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Sensitivity of the thermomechanical response of elastic structures to microstructural changes

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ABSTRACT

This paper is focused on the analysis of the sensitivity of the thermomechanical response of a macroscopic elastic body to changes that occur at the microstructure. This problem is a key issue in material design.

The sensitivity analysis relies on an accurate determination of the effective properties of the heterogeneous material. These effective properties are determined by computational homogenization. And their sensitivities, with respect to the parameters defining the microstructure, are then computed.

For an efficient evaluation of the thermomechanical response, we propose to build response surfaces for the effective material properties. The surfaces are generated in an offline stage, by solving a series of homogenization problems at the microscale. In such a way, the fully online multiscale response analysis reduces to a standard problem at the macroscale. Thus, an important reduction in computational time is achieved, which is a crucial advantage for material design.

The capability of the proposed methodology is shown in light of its application to the design of a thermally-loaded structure with variable microstructure. Considerable improvements in the structural response are achieved.

1. Introduction

As stated by Torquato (2010), the deep knowledge of the sensitivity of the observable macroscopic response of a body to changes in the structure of its constituent material at one or more subscales is the holy grail of materials science. Traditionally, the engineers used to choose from a catalog the best material to build a structure or mechanism with a desired response. In recent years, thanks to the ever-growing power of computers and the maturity of Computational Multiscale Modeling (CMM), an alternative approach is emerging, specially for high-performance applications: the Materials by Design (MbD) approach (McDowell and Story, 1998). MbD consists in designing the structure of a material at a subscale in order to make this material (or the body made of this material) the best-suited for a specific application.

In general, the term subscale refers to a wide range of length scales, from atomistic or molecular to microscopic and mesoscopic, whenever the length scale be much smaller than the dimensions of the structure made of the considered material. This paper is focused on the design of heterogeneous materials, typically composites, by altering their structure at one (and only one) subscale where the material can still be assumed to be a continuum. For the sake of convenience, let us refer to the material at such scale as "microstructure".

Further, we are currently interested in "quantitatively characterized" materials (Kachanov and Sevostianov, 2005), those whose macroscopic or effective physical properties can be expressed as functions of identified microstructural parameters: e.g., fiber orientation in fiber-reinforced polymers (Lund and Stegmann, 2005), density and irregularity factors in materials with isolated inhomogeneities (Kachanov and Sevostianov, 2005; Tsukrov and Kachanov, 2000), size of particles or beads in coating of dental implants (Rungsiyakull et al., 2010; Chen et al., 2013).

From the computational point of view, MbD can be formulated as a structural optimization problem where the cost function is defined at the macrostructure level. The goal is to obtain the distribution of microstructures along the macrostructure domain providing the minimum cost. This approach has been addressed by Rodrigues et al. (2002) and Bendsøe and Sigmund (2003). The so-determined material can be seen as a functionally graded material (FGM) in the sense that the microstructure changes smoothly

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from point to point at the macroscale. Paulino et al. (2009) have studied the microstructural optimization problem for a FGM.

Based on this MbD paradigm, the key point for developing an admissible computational procedure relies on the concept of hierarchical optimization (Rodrigues et al., 2002): the microstructural design problem (the *inner problem*) is uncoupled from the problem of finding the minimum cost function at the macroscale (the *outer problem*). Then, the sensitivity analysis addressed in this work plays an extremely important role during the process of obtaining the minimum cost function of the outer problem.

In our case, the inner problem consists on determining the way the effective properties of quantitatively characterized materials depend on microstructural parameters. In order to solve this problem, recourse can be made to experiments (the most expensive option), homogenization techniques for specific materials having simple microstructural topologies like analytical solutions (Kachanov and Sevostianov, 2005; Tsukrov and Kachanov, 2000), the effective field methods of the Mori–Tanaka type and variational estimates of the Hashin–Shtrikman type, or numerical methods like computational homogenization (CH) (Rungsiyakull et al., 2010; Chen et al., 2013). CH, the most general approach, is preferred in this work.

Then, we proceed to solve the inner problem applying CH over a parameterized Representative Volume Element (RVE). In this way, we build a grid of points (*microparameters vs. homogenized property*) for each one of the independent tensorial components of the physical properties involved in a steady-state thermomechanical problem: the fourth-order elasticity tensor, the second-order thermal expansion tensor, and the second-order thermal conductivity tensor.

After that, recourse is made to the response surface methodology (RSM) in order to fit the grid points for each effective property by a polynomial function of the microparameters. Then, the sensitivity of such property to microstructural changes (i.e., its derivative with respect to the microparameters) is also a polynomial. Let us remark that, using RSM, we do not need either to interpolate a property when the microparameters do not coincide with grid points or to use numerical differentiation. Kamiński (2009) has presented a similar approach to evaluate the sensitivity gradients of the computationally-homogenized properties of random composites. He has considered as microparameter the randomness of the mechanical properties of the microcomponents, and has constructed a response function for each of them.

Regarding the computational cost, let us remind that the seek of the optimal macroscopic response of a structure uses to be a long iterative process. At each iteration, a multiscale problem has to be solved: given the distribution of the microstructure throughout the structure, we obtain the macroscopic distribution of the homogenized properties (solving the inner problem at each sampling point), and then we solve a standard structural problem (the outer problem) to obtain the corresponding macroscopic response. In this work, since the inner problem is solved in an offline way, the outer problem becomes the only online stage, making each iteration as expensive as the solution of a standard problem at the macroscopic scale, i.e., considerably cheaper than the solution of a multiscale problem. This is a major contribution of this paper to the MbD approach.

Further, by accounting for the thermal coupling, this work constitutes a step further in sensitivity analysis of purely mechanical multiscale problems (Fish and Ghouali, 2001; Kamiński, 2014).

Finally, as an example of application, the current technique of sensitivity analysis is applied to determine the effect of microstructural changes on the compliance of a thermally loaded structure made of a bi-material. As result, a considerable improvement of the compliance or the stiffness of the structure can be achieved.

2. The two-scale thermomechanical problem

Let us consider a body $\Omega \subset \mathbb{R}^{\dim}$, Fig. 1, undergoing a steady state thermomechanical loading process: the heat flux q^{wall} and the temperature T^{wall} are prescribed on the boundaries $\partial\Omega_q$ and $\partial\Omega_T$, respectively, while the traction $\mathbf{t}^{\text{wall}}$ and the displacement $\mathbf{u}^{\text{wall}}$ are prescribed on the boundaries $\partial\Omega_\sigma$ and $\partial\Omega_u$, respectively. Considering these boundary conditions, the sets of admissible temperature and displacement fields are

$$\mathcal{T} = \{T(\mathbf{X}) \,|T \in \mathcal{H}^1(\Omega) \text{ and } T = T^{\text{wall}} \text{ on } \partial\Omega_T\}, \tag{1}$$

$$\mathcal{U} = \{\mathbf{u}(\mathbf{X}) \,|\mathbf{u} \in \mathcal{H}^1(\Omega) \text{ and } \mathbf{u} = \mathbf{u}^{\text{wall}} \text{ on } \partial\Omega_u\}, \tag{2}$$

where $\mathcal{H}^1(\Omega)$ is the space of functions having square-integrable first derivatives. The spaces of admissible temperature and displacement variations are

$$\hat{\mathcal{T}} = \{\hat{T}(\mathbf{X}) \,|\hat{T} \in \mathcal{H}^1(\Omega), \text{ and } \hat{T} = 0 \text{ on } \partial\Omega_T\}, \tag{3}$$

$$\hat{\mathcal{U}} = \{\hat{\mathbf{u}}(\mathbf{X}) \,|\hat{u}_i \in \mathcal{H}^1(\Omega), \text{ and } \hat{\mathbf{u}} = \mathbf{0} \text{ on } \partial\Omega_u\}. \tag{4}$$

Then, the current macroscopic thermomechanical problem can be stated in the standard variational format as follows: find $T \in \mathcal{T}$ and $\mathbf{u} \in \mathcal{U}$ satisfying

$$\int_\Omega \mathbf{q}(T) \cdot \nabla_{\mathbf{X}} \widehat{T} \; \mathrm{d}V - \int_{\partial\Omega_q} q^{\text{wall}} \widehat{T} \; \mathrm{d}S = 0, \quad \forall \widehat{T} \in \hat{\mathcal{T}}, \tag{5}$$

$$\int_\Omega \boldsymbol{\sigma}(\mathbf{u}, T) \cdot \nabla^s_{\mathbf{X}} \hat{\mathbf{u}} \; \mathrm{d}V - \int_{\partial\Omega_\sigma} \mathbf{t}^{\text{wall}} \cdot \hat{\mathbf{u}} \; \mathrm{d}S = 0, \quad \forall \hat{\mathbf{u}} \in \hat{\mathcal{U}}, \tag{6}$$

where $\mathbf{q}$ is the macroscopic heat flux vector and $\boldsymbol{\sigma}$ is the macroscopic Cauchy stress tensor. Eq. (5) represents the steady-state heat balance equation in absence of internal heat source, while (6) is the momentum balance equation in absence of body forces and inertial terms.

The problem is completed by the constitutive laws for $\mathbf{q}$ and $\boldsymbol{\sigma}$ at any point $\mathbf{X} \in \Omega$, which are determined in this work from the analysis of the microstructure at this point.

Let the body have a heterogeneous microstructure that, at any point $\mathbf{X} \in \Omega$, is described by a Representative Volume Element (RVE), denoted Ω_μ, shown in Fig. 1. Points in Ω_μ are denoted $\mathbf{y}$. From now on, any quantity $(\cdot)$ described in the domain Ω_μ will be denoted as $(\cdot)_\mu$.

As stated in Appendix A, the macroscopic terms $\mathbf{q}$ and $\boldsymbol{\sigma}$ at $\mathbf{X} \in \Omega$ are defined by the homogenization formulas

$$\mathbf{q} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{q}_\mu \mathrm{d}V_\mu, \tag{7}$$

$$\boldsymbol{\sigma} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \mathrm{d}V_\mu, \tag{8}$$

where $|\Omega_\mu|$ is the volume of Ω_μ.

The constitutive response of the material components at the microscopic level is assumed to be known. Further, for the purpose of this work, the behavior of these microcomponents is assumed to be linear. In such a case, $\mathbf{q}_\mu$ and $\boldsymbol{\sigma}_\mu$ are respectively defined by the Fourier's and Hooke's laws:

$$\mathbf{q}_\mu = -\mathbf{k}_\mu \nabla_{\mathbf{y}} T_\mu, \tag{9}$$

$$\boldsymbol{\sigma}_\mu = \mathbf{C}_\mu \nabla^s_{\mathbf{y}} \mathbf{u}_\mu + \mathbf{d}_\mu \left(T_\mu - T^0\right), \tag{10}$$

where $\mathbf{k}_\mu$ is the thermal conductivity tensor, $\mathbf{C}_\mu$ is the elasticity tensor, $\mathbf{d}_\mu$ is the stress increment per unit temperature, all of them are