Thermo-mechanical homogenization of composite materials

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ABSTRACT

The increased complexity of the materials used for thermo-mechanical applications implies the need of taking into account the microstructure and assessing its behavior. This paper proposes an extension of classical first-order computational homogenization to involve thermo-mechanical effects. The formulation used considers as fully coupled the two physics of the problem, firstly determining the thermal parameters and then considering thermal effects onto the mechanical behavior. The work is completed by benchmark tests to assess the behavior of the new model.

KEYWORDS: First-Order Computational Multiscale Homogenization, Representative Volume Element (RVE), Finite Element Method (FEM)

1. INTRODUCTION

The development of thermo-mechanical homogenization is particularly important since many applications, as aerospace and energy production fields, require this technology. Some examples are heat exchangers or solar space installations, where the thermal effects are not negligible. For instance, space solar panels are made by sandwich composite structure where each layer is composed by different type of material with different thermal properties. The thermal variation during night and day induces strong thermal gradients, therefore the cyclic thermal variation may produce delamination between the layers. As an alternative example, heat exchangers are commonly made by a series of pipes delivering fluid, liquid or a gas. Commonly these pipes are made by steel with a ceramic protective coating. This coating is very important for the correct behavior of the heat exchanger. The best approach for studying its microstructure is the multiscale method that could reproduce the real thermo-mechanical state of this ceramic coating.

The use of multiscale methods for the analysis of composite materials has increased in the last years. At the same time, the microstructure complexity of the composite studied [1,2] has increased as well. The development of several techniques of multiscale homogenization has the aim of determining the effective thermo-mechanical properties of complex materials [3,4,5]. The differences among these techniques are related to the

coupling between the two physics. The strategy proposed in this paper is a fully coupled thermo-mechanical method, as in [6], that was able to solve a non-linear and temperature dependent thermo-mechanical material response at the micro-scale level and then to transmit this information to the macro-scale.

2. FORMULATION

This section summarizes the main concepts and basic equations of classical first-order thermo-mechanical computational homogenization. Standard first-order continuum theory was assumed at both scales. We also assumed static cases, linear elasticity and small displacement conditions. We have used as subscript, for distinguishing the two scales, respectively "μ" for the micro domain and "m" for the macro domain.

The proposed algorithm can be defined by three main phases, as we can see in the Figure 1. We consider an equivalent homogeneous medium at the macro-scale. The first step is the Macro to Micro transition, where the macroscopic strain at any point of the macroscopic mesh, is transferred to the micro-scale. Then, the analysis of the thermal and mechanical micro-scale Boundary Value Problem (BVP) can be performed. Finally, the macro-scale parameters were obtained through homogenization procedures during the Micro to Macro transition step.

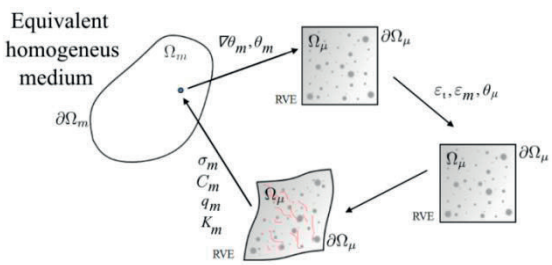

Fig. 1. Work-flow of thermo-mechanical computational homogenization

2.1 Macro to Micro transition

At the macro level, the starting point for a kinematically based computational homogenization method is the assumption that the mechanical strain ε_m, at each point x_m and at a certain instant t, can be obtained as the volume average of the microscopic mechanical strain field ε_μ defined at each point x_μ of the micro-scale domain Ω_μ and at the same instant t as

$$\varepsilon_m(x_m, t) = \frac{1}{V_\mu}\int_{\Omega_\mu} \varepsilon_\mu(x_\mu, t)dV \quad (1)$$

the microscopic strain field could can be expressed as the symmetric gradient of the microscopic displacement field u_μ

$$\varepsilon_m(x_m, t) = \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla^s u_\mu dV \quad (2)$$

In the same way we can define the macro temperature gradient $\nabla\theta_m$, at each point x_m and at each instant t, as the volume average of the microscopic temperature gradient $\nabla\theta_\mu$ defined at each point x_μ of the micro-scale domain and at each instant t

$$\nabla\theta_m(x_m,t) = \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla\theta_\mu(x_\mu,t)dV \quad (3)$$

Without loss of generality we can decompose the micro-scale displacement and temperature as

$$u_\mu(x_\mu,t) = \varepsilon_m(x_m,t)\cdot(x_\mu - x_g) + \bar{u}_\mu(x_\mu,t) \quad (4)$$

$$\theta_\mu(x_\mu,t) = \theta_m(x_m,t) + \nabla\theta_m(x_m,t)\cdot(x_\mu - x_g) + \bar{\theta}_\mu(x_\mu,t) \quad (5)$$

where $\bar{u}_\mu(x_\mu)$ and $\bar{\theta}_\mu(x_\mu)$ are respectively the displacements and the temperature fluctuations with respect to the average fields and x_g (the centroid of the micro-scale).

We also define periodic boundary conditions to be applied on the RVE displacements and temperature fluctuations field

$$\bar{u}_\mu(x_\mu^+,t) = \bar{u}_\mu(x_\mu^-,t)\ \forall\ pair\ \{x_\mu^+, x_\mu^-\} \in \partial\Omega_\mu \quad (6)$$

$$\bar{\theta}_\mu(x_\mu^+,t) = \bar{\theta}_\mu(x_\mu^-,t)\ \forall\ pair\ \{x_\mu^+, x_\mu^-\} \in \partial\Omega_\mu \quad (7)$$

being x_μ^+ and x_μ^- two opposite points on the RVE boundary $\partial\Omega_\mu$.

2.2 Solution of the thermal micro-scale BVP

Using the Fourier equation for heat transfer, the equilibrium of the micro-scale was achieved when the following condition is verified

$$\nabla\theta_m \cdot q_m = \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla\theta_\mu \cdot q_\mu dV \quad (8)$$

taking $\boldsymbol{k_i}$ as a component of conductivity matrix and q_i as a component of heat flux vector. We can defined q_i as

$$q_i = -\boldsymbol{k_i}\frac{\partial\theta}{\partial i}\ with\ (\mathrm{i} = \mathrm{x,y,z}) \quad (9)$$

2.3 Solution of the mechanical micro-scale BVP

For the mechanical phase, the Hill-Mendel Principle of Macro-Homogeneity [7,8] establishes that the macroscopic stress power, product of macro stress tensor σ_m and the macro strain rate $\dot{\varepsilon}_m$, must be equal to the microscopic stress power over the RVE averaged on the volume domain. Hence:

$$\sigma_m : \dot{\varepsilon}_m = \frac{1}{V_\mu}\int_{\Omega_\mu} \sigma_\mu : \dot{\varepsilon}_\mu dV \quad (10)$$

In order to obtain the strain field for the thermo-mechanical homogenization we need to add the contribution from the equilibrium of thermal RVE:

$$\varepsilon_{\mu,thermal} = \alpha(\theta_\mu - \theta_{amb}) \quad (11)$$

where α is the coefficient of thermal expansion, $\varepsilon_{\mu,thermal}$ is the thermal strain contribution and θ_{amb} is the ambient temperature. Thus, the total micro-scale strain can be obtained adding the mechanical strain part $\varepsilon_{\mu,mechanical}$

$$\varepsilon_\mu = \varepsilon_{\mu,mechanical} + \varepsilon_{\mu,thermal} \quad (12)$$

2.4 Micro to Macro transition

Following the achievement of the BVP for each physics, homogenized macroscopic stress tensor and macroscopic heat flux vector, we can also obtain the homogenized tangent operator and the macroscopic conductivity matrix.

The homogenized macroscopic stress tensor can be obtained as the microscopic stress field of the RVE averaged on the volume as

$$\sigma_m = \frac{1}{V_\mu}\int_{\Omega_\mu} \sigma_\mu(x_\mu,t)dV \quad (13)$$

Similarly, even the homogenized macroscopic heat flux vector q_m can be evaluated in the same way through the microscopic heat flux vector of the RVE:

$$q_m = \frac{1}{V_\mu}\int_{\Omega_\mu} q_\mu(x_\mu, t)dV \tag{14}$$

3. IMPLEMENTATION

The implementation of this formulation was based on the splitting of the homogenized problem into two sub-problems that are, every each time increment, uncoupled.
Like classical first order homogenization we assumed that at each integration point of the element of the macro-scale there was an associated RVE, in that case one for each physic. See [9,10] for the definition of the correct size of the RVE.

In this way, the first sub-problem was the thermal one and at this step the mechanical part was suspended. Then, the linear system of equations for the heat transfer was solved and the mechanical part was updated providing the true actual temperature. Sequent the thermal problem was stopped for solving the mechanical equilibrium, thus the stress tensor and the flux vector were found and the thermal part was updated.

The analysis has been performed using Kratos Multiphysics [11,12], a free open-source framework for the development of multidisciplinary solvers, developed at CIMNE, while pre and post-processing have been performed using GiD [13], also developed at CIMNE.

4. VALIDATION AND EXAMPLES

3.1 Benchmark

An analytical benchmark has been studied in order to validate the proposed formulation. The macro-scale geometry was a 2D beam (3000[mm] x 1000[mm]) and the micro-scale was a square of 1[mm] x 1[mm], 1.0e3 times smaller than the macro-scale. The structure was subjected to positive thermal load θ^+ in the upper-side and negative thermal-load θ^- in the down-side. Using a linear-elastic material for the micro-scale, the expected displacement, temperature and the stress/strain distribution were exactly the same as the analytical results. In order to resolve flexional problems with quadrilateral elements we have used a small displacement element modified by Simo, see[14]. After the multiscale analysis, a Direct Numerical Simulation (DNS) was performed with the purpose of verifying once again the formulation. We have also considered a granular geometry, as in Figure 2, for the micro-scale with two materials. An isotropic damage constitutive law was used imposing between the Coefficients of thermal Expansion (CTE), of the two materials, a ratio = 100 in order to appreciate the effective temperature dependent mechanical properties.

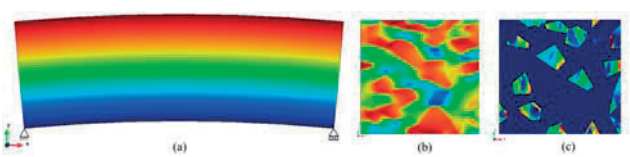

Fig. 2. (a) Temperature distribution on macro-scale, (b) Cauchy Stress in x direction, (c) damage distribution on micro-scale

From Figure 2 we can see how only the application of a thermal gradient can induce a mechanical reaction. In this case we can also see how the material having lower CTE (the blue one in Figure 2) shows a lower strain and it has not been damaged. The damage's distribution of the second material has been caused also by the constriction of the first undamaged material.

3.2 Pipe Section Analysis

As real structure simulation, we have decided to consider a pipe cross-section subjected to radial extended thermal load. The purpose of this analysis was the behavior assessment of an heat exchanger's pipe by means of the proposed simulation method. The macro-scale was made by ceramic material and the micro-scale was assumed as 1x1 cubes, with pholiedra volumes, composed by two materials (MAT_1: ρ=3200(kg/m^3), E=410(GPa), ν=0.14, K=125(W/mK), σ_y=460(MPa), CTE=4.5e^{-6}; MAT_2: ρ=2300(kg/m^3), E=150(GPa), ν=0.22, K=50(W/mK), σ_y=100(MPa), CTE =4.0e^{-6}).

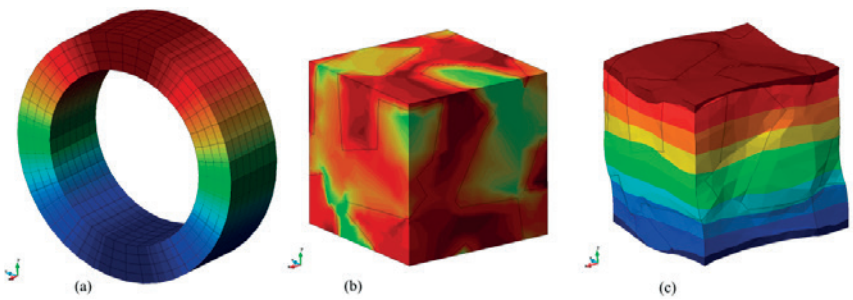

Fig. 3. (a) Temperature distribution on macro-scale, (b) Cauchy Stress in xx direction, (c) gradient temperature distribution on micro-scale.

In Figure 3, where the RVEs are referred to the upper side of the ring, we can observe the preserved periodicity of the displacements in the RVE where the non-homogeneous deformations are induced from the different properties of the material that compose the RVE. It is also possible to observe the different stress distributions that were induced exclusively by thermal gradient.

3. CONCLUSIONS

Thanks to the proposed formulation we are able to establish the homogenized thermo-mechanical properties of a generic macro-structure and also to evaluate the micro-scale response of a granular, or also more complex, geometry. The method has been tested simulating a section of a heat exchanger's pipe under radially depending temperature distribution load. The results of the final simulation denote how the formulation is able to reproduce the expected behavior of the structure. For this reason it can be also used to perform virtual simulations in cases where the experimental ones are difficult or even impossible to be used.

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