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Multi-scale computational homogenization of heterogeneous materials

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ABSTRACT

The mechanical response of a heterogeneous medium results from the interactions of mechanisms spanning several length scales. The computational homogenization method captures direct influence of underlying constituents and morphology with a numerically efficient framework. This study reviews the performance of first order computational homogenization technique with a flat punch indentation problem. Results obtained are benchmarked against those using direct numerical simulations (DNS) with full microstructural details. It is shown that the computational homogenization method is able to capture structural response adequately, even for constituent materials with nonlinear behavior. However, the first order computational homogenization method becomes problematic when localized macroscopic deformation occurs. In this context, some recent trends addressing the issues are discussed.

1 INTRODUCTION

Multi-phase or heterogeneous materials, boasting enhanced mechanical properties compared to the respective constituents, have been the subject of ever increasing interest in recent years. Typical examples include composites, alloys, polycrystals, and metal foams.

The effective material behavior of a heterogeneous material, typically required for engineering design purposes, is highly dependent on the characteristics of the micro-constituents e.g. size, shape, spatial distribution, constitutive relations, and interface properties. Consequently, it is essential to develop a quantitative link between the macro variables and its microstructural counterpart. The task can be achieved by conducting experiments on material samples. But, from economic viewpoint, this approach becomes intractable when many possible combinations of constituents, volume fractions, and load paths have to be considered. As an alternative, Direct Numerical Simulation (DNS) can be performed by incorporating full microstructural details accompanied with a mesh discretization of sufficient resolution. However, it is seldom practical for typical engineering problem due to its inherent high computational cost. To this end, several homogenization methods have been proposed in literature e.g. rule of mixture, self-consistent approaches, asymptotic homogenization theory, and first-order computational homogenization.

The objective of this study is to elaborate on the performance of the first-order computational homogenization technique through a flat punch indentation problem on a perforated plate. Theoretical aspects of this approach are presented in Section 2 and its applicability demonstrated in Section 3.

2 FIRST-ORDER COMPUTATIONAL HOMOGENIZATION

The first-order computational homogenization scheme can be decomposed into four steps: (i) identification of a representative volume element (RVE); (ii) macro to micro transition and solution of boundary value problem (BVP) at the micro scale; (iii) micro to macro transition; and (iv) solution of BVP at the macro level. These steps are illustrated in Figure 1 and detailed in the following sections.

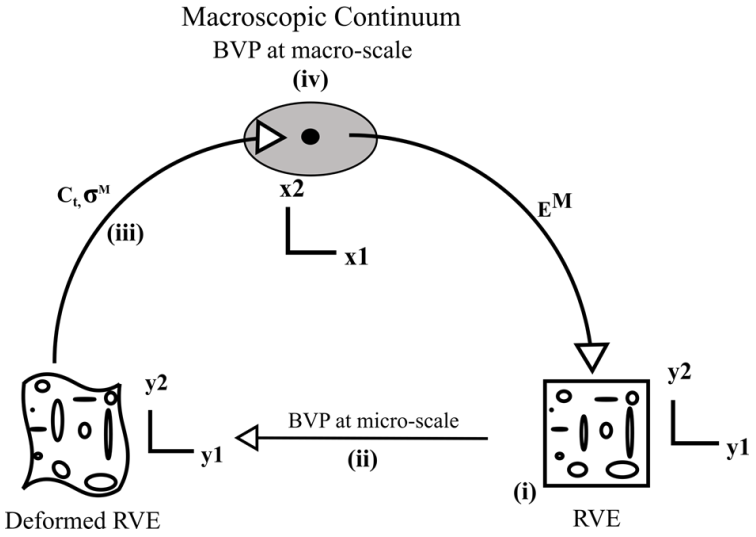

Figure 1. First-order computational homogenization scheme

2.1 Identification of RVE

The representative volume element or RVE can be defined as a sample that reflects the material microstructure, and from which effective material properties can be estimated with desired level of precision. The size of the RVE should be large enough to contain sufficient number of inclusions so that the extracted overall properties are independent of the applied boundary conditions and at the same time sufficiently smaller than the macroscopic characteristic length scale for the continuum assumptions to be valid at the macro level. This condition is known as the principle of separation of scales. In case of a periodic medium, the unit cell can be taken as the representative of the whole domain.

2.2 Macro to micro transition

The objective of this step is to formulate a boundary value problem on the RVE based on macroscopic field values. The local displacement field (**u**) inside the RVE can be decomposed as:

$$\mathbf{u} = \mathbf{E^M}.\mathbf{y} + \mathbf{w} \qquad (1)$$

where **w** is a fluctuation field due to presence of the heterogeneities, **y** represents the local coordinates (see Fig 1) and $\mathbf{E^M}$ is the macroscopic strain tensor.

The kinematic coupling between these two scales is achieved by constraining the volume average of local strain field within the RVE to be equal to $\mathbf{E^M}$, i.e. the volume average of fluctuation field **w** has to vanish. In literature, this requirement is commonly achieved by having periodic boundary conditions for the RVE, which have been shown to provide better estimates for the apparent properties, with smaller RVE sizes. Furthermore, the periodic boundary conditions ensure (i) identical shapes of the opposite edges by imposing equal fluctuation values on analogous points of the RVE; and (ii) stress continuity across the boundaries by satisfying anti-periodic tractions on opposite edges.

2.3 Micro to macro transition

The Hill-Mandel condition, which requires an equivalence of power density between the two scales, is imposed to effect the micro to macro transition. Following this condition, the macroscopic stress tensor ($\boldsymbol{\sigma}^{\mathbf{M}}$) is defined as the volume average of the local stress field (**σ**):

$$\boldsymbol{\sigma}^{\mathbf{M}} = \frac{1}{V}\int_{RVE} \boldsymbol{\sigma} dV \qquad (2)$$

In this study, the tangent stiffness matrix ($\mathbf{C_t}$), defined as $\Delta\boldsymbol{\sigma}^{\mathbf{M}} = \mathbf{C_t}\,\Delta\mathbf{E}^{\mathbf{M}}$, is computed by performing static condensations on structural stiffness matrix of the RVE to improve computational efficiency over the conventional perturbation method (Kouznetsova 2002).

2.4 Boundary value problem at macro-scale

The macro level problem is solved in the commercial software ABAQUS with the following sequence: (i) discretize the macrostructure and assign RVE at each integration points; (ii) compute element stiffness matrices and residual nodal force vectors by using the tangent stiffness, and macroscopic stress tensor provided by RVE analyses, and (iii) check for convergence.

3 EXAMPLE

3.1 Flat punch indentation

This section considers the plane strain flat punch indentation on a perforated plate as illustrated in Figure 2a. The plate comprises of 200 by 40 periodic unit cells. Two different morphologies with the same volume fraction (30%) of voids are considered, as shown in Figure 2b. Displacement boundary condition is applied on the plate surface corresponding to the location of indenters. The matrix material follows an isotropic von Mises plasticity model:

$$\sigma_y = \sigma_o + h\,(\varepsilon_p)^n \qquad (3)$$

with initial yield strength (σ^o) = 400 MPa, hardening modulus (h) = 2 GPa, and n = 0.5. The effective plastic strain is denoted as ε_p. Other material properties of the matrix include: elastic modulus (E) =200 GPa and Poisson ratio (υ) = 0.3.

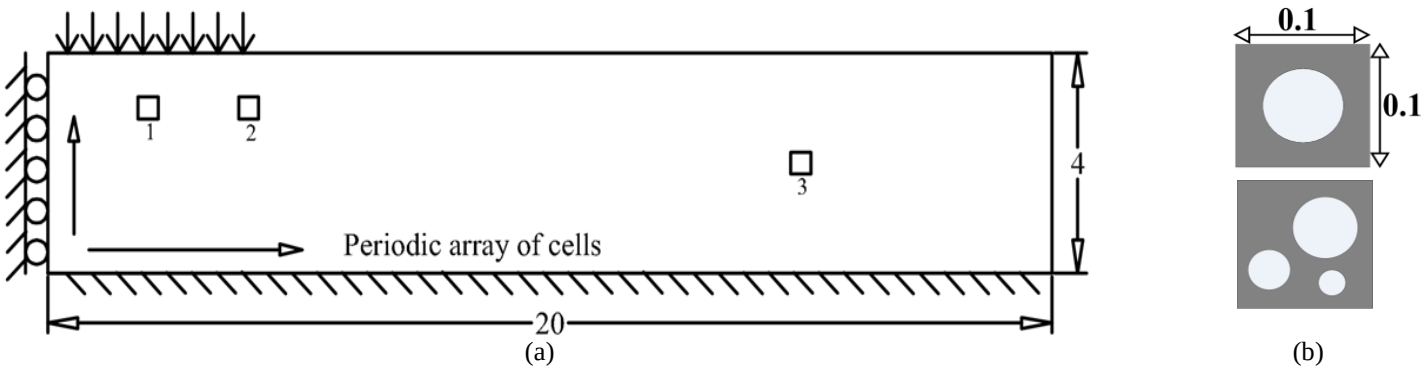

Figure 2. (a) Flat punch indentation of perforated plate. (b) Two different RVEs with same void volume fraction considered

3.2 Results and discussions

The problem is solved using: (i) direct numerical simulation (DNS), and (ii) first-order computational homogenization. In Figure 3, the indentation load (P) vs indentation depth (δ) graphs are presented for the two morphologies considered. From this figure, it can be observed that the mechanical behaviour of the plate is well approximated by the first-order computational homogenization technique. Furthermore, the computational cost is reduced significantly.

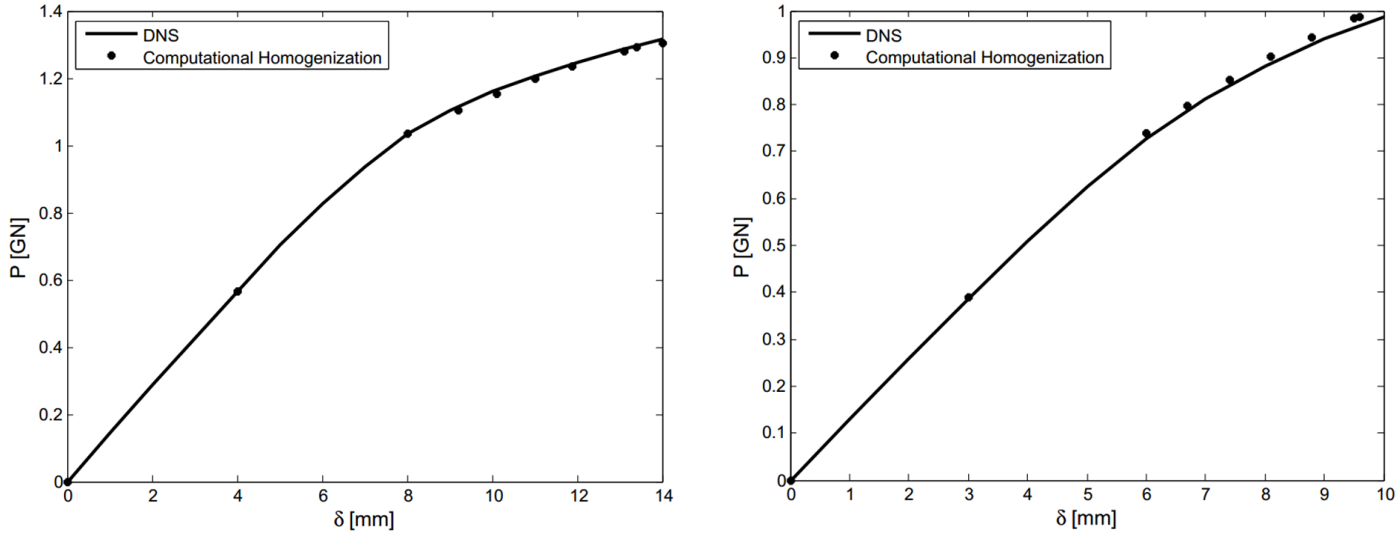

Figure 3. P- δ response of the plate composed of RVEs with one void (left), and three voids (right)

Figure 4 depicts contour plots of the S22 stress component in the deformed RVE at three locations of the macrostructure (see Fig 2). As observed, the deformed shape strongly depends on the macroscopic strain components at the respective locations. Also, maximum stress values inside the RVEs are observed to be much higher than that of homogenized macrostructure due to the stress concentration effect around the hole. For the same reason, macro stress-strain fields obtained from direct numerical simulations and the computational homogenization approach are not directly comparable. However, if fields within the individual cells of the plate are represented by a constant value i.e. the volume average, then S22 contour plots resulting from both approaches exhibit good match, as illustrated in Figure 5.

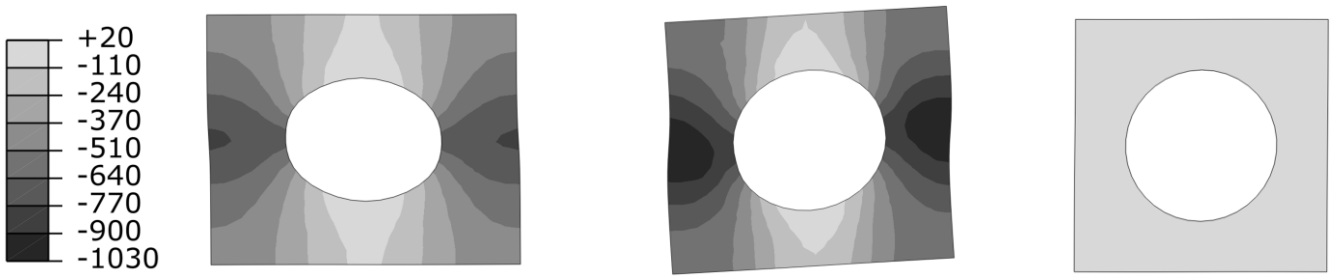

Figure 4. Contour plots for S22 (MPa) inside the deformed RVE at locations 1,2, and 3 in Fig 2a.

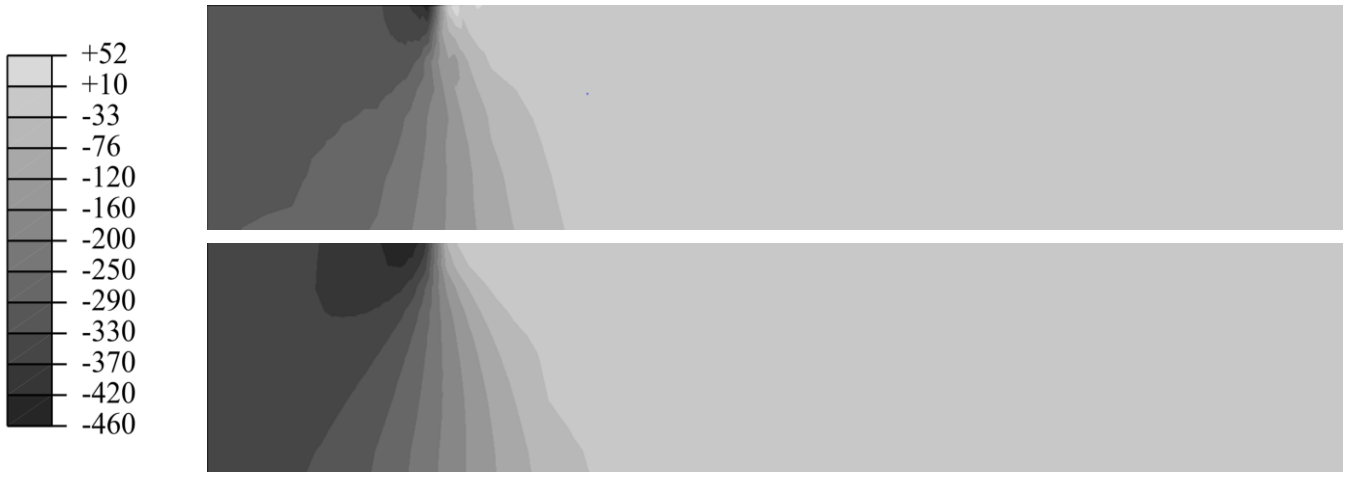

Figure 5. Contour plots for S22 (MPa) obtained from multi-scale computational homogenization (top), and direct numerical simulation (bottom), at the indentation depth of 0.014 m.

4 REMARKS

Multi-scale computational homogenization methods have become increasingly popular with advances in computational resources. These methods do not make any constitutive assumptions at the macro scale. Instead, numerical stress-strain relationships are extracted on the fly at various materials points by solving the RVE boundary value problem. This approach can easily be extended to nonlinear cases; incorporating the effects of large displacements, large rotations, and nonlinear history dependent micro-constituent material behavior. However, because of the inherent quadratic nature of the micro-macro concurrent coupling strategy, it is still computationally expensive. Nevertheless, this concern can be mitigated by making use of parallel computation (Feyel & Chaboche 2000). Despite overall success, this technique suffers from a few limitations e.g. macroscopic localization problems and structural size effects cannot be modeled properly. In this context, extensions of classical homogenization methods have emerged e.g. second-order computational homogenization (Kouznetsova 2002). These methods rely on introduction of higher order gradients to capture the rapid fluctuations within RVE.

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