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A 3D computational homogenization model for porous material and parameters identification

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ABSTRACT

Based on the assumptions of periodicity and separation of two length scales, a 3D computational homogenization model is developed for porous material. The method is implemented based on the finite element method by assuming linear material behavior. Numerical examples show that the variation of pore geometry and spatial distribution will result in much higher level local stress concentration compared to the macroscale smeared out stress, apart from bringing the material properties in transition to transverse isotropy. The convergence studies and the comparison to the reference/analytical solution show that the linear computational homogenization is an effective method for modelling the linear elastic porous materials.

1. Introduction

Porous materials are of significant interest in many engineering applications such as the porphyrite and lamprophyre as high porosity ignites rock, aerated concrete and polyfoam, to name a few. For natural materials, the statistical information of pore structures, void ratio, void geometry and their spatial distribution can be used as the input parameters to analyze the material deformation. For artificial materials, such as polyfoam, the pore distribution can be optimized to improve the material performance and obtain the optimal techno-economy balance. Therefore, for both types of materials, there is a strong need to develop a numerical model for better prediction of the mechanical behavior. The mechanical behavior of porous materials is heterogeneous at various length scales. The microstructure is usually an assembly of complex geometry such as particulate or fibrous inclusions or voids. The material properties and morphology of the microstructure has a significant impact on the macroscopic behavior of the composite materials. The microstructural morphology refers to the shape, size and spatial distribution of the microstructural constituents. Determination of the macroscopic properties of composite materials is an essential problem in many engineering applications. Studying the relation between microstructure and the macroscopic properties not only allows to predict the behavior of the existing composite materials, but also provide a method to design the material microstructure with the desirable macroscopic properties.

The local degradation in the "micro"-structure accompanied by irreversible local geometrical changes [1,2] will result in a nonlinear macroscopic response. The characterization of such behavior by macroscopic closed-form constitutive laws is difficult, due to the complex mathematical model and high computational costs involved in identifying the design parameters [3]. Therefore, the need arises for a strong coupling between the evolving microstructure and the macroscopic response. Numerous modelling strategies have been developed to predict the relations between the microstructure and macroscopic properties in composite materials. The effective medium model is established by Eshelby [4] and further developed by Hashin and Shtrikman [5], Budiansky [6], Mori and Tanaka [7]. The effective medium model is an analytical or semi-analytical method. The macroscopic properties are derived by solving the boundary value problem for a spherical or ellipsoidal inclusion in an infinite matrix. The self-consistent approach of Hill [8], Christensen and Lo [9] is an extension of the effective medium model. The variational bounding method of Hashin and Shtrikman [10], Castañeda and Suquet [11] provide upper and lower bounds for macroscopic properties. Another homogenization approach is asymptotic homogenization method of Bensoussan et al. [12] and Sánchez-Palencia [13]. To generate the complex microstructure and to develop the computational methods, the

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unit cell methods by Nakamura and Suresh [14] and Van der Sluis et al. [15] have been widely used. Early models employ hierarchical multiscale approaches based on analytical or semi-analytical homogenization. However, all the formulations are difficult to extend to the non-linear behavior and coupled field interactions. Recently a multiscale computational homogenization technique has been developed. The homogenization approach have been initiated by Suquet [20], Guedes and Kikuchi [21], Terada and Kikuchi [22], Ghosh et al. [23,24] and developed by Smit et al. [25], Miehe et al. [26], Michel et al. [27], Terada and Kikuchi [28], Ghosh et al. [29], Kouznetsova et al. [30], and Miehe and Koch [31]. A popular homogenization approach is the semi-concurrent FE^2 method [16], which employs Representative Volume Elements (RVEs). The FE^2 approach has been developed inter-alia for non-linear materials [17], higher order models [18] and coupled (thermo-mechanical) problems [19]. In the homogenization method it is not required to estimate constitutive equations at the macroscale, instead the stress–strain law is computed at the critical material points. Existing works on multiscale methods are limited mainly based on the FEM [46,52,53], or coupled FE-molecular dynamics [47,54,56–63,75] techniques. It would be interesting in the future to explore the potential of other novel numerical methods to deal with the moving boundary problems such as meshless methods [39–45,48–51,64–71] and other types of discontinuum based methods [55,72–74].

Past work on the computational homogenization for heterogeneous materials normally assumes the media to be continuous or includes 2D microcracks (line segments) or 3D initial damage tensors, which does not include the volume loss. In otherwords, the void structures were considered explicitly to include 3D microstructural details of the void geometry. In this paper, the computational homogenization is employed and extended for porous materials. The motivation of the present work is to include the 3D porous structures at the microscale model for porous materials, considering the statistical geometry features of the pores. Our interest is to estimate the change in the bulk material properties with the design parameters of pore structures.

The content of the paper is outlined as follows. In Section 2, the homogenization model is described. The implementation issues of the model in ABAQUS are detailed in Section 3. Section 4 shows the performance the model and the effects of microscale porous structures on material parameters at macroscale through two numerical examples. The paper is concluded in Section 5 with the suggested topics for future studies.

2. Computational homogenization of porous material

2.1. Assumptions of the model

The porous material is assumed to be macroscopically homogeneous and microscopically heterogeneous when the microstructure consists of inclusions, grains, interfaces and cavities. Most computational homogenization approaches make two assumptions [32], as illustrated in Fig. 2.1.

The first assumption is the separation of the lengths scale into micro and macro-scales. The microscale length is assumed to be much larger than the molecular dimensions, so that a continuum approach is justified for the microstructural constituents. And the microscale length is much smaller than the macroscale length, so that the microstructural heterogeneities can be reflected. Therefore,

$$l_{molecular} \ll l_{micro} \ll l_{macro} \tag{1}$$

where $l_{molecular}$ is the length at nanoscale; l_{micro}, l_{macro} are the length of micro and macro-scales, respectively.

The second assumption is the periodicity of the microstructures. Most of the homogenization approaches assume that the microstructures vary periodically over the whole macroscopic domain. But in the computational homogenization approach, the microstructures are different corresponding to different macroscopic points and repeat themself in the vicinity of different macroscopic points, such as the microstructures of M and N in Fig. 2.1. According to the periodicity assumption, it is natural to anticipate the periodic variation of the properties and response of the porous material. Two different scales $\boldsymbol{x}$ and $\boldsymbol{y}$, associated respectively to the material properties and responses at the macroscale and microscale, are assumed. The relation between the spatial microscale and macroscale coordinates is as below:

$$y_i = \frac{x_i}{\varepsilon} \tag{2}$$

where x_i ($i = 1,2,3$) are the macroscale coordinates; y_i are the microscale coordinates; $\varepsilon \ll 1$ is a scale factor between the macroscale and the microscale.

By means of the coordinates defined above, the periodicity assumption of the material properties and responses on the microscale can be expressed as given below:

$$f^{\varepsilon}(x_i) \cong f(x_i, y_j) = f(x_i, y_j + KY_j) \quad K = 1,2\ldots \tag{3}$$

where $f^{\varepsilon}(x_i)$ is the properties or response function of the material, the superscript ε indicate that the function $f^{\varepsilon}(x_i)$ registers all the properties or response over the microscale and Y_j is the period of the microstructure.

2.2. The governing equations

Consider a problem domain Ω^{ε} with boundary Γ^{ε} composed of heterogeneous linear elastic material. The microstructure of Ω^{ε} consists of periodically distributed representative volume element associated with smaller domain denoted as Θ. The governing equation of linear elastic problem may be expressed based on the Einstein's convention for tensor notation [33] as

$$\sigma^{\varepsilon}_{ij,x_j} + b_i = 0 \quad \text{in } \Omega^{\varepsilon}, \tag{4}$$

$$\sigma^{\varepsilon}_{ij} = L^{\varepsilon}_{ijmn} e^{\varepsilon}_{mn} \quad \text{in } \Omega^{\varepsilon}, \tag{5}$$

$$e^{\varepsilon}_{mn} = \frac{1}{2}(u^{\varepsilon}_{m,x_n} + u^{\varepsilon}_{n,x_m}) \quad \text{in } \Omega^{\varepsilon}. \tag{6}$$

The displacement and traction boundary conditions applied to the domain are

$$u^{\varepsilon}_i = \overline{u_i} \quad \text{in } \Gamma^{\varepsilon}_u, \tag{7}$$

$$\sigma^{\varepsilon}_{ij} n_j = \overline{t_i} \quad \text{in } \Gamma^{\varepsilon}_t, \tag{8}$$

where the subscript $i, j, m, n \in \{1,2,3\}$, $\sigma^{\varepsilon}_{ij}$, e^{ε}_{mn}, u^{ε}_i, L^{ε}_{ijmn} are the components of stress, strain, displacement and constitutive tensor respectively, b_i is the body force vector, $\overline{u_i}$, $\overline{t_i}$ are the prescribed displacement and traction, Γ^{ε}_u, Γ^{ε}_t are the displacement and traction boundary, n_j is the outward normal vector of the boundary. The subscript x_i, y_i refer to the spatial coordinates of macroscale and microscale. The spatial gradient operator in the governing equations is applied as

$$f^{\varepsilon}_{,x_i} = \frac{\partial f}{\partial x_i} + \frac{1}{\varepsilon}\frac{\partial f}{\partial y_i} \quad f^{\varepsilon}_{,y_j} = \frac{\partial f}{\partial y_i}. \tag{9}$$

2.3. The asymptotic expansion to approximate the displacement field

Assuming the material responses of the macroscale $\boldsymbol{x}$ and the microscale $\boldsymbol{y}$ are related, the displacement field can be approximated by using the asymptotic expansions of ε as in [34] that