}_\mu\cdot\mathbf{n})\,\boldsymbol{y}dA - \int_{\Omega_\mu^e} \mathrm{div}(\boldsymbol{q}_\mu)\,\boldsymbol{y}dV + \int_{\partial\Omega_\mu^i} (\boldsymbol{q}_\mu\cdot\mathbf{n})\,\boldsymbol{y}dA - \int_{\Omega_\mu^i} \mathrm{div}(\boldsymbol{q}_\mu)\,\boldsymbol{y}dV\right] \\ &= \frac{1}{V_\mu}\left[\int_{\partial\Omega_\mu} (\boldsymbol{q}_\mu\cdot\mathbf{n})\,\boldsymbol{y}dA - \int_{\Omega_\mu^e} \mathrm{div}(\boldsymbol{q}_\mu)\,\boldsymbol{y}dV + \int_{\partial\Omega_\mu^i} [\![\boldsymbol{q}_\mu\cdot\mathbf{n}]\!]\boldsymbol{y}dA - \int_{\Omega_\mu^i} \mathrm{div}(\boldsymbol{q}_\mu)\,\boldsymbol{y}dV\right], \end{aligned}$$

then, with the introduction of the strong form of equilibrium eq. (15) in above equation, we obtain the following expression,

$$\boldsymbol{q}(\boldsymbol{x}) = \frac{1}{V_\mu}\left[\int_{\partial\Omega_\mu} t\boldsymbol{y}dA - \int_{\Omega_\mu^e} b^e\boldsymbol{y}dV - \int_{\Omega_\mu^i} b^i\boldsymbol{y}dV\right].$$

Finally, in above equation is established the homogenized heat flux, exclusively in terms of RVE boundary flux and heat source.

2.4 The Hill-Mandel Principle

Based on physical arguments, Hill, 1965; and Mandel, 1971; established that "*the macroscopic stress power must equal the volume average of the microscopic stress power over the RVE*". Then to apply the previously statement on the context of this work, it is necessary to write the Hill-Mandel Principle in terms of the work generated by macroscopic and microscopic virtual temperatures, δu and δu_μ, respectively. That is, at any state of the RVE characterized by a vector field $\boldsymbol{q}_\mu$ in equilibrium, the identity

$$\boldsymbol{q}\cdot\nabla(\delta u) = \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu\cdot\nabla(\delta u_\mu)\,dV, \tag{18}$$

must holds for any kinematically admissible microscopic field $\nabla(\delta u_\mu)$. Within the present scheme, a microscopic gradient of virtual temperature is said to be kinematically admissible if the following representation is satisfied,

$$\nabla(\delta u_\mu) = \nabla(\delta u) + \nabla(\delta\tilde{u}_\mu), \quad \forall\delta\tilde{u}_\mu \in \mathcal{V}_\mu, \tag{19}$$

where $\mathcal{V}_\mu$ is the space of kinematically admissible variation of the virtual temperature fluctuation over the RVE, given by eq. (9). Then, with the *Hill-Mandel principle* established in the previous expression, eq. (18), it is possible to write the following proposition:

Proposition 1 *: The Hill-Mandel principle is satisfied if and only if the virtual works of external flux, t, and internal heat sources, b^e and b^i, on the RVE vanish. That is, the Hill-Mandel Principle is equivalent to the following variational equations:*

$$\int_{\partial\Omega_\mu} t\eta dA = 0; \quad \int_{\Omega_\mu^e} b^e\eta dV = 0; \quad \int_{\Omega_\mu^i} b^i\eta dV = 0, \quad \forall\eta \in \mathcal{V}_\mu, \tag{20}$$

Proof. Introducing eq. (19) into eq. (18), we obtain

$$\begin{aligned} \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu\cdot\nabla(\delta u_\mu)\,dV &= \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu\cdot[\nabla(\delta u) + \nabla(\delta\tilde{u}_\mu)]\,dV \\ &= \left(\frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu dV\right)\cdot\nabla(\delta u) + \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu\cdot\nabla(\delta\tilde{u}_\mu)\,dV \\ &= \boldsymbol{q}\cdot\nabla(\delta u) + \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu\cdot\nabla(\delta\tilde{u}_\mu)\,dV. \end{aligned}$$

Then the identity given by eq. (18) holds if and only if,

$$\int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla\left(\delta\tilde{u}_\mu\right) dV = 0, \quad \forall \delta\tilde{u}_\mu \in \mathcal{V}_\mu.$$

Next, integrating by parts in the previous equation, gives

$$\begin{aligned}\int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla\left(\delta\tilde{u}_\mu\right) dV \;&=\; \int_{\partial\Omega_\mu} \left(\boldsymbol{q}_\mu \cdot \mathbf{n}\right) \delta\tilde{u}_\mu dA - \int_{\Omega_\mu^e} \operatorname{div}\left(\boldsymbol{q}_\mu\right) \delta\tilde{u}_\mu dV + \int_{\partial\Omega_\mu^i} [\![\boldsymbol{q}_\mu \cdot \mathbf{n}]\!] \delta\tilde{u}_\mu dA \\ &\quad - \int_{\Omega_\mu^i} \operatorname{div}\left(\boldsymbol{q}_\mu\right) \delta\tilde{u}_\mu dV.\end{aligned}$$

Taking into account the strong form of equilibrium over the RVE, given by eq. (15), we have

$$\int_{\Omega_\mu} \boldsymbol{q}_\mu \cdot \nabla\left(\delta\tilde{u}_\mu\right) dV = \int_{\partial\Omega_\mu} t\delta\tilde{u}_\mu dA - \int_{\Omega_\mu^e} b^e \delta\tilde{u}_\mu dV - \int_{\Omega_\mu^i} b^i \delta\tilde{u}_\mu dV.$$

From the previous expression, the Hill-Mandel principle is equivalent to the following variational equation,

$$\int_{\partial\Omega_\mu} t\delta\tilde{u}_\mu dA - \int_{\Omega_\mu^e} b^e \delta\tilde{u}_\mu dV - \int_{\Omega_\mu^i} b^i \delta\tilde{u}_\mu dV = 0, \quad \forall \delta\tilde{u}_\mu \in \mathcal{V}_\mu.$$

Further, since $\mathcal{V}_\mu$ has the structure of a vector space (see eqs. (8) and (9)), the above variational equation holds if and only if each of its integrals vanish individually. Finally, with this statement the Proposition 1 is proved. ■

Remark 1 *: The equation (20) establish that the Hill-Mandel principle is equivalent to require that the external flux t and the internal heat sources b^e and b^i of the RVE be purely reactive. That is, the external flux t and the internal heat sources b^e and b^i are reactions to the kinematical constraint (involved in the choice of space $\mathcal{V}_\mu$) imposed upon the RVE and cannot be prescribed independently. Thus, t, b^e and b^i belong to the functional space orthogonal to $\mathcal{V}_\mu$, i.e.*

$$\left(t, b^e \; and \; b^i\right) \in \mathcal{V}_\mu^\perp.$$

Then, once $\mathcal{V}_\mu$ is chosen, the space to which t, b^e and b^i belong is defined in an automatic way.

3. Classes of Multi-Scale Models

Based on the variational approach presented in the above sections, in this one we obtain four classes of multi-scale constitutive models, which are:

(a) Taylor model, or homogeneous micro-cell temperature gradient;

(b) Linear RVE boundary temperature model;

(c) Periodic RVE boundary temperature fluctuation model;

(d) Uniform RVE boundary flux, or the minimum kinematical constraint model.

It is important to note that each model is only a consequence of the choice made for the space of kinematically admissible variation $\mathcal{V}_\mu \subset \tilde{\mathcal{K}}_\mu$.

3.1 Taylor Model

The Taylor model is based on adopting the null space for the space of kinematically admissible variation, i.e.,

$$\mathcal{V}_\mu = \mathcal{V}_\mu^T \equiv \{\mathbf{0}\},$$

consequently the kinematical constraint over the RVE is given by,

$$\tilde{u}_\mu(\boldsymbol{y}) = 0, \quad \forall \boldsymbol{y} \in \bar{\Omega}_\mu.$$

This choise for the space implies that the microscopic temperature field is linear in the variable $\boldsymbol{y}$,

$$u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y}, \quad \forall \boldsymbol{y} \in \bar{\Omega}_\mu,$$

and the micro-cell temperature gradient is *homogeneous*,

$$\nabla u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}), \quad \forall \boldsymbol{y} \in \bar{\Omega}_\mu, \tag{21}$$

moreover, it coincides with the macroscopic temperature gradient at the corresponding point $\boldsymbol{x}$ of the domain Ω.

Then, for this kind of model the internal heat sources b^e and b^i, and the external flux t, are reactions to be determinated. Therefore the orthogonal space $\mathcal{V}_\mu^\perp$ can be any space that has sufficient regularity.

3.1.1 The rule of mixture

Taking into account the expression (12) and the result given by eq. (21), the microscopic heat flux satisfies,

$$\boldsymbol{q}_{\mu}(\boldsymbol{y}) = \mathcal{F}_y(\nabla u_{\mu}(\boldsymbol{y})) = \mathcal{F}_y(\nabla u(\boldsymbol{x})).$$

A case of practical interest arise when the constitutive response functional $\mathcal{F}$ is independent of $\boldsymbol{y}$. In this particular case, the homogenized heat flux (eq. (17)) for the Taylor-based model can be written as,

$$\boldsymbol{q}(\boldsymbol{x}) = \frac{1}{V_{\mu}}\left[\int_{\Omega_{\mu}^{e}} \mathcal{F}(\nabla u(\boldsymbol{x}))\,dV + \int_{\Omega_{\mu}^{i}} \mathcal{F}(\nabla u(\boldsymbol{x}))\,dV\right] = v^{e}\boldsymbol{q}_{\mu}^{e} + v^{i}\boldsymbol{q}_{\mu}^{i}\ , \tag{22}$$

where $\boldsymbol{q}_{\mu}^{e}$ and $\boldsymbol{q}_{\mu}^{i}$ are the (uniform) heat flux resulting, respectively, in the matrix and inclusion of the RVE; and the matrix and inclusion volume fraction are, respectively, given by

$$v^{e} \equiv \frac{V_{\mu}^{e}}{V_{\mu}} \qquad \text{and} \qquad v^{i} \equiv \frac{V_{\mu}^{i}}{V_{\mu}}\ ,$$

with V_{μ}^{e} and V_{μ}^{i} denoting the matrix and inclusion volume of the RVE.

Now, considering multiple inclusions, for example M non-overlapping inclusions, and supposing that each subdomain j can be modelled by a constitutive functional $\mathcal{F}_j(\nabla u)$, i.e., the microscopic constitutive response functional $\mathcal{F}_j$ is independent of $\boldsymbol{y}$, we can write the expression (22) in the following way,

$$\boldsymbol{q}(\boldsymbol{x}) = v^{e}\boldsymbol{q}_{\mu}^{e} + \sum_{j=1}^{M} v_j^{i}\boldsymbol{q}_{\mu j}^{i}\ , \tag{23}$$

where

$$v_j^{i} \equiv \frac{V_{\mu j}^{i}}{V_{\mu}} \qquad \text{and} \qquad \boldsymbol{q}_{\mu j}^{i} = \mathcal{F}_j(\nabla u)\ ,$$

are, respectively, the volume fraction and the (uniform) heat flux of phase j. Thus, with the previous definition we still have,

$$\Omega_{\mu}^{i} = \bigcup_{j=1}^{M}\Omega_{\mu j}^{i}, \qquad V_{\mu}^{i} = \sum_{j=1}^{M} V_{\mu j}^{i}, \qquad \Omega_{\mu}^{e} = \Omega_{\mu}\backslash\Omega_{\mu}^{i} \qquad \text{and} \qquad V_{\mu}^{e} = V_{\mu} - V_{\mu}^{i}\ .$$

where $\Omega_{\mu j}^{i}$ and $V_{\mu j}^{i}$ are the subdomain and the volume of the phase j of the inclusion. That is, the macroscopic heat flux, for this Taylor-based model given by eq. (23), is the weighted average of the heat flux acting at the different microscopic phases. This rule is commonly known as the *rule of mixtures*.

3.2 Linear boundary temperature model

This class of model is derived by assuming that the temperature fluctuation is null on the RVE boundary. Thus, the space $\mathcal{V}_{\mu}$ is chosen as,

$$\mathcal{V}_{\mu} = \mathcal{V}_{\mu}^{L} \equiv \left\{\tilde{u}_{\mu} \in \tilde{\mathcal{K}}_{\mu} : \tilde{u}_{\mu}(\boldsymbol{y}) = 0,\ \forall \boldsymbol{y} \in \partial\Omega_{\mu}\right\}.$$

This choice for the space of kinematically admissible variation assures that the distribution of temperature on the RVE boundary is *linear* in $\boldsymbol{y}$, i.e.,

$$u_{\mu}(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y}, \quad \forall \boldsymbol{y} \in \partial\Omega_{\mu}.$$

In the same way that it happens in the Taylor model, the external flux t belongs to the space of all sufficiently regular functions over RVE boundary $\partial\Omega_{\mu}$. Then, it is necessary to determine this external flux in a posteriori calculus. Due to the definition of space $\mathcal{V}_{\mu}$, the only internal heat sources that satisfies the variational equations (20) are the identically null, i.e.,

$$b^{e}(\boldsymbol{y}) = 0 \quad \forall \boldsymbol{y} \in \Omega_{\mu}^{e}, \ \text{ and } \ b^{i}(\boldsymbol{y}) = 0 \quad \forall \boldsymbol{y} \in \Omega_{\mu}^{i}.$$

3.3 Periodic boundary temperature fluctuations model

This class of constitutive models is appropriated to represent the behavior of materials with periodic microstructure (Michel *et al.*, 1999). So that this periodic representation makes sense, it is necessary that the RVE boundary be composed for N pairs of equal sets of sides

$$\partial\Omega_\mu = \bigcup_{j=1}^{N} \left(\Gamma_j^+, \Gamma_j^-\right),$$

such that, each point $\boldsymbol{y}^+ \in \Gamma_j^+$ has its correspondent point $\boldsymbol{y}^- \in \Gamma_j^-$, and that the normal vectors to the sides $\left(\Gamma_j^+, \Gamma_j^-\right)$ in the points $(\boldsymbol{y}^+, \boldsymbol{y}^-)$ satisfy

$$\mathbf{n}_j^+ = -\mathbf{n}_j^-.$$

The typical examples of shape for periodic RVE boundary are square and hexagonal (see Figure 2).

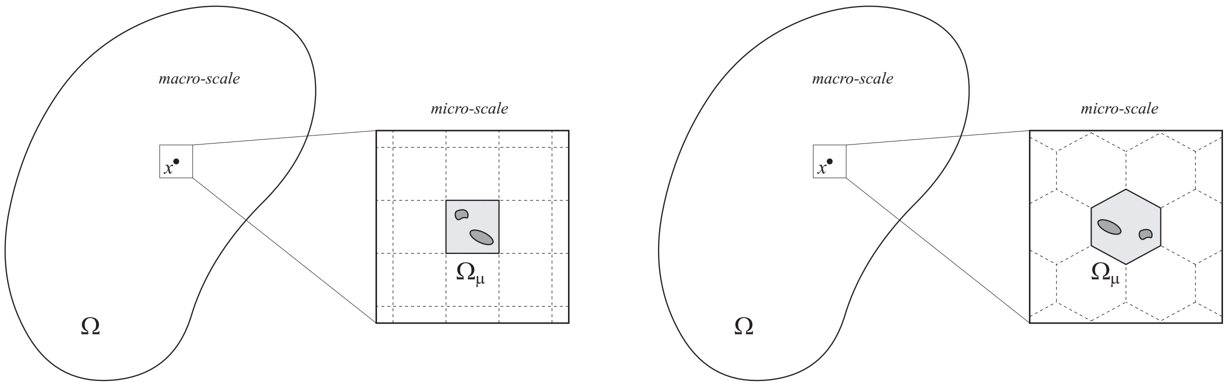

Figure 2. continuum macro-scale with different locals periodic micro-scales

Taking into account the geometric considerations established previously for the RVE boundary, the space $\mathcal{V}_\mu$ for this *periodic boundary temperature fluctuations model* is defined as,

$$\mathcal{V}_\mu = \mathcal{V}_\mu^P \equiv \left\{\tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{u}_\mu\left(\boldsymbol{y}^+\right) = \tilde{u}_\mu\left(\boldsymbol{y}^-\right),\ \forall \text{ pair } \left(\boldsymbol{y}^+, \boldsymbol{y}^-\right) \in \partial\Omega_\mu\right\}.$$

With the above definition for the space $\mathcal{V}_\mu$, it is simple to verify if the condition $\mathcal{V}_\mu \subset \tilde{\mathcal{K}}_\mu$ is satisfied. In fact, it is only necessary to verify that the equation (7) is fulfilled. Then, having assumed the above geometric partition for the RVE boundary, the constraint of set $\tilde{\mathcal{K}}_\mu$ can be written as,

$$\begin{aligned}\int_{\partial\Omega_\mu} \tilde{u}_\mu \mathbf{n} dA &= \sum_{j=0}^{N}\left[\int_{\Gamma_j^+} \tilde{u}_\mu\left(\boldsymbol{y}^+\right)\mathbf{n}_j^+ dA + \int_{\Gamma_j^-} \tilde{u}_\mu\left(\boldsymbol{y}^-\right)\mathbf{n}_j^- dA\right] = \\ &= \sum_{j=0}^{N}\left[\int_{\Gamma_j^+} \tilde{u}_\mu\left(\boldsymbol{y}^+\right)\mathbf{n}_j^+ dA - \int_{\Gamma_j^+} \tilde{u}_\mu\left(\boldsymbol{y}^+\right)\mathbf{n}_j^+ dA\right] = 0.\end{aligned}$$

Remembering that the external heat flux applied to RVE boundary t is orthogonal to $\mathcal{V}_\mu^P$, $t \in \left(\mathcal{V}_\mu^P\right)^\perp$, in order to satisfies the variational equation

$$\int_{\partial\Omega_\mu} t\eta dA = 0 \quad \forall \eta \in \mathcal{V}_\mu^P,$$

it is necessary that the external heat flux be *anti-periodic* on $\partial\Omega_\mu$, i.e.,

$$t\left(\boldsymbol{y}^+\right) = -t\left(\boldsymbol{y}^-\right) \quad \forall \text{ pair } \left(\boldsymbol{y}^+, \boldsymbol{y}^-\right) \in \partial\Omega_\mu.$$

Finally, the internal heat sources, b^e and b^i, orthogonal to $\mathcal{V}_\mu^P$ are,

$$b^e\left(\boldsymbol{y}\right) = 0 \quad \forall \boldsymbol{y} \in \Omega_\mu^e, \text{ and } b^i\left(\boldsymbol{y}\right) = 0 \quad \forall \boldsymbol{y} \in \Omega_\mu^i.$$

3.4 Uniform RVE boundary flux model

For this last model, the choice for the space $\mathcal{V}_\mu$ is the minimum kinematical constraint on the RVE. Thus, the space of kinematically admissible variation is chosen as,

$$\mathcal{V}_\mu = \mathcal{V}_\mu^U \equiv \tilde{\mathcal{K}}_\mu = \left\{ \tilde{u}_\mu \in \mathcal{W} : \int_{\partial\Omega_\mu} \tilde{u}_\mu \mathbf{n} dA = 0 \right\},$$

where $\mathcal{W}$ is a Sobolev's space defined in section 2.1.

In the same manner that in the models presented in the previous sections 3.2 and 3.3, the internal heat sources that satisfy the variational equations (20) are identically null, i.e.,

$$b^e(\boldsymbol{y}) = 0 \quad \forall \boldsymbol{y} \in \Omega_\mu^e, \text{ and } b^i(\boldsymbol{y}) = 0 \quad \forall \boldsymbol{y} \in \Omega_\mu^i.$$

For a constitutive multi-scale model based on the minimum kinematical constraint over the RVE, the compatible external heat flux is given by (de Souza Neto & Feijóo, 2006),

$$t(\boldsymbol{y}) = \boldsymbol{q}_\mu(\boldsymbol{y}) \cdot \mathbf{n}(\boldsymbol{y}) = \boldsymbol{q}(\boldsymbol{x}) \cdot \mathbf{n}(\boldsymbol{y}), \quad \forall \boldsymbol{y} \in \partial\Omega_\mu, \tag{24}$$

where $\boldsymbol{q}(\boldsymbol{x})$ is the macroscopic heat flux associated with material point $\boldsymbol{x}$ of the domain Ω.

Note that with the present variational construction of *minimum kinematical constraint model*, the external flux condition given by eq. (24) is ***not*** imposed a priori. In fact, it is a ***consequence*** of the choice of kinematically admissible fluctuations space $\mathcal{V}_\mu^U$. Due to the condition given by eq. (24), this kind of models is known as *uniform boundary flux model*.

4. Final remarks

In this work, we have applied the variational theory proposed by de Souza Neto & Feijóo (2006) to develop a general kinematic variational framework for infinitesimal multi-scale models in the steady-state heat conduction problem on rigid solids. Several models were presented in section 3. Each one of these models differs in the definition of the kinematically admissible variations space $\mathcal{V}_\mu$. From the choices made for the kinematically admissible variations space $\mathcal{V}_\mu$, we have that each one produces a different estimate for the microscopic temperature u_μ. Generating, as consequence, that the response in macro-scale be different for each model.

With the models developed in the previous sections, the following summary can be constructed:

(a) Taylor model

$$\mathcal{V}_\mu^T \equiv \{\mathbf{0}\};$$

(b) Linear RVE boundary temperature model

$$\mathcal{V}_\mu^L \equiv \left\{ \tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{u}_\mu(\boldsymbol{y}) = 0, \ \forall \boldsymbol{y} \in \partial\Omega_\mu \right\};$$

(c) Periodic RVE boundary temperature fluctuation model

$$\mathcal{V}_\mu^P \equiv \left\{ \tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{u}_\mu(\boldsymbol{y}^+) = \tilde{u}_\mu(\boldsymbol{y}^-), \ \forall \text{ par } (\boldsymbol{y}^+, \boldsymbol{y}^-) \in \partial\Omega_\mu \right\};$$

(d) Uniform RVE boundary flux model

$$\mathcal{V}_\mu^U \equiv \tilde{\mathcal{K}}_\mu = \left\{ \tilde{u}_\mu \in \mathcal{W} : \int_{\partial\Omega_\mu} \tilde{u}_\mu \mathbf{n} dA = 0 \right\}.$$

From the above box, it is simple to see the following relation between the obtained models,

$$\mathcal{V}_\mu^T \subset \mathcal{V}_\mu^L \subset \mathcal{V}_\mu^P \subset \mathcal{V}_\mu^U.$$

That is, the Taylor model and uniform RVE boundary flux model are the upper and lower limits, respectively, for all possible choices of kinematical constraint for the admissible variation space $\mathcal{V}_\mu$.

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