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Evaluation of stresses at the macro level based on computational micromechanics under finite strains

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ABSTRACT

A post-processing methodology to evaluate stresses at the macro level is presented. The methodology involves homogenization of a Representative Volume Element (RVE) or Unit Cell at the micro level by means of control nodes, with the consequence that numerical integration in the domain is not needed. This can be employed in cases of infinitesimal or finite strains; elastic, hyper-elastic or elastic-plastic materials under quasi-static processes. The paper shows that evaluation of stresses or material properties can be done in a RVE of simple shape, such as a prism, or in a RVE of complex shape, such as a truncated octahedron, using the proposed methodology. Use of the methodology is illustrated for cases under various conditions, for which comparison with independent results shows excellent agreement.

1. Introduction

Modeling of heterogeneous materials in terms of their microstructural characteristics, including volume fraction of each constituent, type and shape of inclusions, internal defects, is carried out at present by means of micro-mechanics (Nemat-Nasser and Hori, 1999). At least two scales are considered: a microscopic scale, in which details of the microstructure are represented, and a macroscopic scale in which an homogeneous material is considered to represent the heterogeneous properties by means of an equivalence. The region of heterogeneous material at the micro level necessary to capture the macroscopic behavior is taken as a Representative Volume Element (RVE) or a Unit Cell (UC), and analytical or numerical procedures are employed next to model the behavior at a macro level.

Computational Micro Mechanics (CMM) takes advantage of computational procedures to represent details of behavior which would not be accessible by analytical techniques (Zohdi and Wriggers, 2008); however, the cost of employing CMM in two-scale problems is the need to employ large computer resources, so that there are motivations to reduce computational cost whenever possible. Homogenization is a key ingredient in CMM modeling and improvements in this part of the process may yield considerable improvements in performance.

Homogenization is commonly employed in two steps of the modeling process: (a) the approximate solution of the boundary value problem by means of numerical methods; and (b) the post-processing of results to evaluate variables of interest at the macro level, such as stresses, elastic properties, etc. This work focuses on the second stage, i. e. the post-processing homogenization.

Homogenization post-processing may be oriented to compute stresses at the macro level based on micromechanics information. For small strains, the usual definition of macro stress is given by Nemat-Nasser and Hori (1999)

$$\boldsymbol{\sigma} = \frac{1}{V}\int_V \sigma^m \, dV \qquad (1)$$

where $\boldsymbol{\sigma}$ is the stress at the macro level; $\boldsymbol{\sigma}^m$ is the Cauchy stress in the RVE; and V is the volume of the RVE. Index m on top of a variable indicates that it belongs to the microscopic scale. A similar expression is employed for large strains, but integration is performed on the current configuration rather than the initial configuration, as discussed in de Souza-Neto and Feijóo (2008).

Within the context of small strain problems, the definition of the macroscopic stress emerges, after Gauss theorem is used, in the form

$$\boldsymbol{\sigma} = \frac{1}{V}\int_{\partial V} \mathbf{X} \otimes \mathbf{t} \, dS \qquad (2)$$

where ∂V is the boundary of the RVE; $\mathbf{X}$ is the coordinate of a point at ∂V; $\mathbf{t}$ is the traction vector in ∂V. The Cartesian components of the tensor product between two vectors $\mathbf{a}$ and $\mathbf{b}$ are

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written as

$$[\mathbf{a} \otimes \mathbf{b}]_{ij} = a_i b_j \tag{3}$$

Numerical implementation of Eq. (1) may be performed for infinitesimal strains, as explained by Barbero (2013), or for finite strains, as discussed by Abadi (2010) and Guo et al. (2014), among others.

Zahr-Viñuela and Pérez-Castellanos (2011) implemented two homogenization processes in the evaluation of macro stresses with finite strains, identified by the authors as "external measure" and "internal measure". Macroscopic stresses are evaluated in the first case by means of a force which is applied to a control node divided by the actual cross area. In the internal measure, the integral in Eq. (1) is approximated as

$$\sigma_{ij} = \frac{1}{v}\sum_{k=1}^{N}\sigma_{ij}^{k} v_k \tag{4}$$

where $\sigma^k{}_{ij}$ is the *ij* component of the microscopic Cauchy tensor at the *k* Gauss point in the element used in the discretization of the RVE; v_k is the weight factor for numerical integration (in terms of volume in the current configuration associated with Gauss point *k*) for a mesh with *N* Gauss points; and *v* is the volume in the current configuration of the RVE. All these variables depend on time.

An alternative formulation for finite strains has been presented by Dijk (2015) for computational homogenization based on virtual work and the Hill-Mandel Principle for periodic boundary conditions. Dijk employs Lagrange multipliers so that the stress measures at macro level become conjugate forces of the macro strains, or vice versa; this formulations is limited to RVE with periodic boundaries

The computation of macro stresses by means of a simple equation was reported by Li and Wongsto (2004), based on an energy equivalence between micro and macro scales (Hill-Mandel condition, see Nemat-Nasser and Hori, 1999). The studies in Li and Wongsto (2004) were applied to particle-reinforced composites, for RVE with shapes adequate to model different packaging configurations of particles. In the mid-1990s, Sun and Vaidya (1996) presented a similar idea but did not apply their methodology to complex shapes. In both Li and Wongsto (2004), and Sun and Vaidya (1996) the problem was formulated for infinitesimal strains.

A methodology for post-processing stresses is presented in this work for finite strains; this is abbreviated as PPM-FS (Post-Processing Methodology for Finite Strains) and should be applicable to linear as well as to nonlinear problems. The goal is to deal with UC problems with internal cracks in contact including material nonlinearity, i.e. plasticity or hyper-elasticity, and geometric nonlinearity. Complex RVE shapes are also of interest, such as a truncated octahedron.

Notice that economies in time and computational cost may be small with respect to the time required to solve the RVE; however, the present methodology avoids the complexities associated with numerical integration.

2. Post-processing methodology

2.1. Geometry of unit cells considered

Two types of UC shown in Fig. 1 are investigated in this work: A prism having a parallelogram with equal sides at the base; and the truncated octahedron. The latter case has been employed in the literature to represent particle-reinforced composites (Li and Wongsto, 2004), crystalline structures (Delannay et al., 2006), and open cell materials such as metal foam (Dharmasena and Wadley, 2002). In the present research both RVE geometries are used to model a composite material reinforced with unidirectional fibers.

Periodicity vectors, as described for example in Oller et al. (2005), are here employed to model the microstructure in a periodic material. Three periodicity vectors are used for a UC, as shown in Fig. 1: For the prismatic UC, these vectors are

$$\mathbf{P1} = lf\,\mathbf{i};\ \ \mathbf{P2} = 2b\,\mathbf{j};\ \ \mathbf{P3} = 2b\cos(\theta)\mathbf{j} + 2b\sin(\theta)\mathbf{k} \tag{5}$$

where *lf* is the fiber length; and θ and *b* are shown in Fig. 2a. The relation of θ and *b* with *Vf* (fiber volume fraction) may be written as

$$b = Rf\sqrt{\frac{\pi}{4Vf\sin(\theta)}} \tag{6}$$

were *Rf* is the fiber radius. For the truncated octahedron, the periodicity vectors are

$$\mathbf{P1} = lf_o\mathbf{i};\quad \mathbf{P2} = \frac{lf_o}{3}\mathbf{i} + lf_o\sqrt{\frac{2}{3}}\mathbf{j} + \frac{\sqrt{2}}{3}lf_o\mathbf{k};$$

$$\mathbf{P3} = \frac{2}{3}lf_o\mathbf{i} + \frac{2\sqrt{2}}{3}lf_o\mathbf{k} \tag{7}$$

where lf_o is the fiber length, computed in terms of length *le* shown in Fig. 2

$$lf_o = \sqrt{6}\,le;\quad \text{with}\quad le = Rf\sqrt{\frac{\pi\sqrt{3}}{8Vf}} \tag{8}$$

2.2. Periodic boundary conditions under finite strains

Periodic Boundary Conditions (PBC) have been described in the literature on computational micro-mechanics, such as Guo et al. (2007, 2014) and Abadi (2010), and were used in this work to represent a periodic composite at finite strains. Following the nomenclature adopted in Zahr-Viñuela and Pérez-Castellanos (2011), two points in a microstructure are identified as "corresponding points" if the position of one of them may be obtained as the position of the other one plus a linear combination of the periodicity vectors using integer coefficients. To illustrate the concept, periodicity vectors $\mathbf{P_1}$ and $\mathbf{P_2}$ are shown in Fig. 3. The points in pairs: (C_0; C_1), (C_0; C_2) and (C_0; C_3) are corresponding points.

The boundary conditions are relations involving the forces and displacements at the boundary of the cell (Guo et al., 2007, 2014). If the traction vector at a boundary point and its corresponding boundary point are $\mathbf{t}^+$ y $\mathbf{t}^-$ respectively, then the following condition should be satisfied at all boundary pairs of points

$$\mathbf{t}^+ = -\mathbf{t}^- \tag{9}$$

Assuming that the locations at a boundary point, in the actual configuration, are written as $\mathbf{x}^+$ and at its corresponding point as $\mathbf{x}^-$, then the condition

$$\mathbf{x}^+ - \mathbf{x}^- = \mathbf{F}(\mathbf{X}^+ - \mathbf{X}^-) \tag{10}$$

applies at all boundary points (Guo et al., 2014, Eq. (9)), where $\mathbf{X}^+$ and $\mathbf{X}^-$ are the locations of the points in the reference configuration; and $\mathbf{F}$ is the imposed macroscopic deformation gradient.

Eq. (10) is next written as a function of nodal displacements at the boundary in order to facilitate implementation in the general purpose finite element package ABAQUS (2009) by means of command termed ∗EQUATION. The deformation gradient can be written as

$$\mathbf{F} = \nabla\mathbf{U} + \mathbf{I} \tag{11}$$

where $\nabla\mathbf{U}$ is the macroscopic displacement gradient in the reference configuration; and $\mathbf{I}$ is the identity tensor. The components of operator ∇ are

$$[\nabla(\cdot)]_{ij} = \frac{\partial(\cdot)_i}{\partial X_j} \tag{12}$$