Generalized micro-to-macro transitions of microstructures for the first and second order continuum

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Abstract

This paper deals with the first-order and second-order computational homogenization of a heterogeneous material undergoing small displacements. Typically, in this approach a representative volume element (RVE) of nonlinear heterogeneous material is defined. An a priori given discretized microstructure is considered, without focusing on detailed specific discretization techniques. The key contribution of this paper is the formulation of equations coupling micro- and macro-variables and the definition of generalized boundary conditions for the microstructure. The coupling between macroscopic and microscopic level is based on Hill's averaging theorem. We focus on deformation-driven microstructures where overall macroscopic deformation is controlled.

Keywords: Computational homogenization; Microstructures; Elastic–plastic composite

1. Introduction

A wide range of materials produced by industry, as well as natural materials, are heterogeneous at a certain scale of observation. The macroscopic (equivalent) properties of a heterogeneous material should describe the essence of microstructural response. They must be independent of its macrostructural loads or geometry. The micro-to-macro transitions have to be consistent with basic principles of continuum mechanics, i.e. they are subjected to principles of conservation of mass, momentum, energy, and to the Clausius–Duhem inequality [1].

A comprehensive review of the overall properties of heterogeneous materials is provided by [2,3]. Equivalent material properties are obtained as a result of analytical or semi-analytical solution. In recent years, a promising alternative approach has been developed, i.e. computational homogenization [4]. This micro–macro modelling procedure does not lead to closed-form constitutive relations, but computes on-line the strain–stress relationship at a selected point with attributed detailed microstructure assigned to that point [4]. This approach does not require any constitutive assumption on the macro level and enables the incorporation of nonlinear geometric and material equations [5]. The computational homogenization analysis is possible for any discretization technique in space and time.

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2. First-order computational homogenization

To couple the micro- and macro-strain tensors we define overall macro strain $\bar{\varepsilon}$ as a volume average of microstructural strain tensor $\boldsymbol{\varepsilon}$:

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_{v} \boldsymbol{\varepsilon}\, \mathrm{d}V = \frac{1}{V}\int_{\boldsymbol{\Gamma}} \mathbf{n} \otimes \mathbf{u}\, \mathrm{d}\Gamma \tag{1}$$

where $\mathbf{u}$ is displacement vector and $\mathbf{n}$ is the outer normal vector of the representative volume element (RVE) This relation is valid only if the following boundary condition is fulfilled:

$$\int_{\boldsymbol{\Gamma}} \mathbf{n} \otimes (\mathbf{u} - \bar{\varepsilon} \cdot \mathbf{x})\, \mathrm{d}\boldsymbol{\Gamma} = 0 \tag{2}$$

which forces RVE boundary to deform on average according to the prescribed strain $\bar{\varepsilon}$. The relation for macroscopic stress tensor $\bar{\boldsymbol{\sigma}}$ is defined in terms of micro stress $\boldsymbol{\sigma}$ as

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_{V} \boldsymbol{\sigma}\, \mathrm{d}V = \frac{1}{V}\int_{\boldsymbol{\Gamma}} \mathrm{x} \otimes \mathrm{t}\, \mathrm{d}\boldsymbol{\Gamma} \tag{3}$$

The average microscopic stress work has to be equal to the local macroscopic stress work, thus an additional boundary condition has to be satisfied:

$$\int_{\Gamma} \mathbf{t} \cdot (\mathbf{u} - \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x}) \, \mathrm{d}\boldsymbol{\Gamma} = 0 \tag{4}$$

Summarizing, rewriting Eqs. (2) and (4) gives us a generalized boundary condition. Applying this formulation, particular classical boundary conditions are included as special cases, i.e. linear displacements, constant tractions and periodic displacements. We note that these equations are consistent with the deformation-driven approach.

The first-order computational homogenization strategy provides a way to determine the macroscopic response of a heterogeneous material with an accurate account for microstructural characteristics [4]. Despite numerous attractive characteristics, there are some limitations. One of them is that a microstructural length scale must be negligible in comparison with a macrostructural characteristic length. Changing the scale of the entire macrostructure must lead to identical results and, if we change micro the scale of RVE, the average micro strain and stress must not change, see Eqs. (1) and (3).

3. Second-order computational homogenization

The definitions of macroscopic strain and stress tensors for second-order homogenization consistent with prescribed deformation and Hill's theorem yield Eqs. (1) and (3). The relation between the macroscopic second gradient of displacement $\bar{\boldsymbol{\eta}}$ and microscopic variables which do not lead to higher-order boundary conditions is based on averaging the relation betwen macro and micro quantities:

$$\mathrm{grad}\mathbf{u} = \bar{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\eta}} \cdot \mathrm{x} \tag{5}$$

Multiplying Eq. (5) by the position vector $\mathbf{x}$ and scaling by the RVE volume leads to an additional static boundary condition in terms of displacements:

$$\begin{aligned} \bar{\boldsymbol{\eta}} : \int_{V} (\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{1} + \mathbf{x} \otimes \mathbf{1} \otimes \mathbf{x} + \mathbf{1} \otimes \mathbf{x} \otimes \mathbf{x}) \, \mathrm{d}V \\ = \int_{\Gamma} \mathbf{n} \otimes \mathbf{u} \otimes \mathbf{x} \, \mathrm{d}\boldsymbol{\Gamma} \end{aligned} \tag{6}$$

which forces the RVE boundary to deform on average according to the prescribed second gradient of displacements $\bar{\boldsymbol{\eta}}$. We define the higher-order stress:

$$\bar{\boldsymbol{\tau}} = \frac{1}{V} \int_{V} (\mathbf{1} \otimes \mathbf{x} + \mathbf{x} \otimes \mathbf{1}) \cdot \boldsymbol{\sigma} \, \mathrm{d}V = \frac{1}{2V} \int_{\Gamma} \mathbf{x} \otimes \mathbf{x} \otimes \mathrm{t.} \, \mathrm{d}\boldsymbol{\Gamma} \tag{7}$$

This relation satisfies the Hill averaging theorem if an additional condition boundary has the form:

$$\int_{\Gamma} \mathrm{t} \cdot (\mathbf{u} - \bar{\boldsymbol{\varepsilon}} \cdot \mathrm{x} \; - \frac{1}{2} \bar{\boldsymbol{\eta}} : \mathrm{x} \otimes \mathrm{x}) \, \mathrm{d}\boldsymbol{\Gamma} = 0 \tag{8}$$

Summarizing, Eqs. (2) and (6) are boundary conditions enforcing the deformation of the RVE boundary on average according to the prescribed strain and second gradient of displacements. Equation (8) ensures that local macroscopic stress work is equal to microscopic stress work. By considering higher-order deformation and stress tensors the second-order homogenization approach deals with the microstructural size in a natural way. Thus, the size effect is taken into account. We note that this approach preserves the microstructural RVE problem as a classical boundary value problem, while on macroscopic level the higher-order continuum model is applied [4].

4. Computational aspects

It can be noted that a multiscale algorithm is parallel by its nature. All RVE calculations for one iteration can be preformed at the same time. This gives the motivation to develop a parallel implementation. The boundary value problem on the macro and micro scale was discretized by use of the finite element method. It can be shown that the overall stress and tangent moduli of microstructure may be computed exclusively in terms of discrete forces and stiffness properties of boundary. Incorporated by a dual Lagrangian multiplier method [2,5], the boundary conditions of the RVE generate an algorithm for finding equilibrium states and overall properties of microstructures.

5. Example

The application of the formulation outlined above is demonstrated by a numerical example. A simple constitutive response for the constituents of the microstructure is used, i.e. isotropic J2 plasticity with linear isotropic hardening. The elastic microstructural constituents are described by Hooke's equations. The scheme of macrostructure and two microstructures *a* and *b* are shown in Fig. 1. Only displacement boundary conditions are applied to macrostruture and load was displacement controlled. It was assumed that the microscale characteristic size is small compared with macroscale characteristic size. So that first-order computational homogenization was applied. In Fig. 2 the equilibrium paths for different micro-to-macro transitions and RVE geometries are shown. The homogeneous

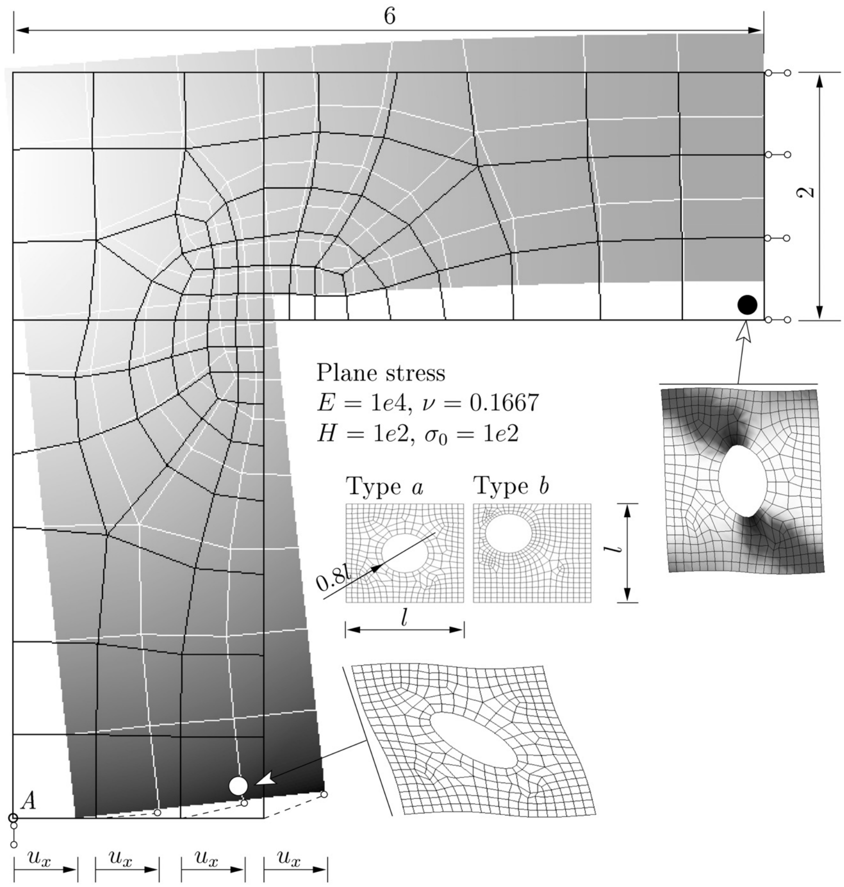

Fig. 1. Deformation of macrostructure and distribution of equivalent plastic strain in deformed RVE with periodic boundary condition.

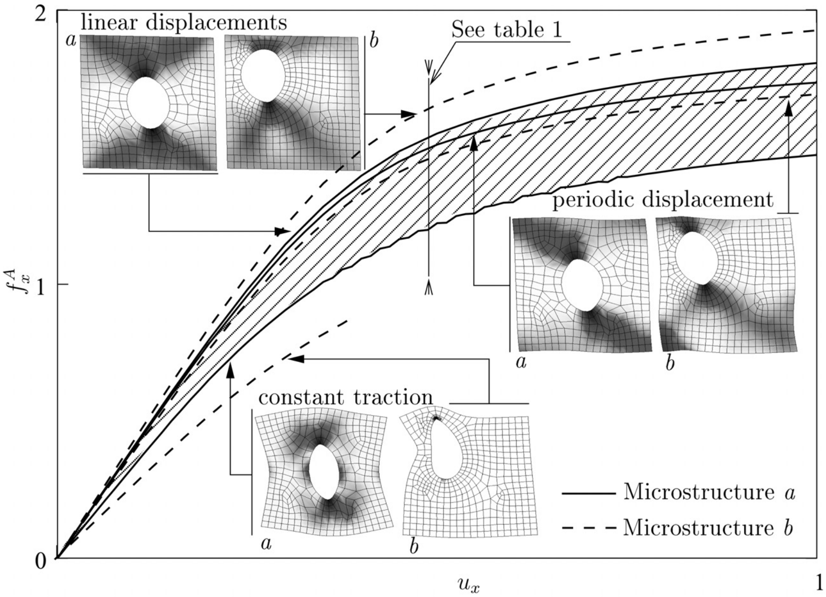

Fig. 2. Equilibrium paths and distribution of equivalent plastic strain on deformed RVE for three classical micro-to-macro transitions.

Table 1

Horizontal nodal force f_x at point A for horizontal displacement $u_x = 0.5$ (see Fig. 1)

	fAx, Microstructure a	fAx, Microstructure b	%
Displacement b.c.	1.55	1.66	6.6%
Periodic b.c.	1.51	1.47	2.6%
Traction b.c.	1.22	not converged	–

displacement and stress boundary conditions provide the upper and lower bounds of the response. The solution of periodic deformation lies between them. Table 1 summarizes the macro displacements for different tests, and demonstrates the inability of stress and displacement boundary conditions to capture a periodic composite.

6. Conclusions

A computational homogenization concept for heterogeneous materials undergoing small deformations has been developed. Generalized boundary conditions have been formulated for deformation driven microstructure. An example has been presented, which covers elastic-plastic microstructures of simple geometry and macrostructure response for first-order continuum. The implementation of algorithm for second-order continuum is currently developed.

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References

[1] Eringen AC. Mechanics of Continua. New York: John Wiley & Sons, 1967.
[2] Nemat-Nasser S, Suresh S. Micromechanics: Overall properties of Heterogenous Materials. Amsterdam: Elsevier, 1993.
[3] Strzelecki T. Mechanics of Heterogenous Media, Homogenization Theory (in Polish). Wrocław: Dolnośląskie Wydawnictwo Edukacyjne, 1996.
[4] Kouznetsova VG. Computational Homogenization for the Multi-scale Analysis of Multi-scale and Multi-phase Materials. Eindhoven: Eindhoven University of Technology, 2002.
[5] Miehe C, Koch A. Computational micro-to-macro transitions of discretized microstructures undergoing small strains. Arch Appl Mech 2002;72:300–317.