Asociación Argentina
de Mecánica Computacional

Mecánica Computacional Vol XXXIV, págs. 2945-2957 (artículo completo)
Sebastián Giusti, Martín Pucheta y Mario Storti (Eds.)
Córdoba, 8-11 Noviembre 2016

CONSTITUTIVE MULTISCALE MODELING OF HEAT DIFFUSION REACTION PROBLEMS

Andrés R. Valdez[a]

[a]*Programa de Pós-Graduação em Modelagem Computacional, Universidade Federal de Juiz de Fora, Juiz de Fora, MG, Brazil,*

Keywords: Non linear heat transfer, Multiscale modeling, Constitutive coefficient definition, Homogenization

Abstract. This article describes a homogenization procedure based on Multiscale analysis. Such homogenization techniques are important for computer-modeling of heterogeneous materials when the heterogeneities measures allows us to have separation of scales. Multiscale analysis is a reliable technique to understand material responses in where the micro structure is mainly characterized by heterogeneities. The described Multiscale procedure relies on a unified variational basis: (i) Kinematic Admissibility, where the micro-macro kinematics are established and properly linked, (ii) Duality, where the force and stress like physical quantities are characterized, and (iii) Principle of Multiscale Virtual Power, where the homogenization rules are established. For academic purposes a one dimensional numeric implementation is done. We compare the constitutive modeling laws for heat transfer phenomenon, when considering Multiscale analysis and neglecting it.

1 INTRODUCTION

The article is devoted to understand the consequences for evaluating constitutive coefficients, when considering homogenization of virtual power at two scales. Heat transfer through porous media covers a brand of challenging modeling phenomenas, which still has special interest in chemical, mechanical, geological, environmental and petroleum sciences. For these reasons, an accurate description of the effective *linear* thermal conductivity for various porous media, reads great practical interest in the efficient design of industrial equipment.

The whole constitutive modeling theory relies on a particular case of Multiscale modeling, whose variational foundations are shown in the works of Hill (1965); Mandel (1971); Hughes et al. (1998); Blanco et al. (2014). The Variational schemes allows us to resume in one integral equation, every element involved in the problem, such as: Equilibrium equation, Constitutive equation, Boundary conditions. Every local movement equation[1] can be obtained from Variational equations. An important fact is that the Variational framework induces the solution finding procedure.

The article is organized as follows. Section 2 describes a general procedure for obtaining a self consistent variational Multiscale technique based on the concept of Representative Volume Element. Section 3 describes the direct consequences of evaluating the *Principle of Kinematic Admissibility*. Sections 4 and 5 are devoted to characterize the concept of internal and external powers, concluding on the *Principle of Multiscale Virtual Power Balance*. We show in Sections 6 and 7 a numeric implementation, based on Finite Element Method. Section 8 unveils the discrepancies between the classic constitutive modeling and the Multiscale procedure developed in this article. Finally the concluding remarks are shown in Section 9.

2 MULTISCALE MODELING BASIC CONCEPTS

The main stream in Multiscale modeling techniques for PDE's based phenomena was leaded by Allaire (1992). That pioneer work was destined to study the homogenization of partial differential equations with periodic oscillating coefficients. The type of studied equations are often used to model several physical problematic situations; where periodic media arise as a predominant characteristic. Quite often the size of the period is small compared to the domain sampling size. In Allaire (1992) there is a search of macroscopic, or averaged description, when the periodical characteristic turns singular, then consequently asymptotic analysis is performed. During the last 20 years a new proposal was introduced by Hughes et al. (1998). This nouvelle reflexion continues using asymptotic analysis but there is a lack of periodic constraints.

Based on the recently published work of Blanco et al. (2014) the entire Multiscale modeling procedure relies on three fundamental principles:

i Kinematic Admissibility, where the micro-macro kinematics are established and properly linked.

ii Duality, where the force and stress like physical quantities are characterized.

iii Principle of Multiscale Virtual Power, where the homogenization rules are established.

In this article the proposed Multiscale method is based on the idea that every point $x(\Omega)$ at the macro-scale body, who occupies the domain Ω, is associated to *Representative Volume Element* (RVE) with domain Ω_μ, see Figure 1. At the RVE, every point has coordinates denoted

[1] often called Euler-Lagrange equations

with $y_\mu(\Omega_\mu)$. Here and in what follows the micro domain variables are denoted as $(\cdot)_\mu$ and the macro variables would not carry any extra notation.

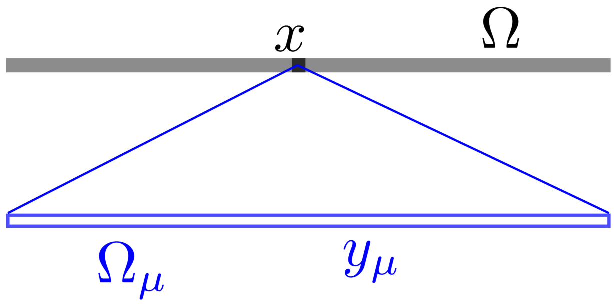


Figure 1: Schematic definition of the 1 dimensional RVE concept.

3 ADMISSIBLE KINEMATICS SETS

The procedure to establish the micro-scale admissible set of motion actions, is based in what Blanco et al. (2014) appointed as *Principle of Kinematic Admissibility*, this principle is supported in the following four statements:

a Definition of the governing kinematics at the macro and micro-scales,

b Definition of insertion operator, that describes how the macro-scale variables are inserted into the micro-scale,

c Definition of homogenization operator, that specifies how the micro-scale variables are averaged, yielding a macro-scale kinematic quantity,

d Definition of the kinematic admissible set for micro-scale variables.

The adopted notation for this article is the following scalar function fields are denoted with u, v. $p-$measurable space functions are denoted with $L^p(\Omega)$, the corresponding Sobolev spaces, $W^{m,p}(\Omega)$, are defined with the usual norms; recalling $H^m(\Omega)$ as the Hilbert space. For Hilbert spaces, the inner product is introduced as $(\cdot;\cdot)$, and the duality is represented with $\langle\cdot;\cdot\rangle$.

3.1 Macro-scale Kinematics

We define the temperature field considering the following rule:

$$\begin{aligned} u : \Omega &\to \mathbb{R} \\ x &\mapsto u(x), \end{aligned}$$

and temperature's gradient vector,

$$\begin{aligned} \mathbb{D} : \mathbb{R} &\to \mathcal{W} \\ u &\mapsto u'. \end{aligned}$$

The kinematic admissible set of temperature changes is written as follows:

$$\mathrm{Kin}\mathcal{U} = \{\, u \in \mathcal{U} \equiv H^m(\Omega) \; + \; extra\ constraints\}; \tag{1}$$

once defined the set of all admissible temperature fields the admissible variations set is defined as follows:

$$\mathrm{Var}\,\mathcal{U} = \{\, u_1 - u_2 \,\in\, \mathrm{Var}\,\mathcal{U} \,:\, u_1, u_2 \,\in\, \mathrm{Kin}\,\mathcal{U}\,\}; \tag{2}$$

due to the previous construction $\mathrm{Kin}\,\mathcal{U}$ can be viewed as a linear manifold of $\mathrm{Var}\,\mathcal{U}$, and this last is a vector space.

3.2 Micro-scale Kinematics

The kinematic description of the micro-scale phenomena is scheduled to be complete with the definition of temperature field to be read as:

$$\begin{aligned} u_\mu : \Omega_\mu &\to \mathbb{R} \\ y_\mu &\mapsto u_\mu(y_\mu), \end{aligned} \tag{3}$$

and temperature's gradient vector,

$$\begin{aligned} \mathbb{D} : \mathbb{R} &\to \mathcal{W}_\mu \\ u_\mu &\mapsto u'_\mu. \end{aligned} \tag{4}$$

3.3 Insertion, Homogenization operator

The kinematic insertion data from macro to micro-scale, is going to be done applying a first order asymptotic expansion, yielding the next expression:

$$\begin{cases} u_\mu\,(y_\mu) = u + u'\,y_\mu + \tilde{u}_\mu\,(y_\mu) \\ u'_\mu\,(y_\mu) = u' + \tilde{u}'_\mu\,(y_\mu), \end{cases} \tag{5}$$

where $\tilde{u}_\mu$ denotes the Fluctuation for micro-scale temperature field.

The kinematic homogenization data from micro to macro-scale, is going to be done by averaging the micro-scales kinematics, recalling the following expression:

$$\begin{cases} u\,\,|\Omega_\mu| = \displaystyle\int_{\Omega_\mu} u + u'\,y_\mu + \tilde{u}_\mu\,(y_\mu)\,\,d\Omega_\mu \\ u'\,\,|\Omega_\mu| = \displaystyle\int_{\Omega_\mu} u' + \tilde{u}'_\mu\,(y_\mu)\,\,d\Omega_\mu, \end{cases} \tag{6}$$

where $|\Omega_\mu|$ denotes the measure of the RVE.

Every admissible Fluctuation for micro-scale's motion action, lies in the following linear manifold:

$$\begin{aligned} \mathrm{Kin}\,\tilde{\mathcal{U}}_\mu = \{\, w \,\in\, \tilde{\mathcal{U}}_\mu \equiv\, H^m(\Omega_\mu) \,\, & \int_{\Omega_\mu} w\,(y_\mu)\,\,d\Omega_\mu = 0\,, \\ & \int_{\partial\Omega_\mu} w\,(y_\mu) \otimes\, n_\mu\,\,d\partial\Omega_\mu = 0\}; \end{aligned}$$

every admissible variation for Fluctuation for micro-scale's motion action, lies in the following subspace:

$$\mathrm{Var}\,\tilde{\mathcal{U}}_\mu = \{\, u_1 - u_2 \,\in\, \mathrm{Var}\,\tilde{\mathcal{U}}_\mu \,:\, u_1, u_2 \,\in\, \mathrm{Kin}\,\tilde{\mathcal{U}}_\mu\,\}.$$

Every admissible micro-scale's motion action lies in the following linear manifold:

$$\mathrm{Kin}\,\mathcal{U}_\mu = \{\, w_\mu \,\in \mathcal{U}_\mu \equiv\; H^m(\Omega_\mu)\, w_\mu = w + w'\, y_\mu + \tilde{w}\,(y_\mu), \tilde{w} \,\in\, \mathrm{Kin}\,\tilde{\mathcal{U}}_\mu, \\ \mathrm{Dirichlet's\,B.C,}\,\};$$

every admissible micro-scale's variation motion action lies in the following subspace:

$$\mathrm{Var}\,\mathcal{U}_\mu = \{\, u_1 - u_2 \,\in\, \mathrm{Var}\,\mathcal{U}_\mu \,:\, u_1, u_2 \,\in\, \mathrm{Kin}\,\mathcal{U}_\mu\,\}.$$

The previous micro-scale's constraints determines the so called *minimal kinematic constrained spaces* compatible with the model. The enforcement of extra kinematic constraints is fully available. When regarding on classical extra constraints, compatibles with the kinematic model, the following constrained models can be generated:

i Voigt-Talyor. This extra constraint relies on the fact that a null prescription of the micro-scale fluctuation field is considered on the RVE, see Figure 2. Consequently,

$$\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu = \{0\};$$

ii Linear boundary fluctuation. This extra constraint relies on the fact that a null prescription of the micro-scale fluctuation field is considered over the RVE's boundary, see Figure 2. Consequently,

$$\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu = \{\, w \,\in\, \tilde{\mathcal{U}}_\mu \equiv\; H_0^m(\Omega_\mu)\; \int_{\Omega_\mu} w\,(y_\mu)\; d\Omega_\mu = 0\,, \\ \int_{\partial\Omega_\mu} w\,(y_\mu) \otimes\, n_\mu\; d\partial\Omega_\mu = 0\};$$

iii Periodic boundary values for fluctuations. It is assumed that over the boundaries of two contiguous RVE's, the fluctuation's jump is forced to be null.

4 DUALITY DEFINITIONS, EXTENSION OF POWER

Previous sections were employed to describe the kinematic aspects of temperature field and temperature's gradient vector. The objective of this section is to measure the expended power, to perform changes in temperatures and temperature's gradients. It is possible to distinguish two different powers, referred to the kinematic changes mentioned before.

4.1 Internal macro-scale Power

We define internal power as the expended power when considering changes in the temperature's gradient vector defined over a measurable vector space $\mathcal{W}$. The Internal Power of the media is considered to be a linear and continuous functional, then it can be mathematically expressed as

$$P_i : \mathcal{W}^* \times \mathcal{W} \rightarrow \mathbb{R},$$

the space $\mathcal{W}^*$ is the dual space of $\mathcal{W}$. Using Riesz Representation theorem, the linear operator has unique representation,

$$P_i(\mathbb{D}(u)) = -\,\langle \mathbb{T}; \mathbb{D}(u) \rangle\,;$$

the negative sign is because a mechanical convention. The new element $\mathbb{T} \,\in\, \mathcal{W}^*$ is called Heat Flux.

4.2 External macro-scale Power

The external macro-scale power addresses the expended power to perform changes in the temperature. The system of external forces f compatible with the kinematic model is characterized by a linear and continuous functional in $\mathcal{U}$. The set of all these linear and continuous functional define the space of external forces $\mathcal{U}^*$, where $\mathcal{U}^*$ is the dual space of $\mathcal{U}$; then it can be mathematically expressed as

$$P_e : \mathcal{U}^* \times \mathcal{U} \to \mathbb{R},$$

using Riesz Representation theorem, the linear operator has unique representation,

$$P_e(u) = \langle f; u \rangle .$$

4.3 Internal micro-scale Power

We define the internal power at the micro-scale as a linear and continuous functional, then it can be mathematically expressed as

$$P_{i\,\mu} : \mathcal{W}_\mu^* \times \mathcal{W}_\mu \to \mathbb{R},$$

the space $\mathcal{W}_\mu^*$ is the dual space for $\mathcal{W}_\mu$. Using Riesz Representation theorem, the linear operator has unique representation,

$$P_{i\,\mu}(\mathbb{D}(u_\mu)) = -\langle \mathbb{T}_\mu; \mathbb{D}(u_\mu) \rangle .$$

4.4 External micro-scale Power

The system of external forces $f_\mu + \mathcal{R}_\mu$ compatible with the kinematic model is characterized by a linear and continuous functional in $\mathcal{U}_\mu$. The set of all these linear and continuous functional define the space of external forces $\mathcal{U}_\mu^*$, the space $\mathcal{U}_\mu^*$ is the dual space of $\mathcal{U}_\mu$; then it can be mathematically expressed as

$$P_{e\,\mu} : \mathcal{U}_\mu^* \times \mathcal{U}_\mu \to \mathbb{R},$$

using Riesz Representation theorem, the linear operator has unique representation,

$$P_{e\,\mu} = \langle f_\mu - \mathcal{R}_\mu; u_\mu \rangle ;$$

5 PRINCIPLE OF MULTISCALE VIRTUAL POWER BALANCE

A special attention is given when setting equal the virtual power associated with an arbitrary point $x \in \Omega$ of the macro-scale, with the virtual power of the associated RVE. Hence the Principle of Multiscale Virtual Power balance is about to be established. The consequences, of modeling employing this methodology strictly based on Germain (1973); Maugin (1980) reads the following facts:

i Micro-scale equilibrium equation, written in terms of variational arguments,

ii Retrieves an homogenization rule for generalized fluxes type loadings,

iii Retrieves an homogenization rule for generalized force type loading.

Axiom 1 (Principle of Multiscale Virtual Power Balance.) *The total macro-scale virtual power at an arbitrary point $x \in \Omega$ must be equal to the total micro-scale virtual power at the corresponding RVE, for all kinematic admissible macro and micro-scale virtual motion actions.*

This principle itself regards a variational statement version of the celebrated *Hill-Mandel* Principle of Macro homogeneity, Hill (1965); Mandel (1971), where only internal power balance is considered. The Principle of Multiscale Virtual Power is written in terms of the dual power properties mentioned before recalling the next expression,

$$P_i(\mathbb{D}(\hat{u})) + P_e(\hat{u}) = P_{i\,\mu}(\mathbb{D}(\hat{u}_\mu)) + P_{e\,\mu}(\hat{u}_\mu)$$
$$\forall\, \hat{u}_\mu \in \mathrm{Var}\,\mathcal{U}_\mu,\ \forall\, \hat{u} \in \mathrm{Var}\,\mathcal{U}. \tag{7}$$

5.1 Micro-scale Equilibrium

When setting null every admissible variations of the macro temperature field, $u \in \mathrm{Kin}\,\mathcal{U}$, the following expression is obtained, for the micro-scale equilibrium:

$$\int_{\Omega_\mu} -\left\langle \mathbb{T}_\mu; v'_\mu\,(y_\mu)\right\rangle + \langle f_\mu; v_\mu\,(y_\mu)\rangle - \langle \mathcal{R}_\mu; v_\mu\,(y_\mu)\rangle \; d\Omega_\mu = 0$$
$$\forall\, v_\mu \in \mathrm{Var}\,\tilde{\mathcal{U}}_\mu. \tag{8}$$

5.2 Dual Flux like Homogenization rule

When regarding the heat fluxes definition by using the internal power duality, yields the following expression for internal power:

$$-\left\langle \mathbb{T}; \mathbb{D}(\hat{u})\right\rangle\, |\Omega_\mu| = \int_{\Omega_\mu} -\langle \mathbb{T}_\mu; \hat{u}'\,(y_\mu)\rangle + \langle f_\mu; \hat{u}'\, y_\mu\rangle - \langle \mathcal{R}_\mu; \hat{u}'\, y_\mu\rangle \; d\Omega_\mu$$
$$\forall\, \hat{u} \in \mathrm{Var}\,\mathcal{U}, \tag{9}$$

consequently, the heat flux homogenization rule relies the following equation,

$$\mathbb{T}\; |\Omega_\mu| = \int_{\Omega_\mu} \mathbb{T}_\mu + [\mathcal{R}_\mu - f_\mu] \otimes y_\mu \; d\Omega_\mu \tag{10}$$

5.3 Dual Force like Homogenization rule

The force like homogenization rule is based on the averaging of both external powers, reading the following expression:

$$\langle f; \hat{u}\rangle\; |\Omega_\mu| = \int_{\Omega_\mu} \langle f_\mu; \hat{u}\rangle + \langle \mathcal{R}_\mu; \hat{u}\rangle \; d\Omega_\mu$$
$$\forall\, \hat{u} \in \mathrm{Var}\,\mathcal{U} \tag{11}$$

Consequently, the force homogenization rule relies on the following equation,

$$f\; |\Omega_\mu| = \int_{\Omega_\mu} f_\mu + \mathcal{R}_\mu \; d\Omega_\mu \tag{12}$$

6 NUMERIC PROCEDURES

Let there be a properly defined, minimization environment for setting the bases of the micro-scale steady heat transfer. Let us consider the effects of diffusion and reaction in heat's transport to write a minimization scheme, allowing us to define *temperature* as the solution field for the following problem,

Problem 2 (On primal formulation) *Given a regular domain Ω_μ, a source function f_μ defined over an $L^2(\Omega_\mu)$ space, find a field denoted with u_μ, defined over the Hilbert space $\mathrm{Kin}\,\mathcal{U}_\mu$, such that holds true*

$$\mathcal{J}(u_\mu) \leq \mathcal{J}(w_\mu)\,\forall\, w_\mu \,\in\, \mathrm{Kin}\,\mathcal{U}_\mu,$$

where the functional $\mathcal{J}(\cdot) : \mathcal{U}_\mu \rightarrow \mathbb{R}$ is defined as follows:

$$\mathcal{J}(w_\mu) = \frac{1}{2}\int_{\Omega_\mu} \left\langle \mathbb{T}(w_\mu); w'_\mu \right\rangle + 2\,\left\langle \mathcal{R}(w_\mu); w_\mu \right\rangle - 2\,\left\langle f_\mu; w_\mu \right\rangle\, d\Omega_\mu$$

We characterize the micro-scale constitutive behavior with the following expressions:

- Micro-scale constitutive behavior for the heat flux vector, let us consider valid Fourier law, parametrized by:

$$\begin{aligned} \mathbb{T}_\mu &= \alpha\, u'_\mu \\ &= \alpha\, \left(u' + \tilde{u}'_\mu\right) \end{aligned} \tag{13}$$

- Micro-scale constitutive behavior for the reactive phenomena, let us consider valid a reaction, parametrized by:

$$\begin{aligned} \mathcal{R}_\mu &= \beta\, u_\mu \\ &= \beta\, \left(u + u'\, y_\mu + \tilde{u}_\mu\right) \end{aligned} \tag{14}$$

- Micro-scale heat source, let us consider a uniform heat source parametrized by:

$$f_\mu = 1.0 \tag{15}$$

Consequently the following variational problem is written:

Problem 3 (Micro-scale Variational Equation) *Given a regular domain Ω_μ, a source function f_μ defined over an $L^2(\Omega_\mu)$ space, find the temperature field denoted with $\tilde{u}_\mu$, defined over the Hilbert space $\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu$, such that holds true*

$$\begin{aligned} &\int_{\Omega_\mu} -\left\langle \alpha\,\left(u' + \tilde{u}'_\mu\right); v'_\mu \right\rangle + \left\langle f_\mu; v_\mu \right\rangle - \left\langle \beta\,\left(u + u'\,y_\mu + \tilde{u}_\mu\right); v_\mu \right\rangle\, d\Omega_\mu = 0 \\ &\forall\, v_\mu \,\in\, \mathrm{Var}\,\tilde{\mathcal{U}}_\mu. \end{aligned} \tag{16}$$

Where u and u' are considered constants in the RVE.

Corollary 4 (Uniqueness) *The uniqueness of the solution for the Problem 3, who is a variational version for the minimization Problem 2, is strictly subjected to convex Functionals. To show that the functional $\mathcal{J}(\cdot)$ is convex, the second gateaux derivative is calculated,*

$$\delta^2 \mathcal{J}\left(\tilde{u}_\mu; v_\mu\right) = \int_{\Omega_\mu} \left\langle \alpha\, v'_\mu; v'_\mu \right\rangle + \left\langle \beta\, v_\mu; v_\mu \right\rangle\, d\Omega_\mu, \tag{17}$$

then the functional $\mathcal{J}(\cdot)$ is convex if

$$\delta^2 \mathcal{J}\left(\tilde{u}_\mu; v_\mu\right) > 0\ \forall\, v_\mu\ \in\ \mathrm{Var}\,\tilde{\mathcal{U}}_\mu. \tag{18}$$

Recalling that the coefficients α and β, when both are positive, yields the functional $\mathcal{J}(\cdot)$ as a convex functional. [2]

6.1 Finite Element Approximation

Let us consider an arbitrary partition denoted with Ω_μ^h where the union of every partition reads the domain Ω_μ. Within this partition, let there be possible to use $\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu^h$ and $\mathrm{Var}\,\tilde{\mathcal{U}}_\mu^h$ as conforming finite element spaces.

The Finite element approximation, for the micro-scale Variational diffusive reactive phenomena addressed in Problem 3, yields a discrete counterpart:

Problem 5 (Galerkin's approximation for micro-scale Variational Equation) *Given a regular domain Ω_μ^h, a source function f_μ defined over an $L^2(\Omega_\mu^h)$, find the temperature field denoted with $\tilde{u}_\mu^h$, defined over the Hilbert space $\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu^h$, such that holds true*

$$\begin{aligned}&\sum_h \int_{\Omega_\mu^h} - \left\langle \alpha\, \left(u' + \tilde{u}_\mu^{h\prime}\right); v_\mu^{h\prime} \right\rangle + \left\langle f_\mu; v_\mu^h \right\rangle - \left\langle \beta\, \left(u + u'\, y_\mu + \tilde{u}_\mu^h\right); v_\mu^h \right\rangle\, d\Omega_\mu^h = 0 \\ &\forall\, v_\mu^h\ \in\ \mathrm{Var}\,\tilde{\mathcal{U}}_\mu^h.\end{aligned} \tag{19}$$

Where u and u' are considered constants in the RVE.

Let us consider a conforming finite element space spanned with first order polynomials, this reads the following expression:

$$\mathrm{Kin}\,\tilde{\mathcal{U}}_\mu^h = \mathrm{span}\{P_1(\Omega_\mu^h)\} \tag{20}$$

$$\mathrm{Var}\,\tilde{\mathcal{U}}_\mu^h = \mathrm{span}\{P_1(\Omega_\mu^h)\} \tag{21}$$

When considering the established conforming approximation, the local problem's Elemental Stiffness matrix is obtained and shown next:

$$\int_{\Omega_\mu^h} \left\langle \alpha\, \tilde{u}_\mu^{h\prime}; v_\mu^{h\prime} \right\rangle + \left\langle \beta\, \tilde{u}_\mu^h; v_\mu^h \right\rangle\, d\Omega_\mu^h\ \rightarrow A = \frac{1}{h}\begin{bmatrix} \dfrac{\beta\, h^2 + 3\,\alpha}{3} & \dfrac{\beta\, h^2 - 6\,\alpha}{6} \\ \dfrac{\beta\, h^2 - 6\,\alpha}{6} & \dfrac{\beta\, h^2 + 3\,\alpha}{3} \end{bmatrix} \tag{22}$$

[2] The only member from $\mathrm{Var}\,\tilde{\mathcal{U}}_\mu$ who can set null the second gateaux derivative is the null vector.

The corresponding monolithic tridiagonal Global Stiffness matrix's cell, is schematic written as follows;

$$A_h = \frac{1}{h}\begin{bmatrix} \frac{\beta\, h^2 + 3\,\alpha}{3} & \frac{\beta\, h^2 - 6\,\alpha}{6} & 0.0 \\ \frac{\beta\, h^2 - 6\,\alpha}{6} & 2\,\frac{\beta\, h^2 + 3\,\alpha}{3} & \frac{\beta\, h^2 - 6\,\alpha}{6} \\ 0.0 & \frac{\beta\, h^2 - 6\,\alpha}{6} & \frac{\beta\, h^2 + 3\,\alpha}{3} \end{bmatrix} \tag{23}$$

In order to solve the linear algebraic system, the local Loading vector, is written next;

$$\int_{\Omega_\mu^h} \left\langle f_\mu - \alpha\, u' - \beta\, u - \beta\, u'\, y_\mu ; v_\mu^{h\prime} \right\rangle \, d\Omega_\mu^h \rightarrow F = \frac{-1}{2}\begin{bmatrix} \beta\, h\, u + 2\,\alpha\, u' - f_\mu\, h \\ \beta\, h\, u + 2\,\alpha\, u' - f_\mu\, h \end{bmatrix}, \tag{24}$$

It is important to emphasize that the macro quantities like u and u', are considered as external loadings.

7 NUMERIC EXPERIMENTS

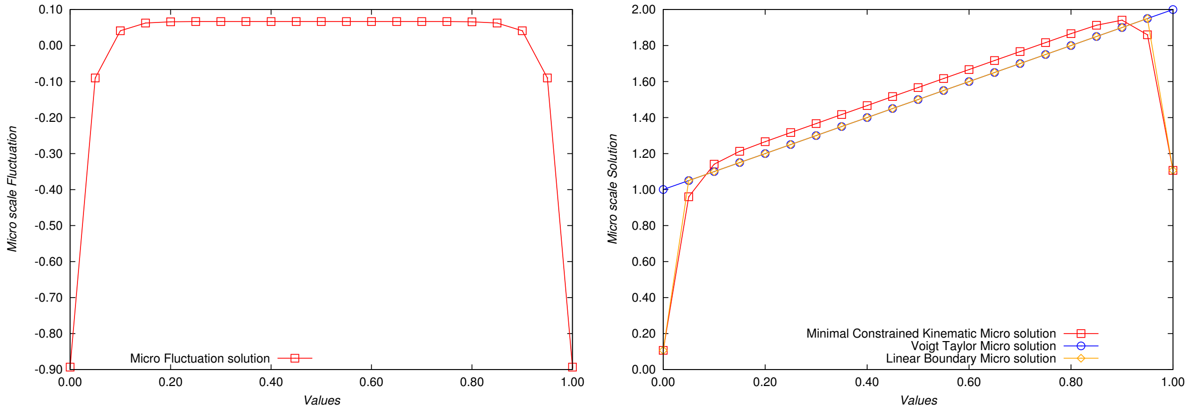
To illustrate the performance of the Multiscale modeling when characterizing the macro-scale loadings, compatible with the established kinematics, we present several academic examples, in which the micro-scale modeling is addressed in Problem 2, when considering finite element method, the classic Galerkin method reads a linear algebraic system. The micro-scale parameters are shown in Table 1

Parameter	Symbol	Value
Diffusive coefficient	α	1.0E-3
Reactive coefficient	β	1.0
Macro Temperature	u	1.0
Macro Temperature's Gradient	u'	1.0
Source load	f_μ	1.0

Table 1: Numeric Simulation parameters

The micro-scale fluctuation solution field is obtained, when solving the variational Problem 5; the micro-scale solution is obtained by applying (5). We show in Figure 2(a) the minimal constrained solution for the micro-scale fluctuation solution field. To compare the consequences of considering extra constraints, we show in Figure 2(b) the micro-scale solution fields for *Voigt Taylor, Linear boundary, and minimal constrained* spaces.

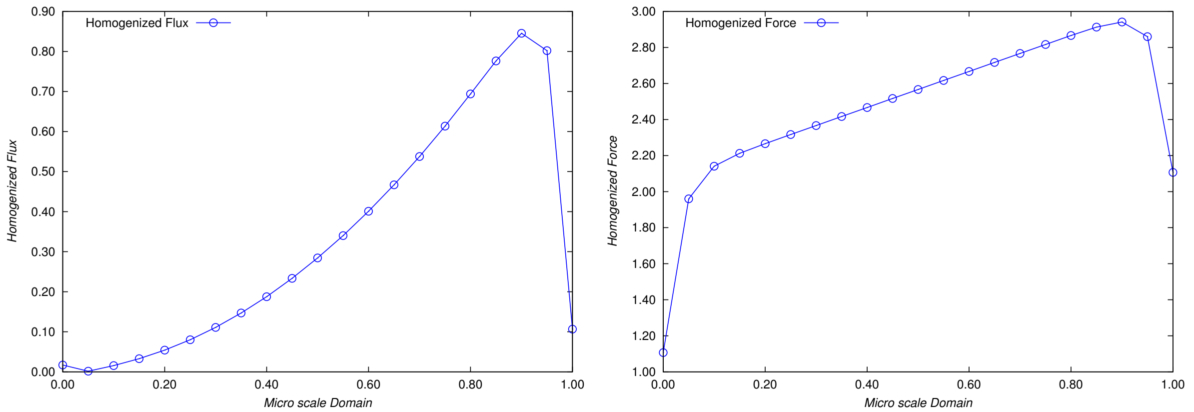
Once calculated the micro-scale solution, the homogenization rules for heat fluxes and loadings can be computed with (6). Considering the minimal constrained space for fluctuation fields, macro-scale heat fluxes and macro-scale force loadings are evaluated and shown in Figure 3.



(a) Minimal Kinematic constrained fluctuation solution field

(b) Comparison between micro-scale's solutions models

Figure 2: Several micro-scale solution fields



(a) RVE's Homogenized heat flux evolution.

(b) RVE's Homogenized loading source evolution.

Figure 3: Extended Hill Mandel Macro homogeneity Principle results

8 CONSTITUTIVE MULTISCALE MODELING

When neglecting the Multiscale modeling results, heat flux and source loading are implicit defined with measures of power, as linear functions. Those functions were written before, as:

$$\begin{cases} P_i : \mathcal{W}^* \times \mathcal{W} \to \mathbb{R}, \\ P_e : \mathcal{U}^* \times \mathcal{U} \to \mathbb{R}, \end{cases}$$

in where both linear operators, have unique representation due to Riesz Representation theorem, yielding the following expressions;

$$\begin{cases} P_i(\mathbb{D}(u)) = -\langle \mathbb{T}; \mathbb{D}(u) \rangle \, , \\ P_e(u) = \langle f; u \rangle \, . \end{cases}$$

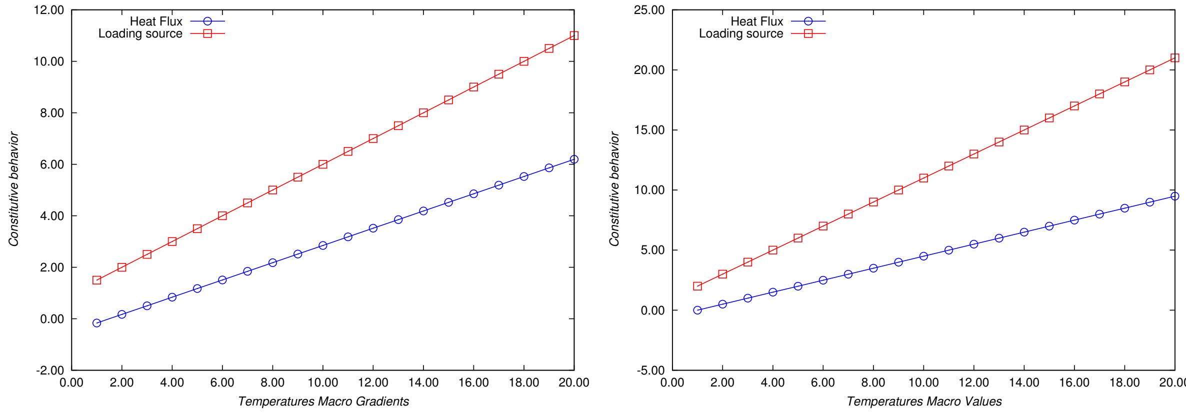
On the other hand when employing Multiscale modeling as a result of combining dual power measures with kinematic admissibility, the constitutive theory for defining heat flux, source loadings reads several updates. Those several updates were the homogenization rules for heat flux and source loading, shown in Equation (10) and Equation (12) respectively. The homogenization rules states that:

$$\begin{cases} \mathbb{T} = \gamma\ (u'; u) \\ f = \psi\ (u'; u)\,. \end{cases} \tag{25}$$

The dependencies between loading type functions (heat flux, source loading), and motion actions (temperature's gradient, temperature) does not fit good with the classical characterization described in Noll (1958), for constitutive behavior.

We employ the Multiscale modeling technique to characterize constitutive behavior. Considering linear variations as shown in Equation (26), we show in Figure 4 the dependencies between loadings and motion actions variations.

$$\begin{cases} u_{(i)} = u_{min} + \dfrac{u_{max}}{20}\, i, \\ u'_{(i)} = u'_{min} + \dfrac{u'_{max}}{20}\, i. \end{cases} \tag{26}$$



(a) Homogenized quantities dependence on Macro temperature's Gradient

(b) Homogenized quantities dependence on Macro temperature's variations

Figure 4: Constitutive modeling for heat fluxes and source loadings

Regarding Noll (1958), the expected behavior between heat fluxes and temperatures variation should be characterized with an horizontal line. In addition to this, the classic constitutive modeling suggests us to neglect variations between temperature's gradients and source loads. The Constitutive modeling based in Multiscale technique, retrieves us a different behavior.

9 CONCLUSIONS

Based on three principles *Kinematic Admissibility*, *Duality* and *Principle of Multiscale Virtual Power* the entire Multiscale modeling is presented. In this context a major extension for the *Hill-Mandel* macro homogeneity principle is obtained, when considering at the micro-scale the effects of diffusion and reaction in heat transfer.

The Multiscale modeling procedure, shown in this work, requires the solution finding of an Equilibrium equation at the micro-scale. Within the variational foundations of the problem, a classic straightforward Finite Element Method is used.

The discussion is presented for an academic one-dimensional model where the classical Finite element theory embedded in Galerkin's conforming approximation is used yielding an important fact. When solving the micro equilibrium Problem 5 (as an extension of the continua counterpart Problem 3) the macro-scale quantities like temperature (u), and temperature's gradient (u') produces no changes in the stiffness matrix (rather elemental either global). This allows us to perform a low cost calculus.

The easy query calculus procedure allows us to study the dependencies between the general loadings and the associated motion actions always aided with variational arguments. With in this context a non classic behavior is obtained between the general loadings and motion actions.

ACKNOWLEDGEMENT

The authors would like to thank the resources provided by the Brazilian research council FAPEMIG

REFERENCES

Allaire G. Homogenization and two-scale convergence. *SIAM Journal on Mathematical Analysis*, 23(6):1482–1518, 1992. ISSN 0036-1410. doi:10.1137/0523084.

Blanco P.J., Sánchez P.J., de Souza Neto E.A., and Feijóo R.A. Variational Foundations and Generalized Unified Theory of RVE-Based Multiscale Models. *Archives of Computational Methods in Engineering*, 2014. ISSN 1134-3060. doi:10.1007/s11831-014-9137-5.

Germain P. On the method of virtual power in continuum mechanics. *SIAM Journal on Applied Mathematics*, 25(3):556–575, 1973. ISSN 1559-3959. doi:10.2140/jomms.2009.4.281.

Hill R. A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, 13(4):213 – 222, 1965. ISSN 0022-5096. doi:http://dx.doi.org/10.1016/0022-5096(65)90010-4.

Hughes T.J., Feijóo G.R., Mazzei L., and Quincy J.B. The variational multiscale method—a paradigm for computational mechanics. *Computer Methods in Applied Mechanics and Engineering*, 166(1-2):3–24, 1998. ISSN 00457825. doi:10.1016/S0045-7825(98)00079-6.

Mandel J. Plasticité classique et viscoplasticité, courses and lectures no. 97, int. *Center for Mech., Springer, Udine*, 1971.

Maugin G.a. The method of virtual power in continuum mechanics: Application to coupled fields. *Acta Mechanica*, 35(1-2):1–70, 1980. ISSN 00015970. doi:10.1007/BF01190057.

Noll W. A mathematical theory of the mechanical behavior of continuous media. *Archive for Rational Mechanics and Analysis*, 2(1):197–226, 1958. ISSN 00039527. doi:10.1007/BF00277929.