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COMPUTATIONAL ALGORITHM FOR HOMOGENIZED COEFFICIENTS OF HYPERELASTIC HETEROGENEOUS MATERIALS UNDERGOING LARGE DEFORMATIONS*

Vladimír Lukeš, Eduard Rohan, Robert Cimrman

Abstract

This article deals with an algorithm for numerical modelling of hyperelastic heterogeneous materials undergoing large deformations. The microstructure of these materials is changing (deforming) during a loading process, the changes in the microstructure depend on macroscopic deformations. To compute macroscopic responses, we must know material stiffness parameters and stresses in the heterogeneous structure. These effective parameters are obtained by solving microscopic problems. The number of microproblems is enormous, because in each iteration step (due to geometrical and material nonlinearities) it is needed to evaluate the effective material parameters in each macroscopic quadrature point. To reduce a computational time a parallel algorithm is presented.

1. Introduction

The problem of computing large deformations in heterogeneous media is characterised by non-uniform change in microstructure, the macroscopic properties depend on the spatial position. Starting with perfect periodic distribution of heterogenities in the reference state, due to nonuniform deformation the material becomes functionally graded. This results in a sequence of macroscopic and local microscopic problems. The assumption of periodicity in the microstructure is crucial for the application of the presented homogenization method.

If we consider large deformations, the mathematical model becomes nonlinear. For obtaining numerical solutions it is needed to linearize the model and solve it iteratively. For linearization the incremental updated Lagrangian (UL) formulation is employed, cf. [4].

2. Homogenized model

Assuming periodic heterogenities and existence of the representative volume element at the microscopic level, we apply the two scale method of homogenization ([4], [1], [6]) to derive effective material parameters at the macroscopic level. The periodic representative cell consists, in our case, of an hyperelastic matrix with an incompressible or compressible inclusion, see Fig. 1. We consider two scales, the

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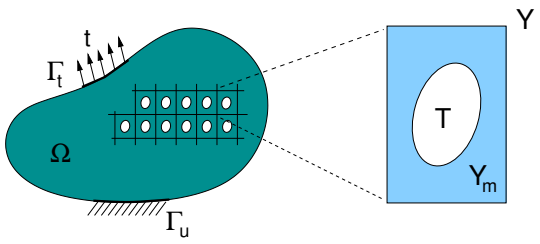

Fig. 1: *Macro and micro domain.*

macroscopic scale (associated with the macroscopic coordinates x) and the *microscopic scale* (y coordinates). These two scales are related by a non-dimensional parameter ε

$$y = x/\varepsilon, \quad \varepsilon > 0. \tag{1}$$

In the homogenization process, we assume that the heterogenities are very small and we take $\varepsilon \longrightarrow 0_+$. We assume the locally periodic heterogeneous microstructure formed as copies of the single representative cell Y, which is decomposed into the hyperelastic matrix Y_m and inclusion T ($Y = Y_m \cup T \cup \partial T, \quad Y_m \cap T = \emptyset$).

For the hyperelastic matrix the neo-Hookean constitutive law is assumed ([3]). The Kirchhoff stress $\boldsymbol{\tau}$, required by the UL formulation, is defined in terms of the hydrostatic pressure p and the deformation gradient $\boldsymbol{F}$:

$$\boldsymbol{\tau} = J\boldsymbol{I}\, p + \mu J^{-2/3}\, dev\, \boldsymbol{b}, \tag{2}$$

where $J = det\, \boldsymbol{F}$, $\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^T$, $dev\, \boldsymbol{b}$ denotes the deviator of the tensor $\boldsymbol{b}$ and μ is the shear stiffness. If the material is compressible, the pressure is given by the following constitutive law

$$p = -\gamma(J-1), \tag{3}$$

where γ is the bulk modulus. For incompressible materials p is the Lagrange multiplier associated with the constraint $J - 1 = 0$. The material coefficients are defined in the microscopic domain Y according to the decomposition:

$$\mu = \begin{cases} \mu_1, & \boldsymbol{x} \in Y_m \\ 0, & \boldsymbol{x} \in T \end{cases}, \qquad \gamma = \begin{cases} \gamma, & \boldsymbol{x} \in Y_m \\ \gamma_T, & \boldsymbol{x} \in T \end{cases}, \tag{4}$$

where $\gamma_T = 0$ for the compressible inclusion and $\gamma_T \longrightarrow +\infty$ for the incompressible one.

The two scale model (in case of the compressible inclusion) involves the microscopic problems for the characteristic response functions $\boldsymbol{\chi}$ and $\boldsymbol{\pi}$, which must be defined for all $\boldsymbol{x}$ in the macroscopic domain Ω by solving the boundary value problems which are defined below.

Microscopic problem: For fixed $\boldsymbol{x} \in \Omega$ and local (deformed) reference microscopic configuration associated with the domain $Y(\boldsymbol{x})$, find $\boldsymbol{\chi} \in H_{\#}(Y)$, $\boldsymbol{\pi} \in L^2(Y)$ such that $(r, s = 1, 2, 3)$:

$$a_{Y_m}\left(\boldsymbol{\chi}^{rs} - \boldsymbol{\Pi}^{rs},\ \boldsymbol{w}\right) - \left(\boldsymbol{\pi}^{rs},\ div_y \boldsymbol{w}\right)_{Y_m} = 0, \quad \forall \boldsymbol{w} \in H_{\#}(Y_m), \tag{5}$$

$$\frac{1}{\gamma}\left(\frac{1}{J}\boldsymbol{\pi}^{rs},\ q\right)_{Y_m} + \left(q,\ div_y\left(\boldsymbol{\chi}^{rs} - \boldsymbol{\Pi}^{rs}\right)\right)_{Y_m} = 0, \quad \forall q \in L^2(Y_m), \tag{6}$$

where $\Pi_i^{rs} \equiv y_s\,\delta_{ri}$ (δ – Kronecker delta), $H_{\#}(Y) \equiv \{\boldsymbol{v} \in [W^{1,2}(Y)]^3 |\ \boldsymbol{v}$ is Y periodic, $\int\limits_Y \boldsymbol{v}(\boldsymbol{y})\,\mathrm{d}y = 0\}$ is the space of admissible displacements ($W^{1,2}(Y)$ is the Sobolev space) and the bilinear form $a_{Y_m}(\boldsymbol{u}, \boldsymbol{v})$ is defined as follows:

$$a_{Y_m}(\boldsymbol{u}, \boldsymbol{v}) = \int\limits_{Y_m} D_{ijkl}^{tTK}\, e_{kl}^y(\boldsymbol{u})\, e_{ij}^y(\boldsymbol{v})\frac{1}{J}\,\mathrm{d}y + \int\limits_{Y_m} \tau_{ij}\,\delta_{kl}\,\partial_i^y u_k\,\partial_j^y v_l \frac{1}{J}\,\mathrm{d}y. \tag{7}$$

By superscripts x and y we denote the partial derivative w.r.t. x_i and y_i respectively, $e_{ij}(\boldsymbol{u}) = \frac{1}{2}\left(\partial_j^y u_i + \partial_i^y u_i\right)$ is the linear strain tensor and D_{ijkl}^{tTK} is the tangential stiffness tensor related to the Kirchhoff stress.
Macroscopic problem: For the given homogenized stiffness tensor $\hat{\mathcal{Q}}_{ijkl}$

$$\hat{\mathcal{Q}}_{ijkl} \equiv \frac{1}{|Y|}\left[a_{Y_m}\left(\boldsymbol{\Pi}^{kl} - \boldsymbol{\chi}^{kl},\ \boldsymbol{\Pi}^{ij} - \boldsymbol{\chi}^{ij}\right) + \frac{1}{\gamma}\left(\frac{1}{J}\pi^{ij},\ \pi^{kl}\right)_{Y_m}\right] \tag{8}$$

and the average Cauchy stress $\hat{\mathcal{S}}_{ij}$

$$\hat{\mathcal{S}}_{ij} \equiv \frac{1}{|Y|}\int\limits_Y \tau_{ij} J^{-1}\,\mathrm{d}y, \tag{9}$$

evaluated by means of the microproblem solutions, compute the macroscopic displacements (increments) $\Delta\boldsymbol{u}^0 \in V(\Omega)$ so that

$$\int\limits_\Omega \hat{\mathcal{Q}}_{ijkl}\,\partial_l^x \Delta u_k^0\,\partial_j^x v_i\,\mathrm{d}x = L(\boldsymbol{v}) - \int\limits_\Omega \hat{\mathcal{S}}_{ij}\, e_{ij}^x(\boldsymbol{v})\,\mathrm{d}x, \quad \forall \boldsymbol{v} = V_0(\Omega). \tag{10}$$

The virtual work of all external forces is denoted by $L(\boldsymbol{v})$ and the spaces of the admissible displacements $V(\Omega)$ a $V_0(\Omega)$ are defined as

$$\boldsymbol{V} = \left\{\boldsymbol{v} \in \left[W^{1,2}(\Omega)\right]^3 |\ v_i = \Delta\bar{u}_i \text{ on } \Gamma_u, i = 1,2,3\right\}, \tag{11}$$

$$\boldsymbol{V}_0 = \left\{\boldsymbol{v} \in \left[W^{1,2}(\Omega)\right]^3 |\ v_i = 0 \text{ on } \Gamma_u, i = 1,2,3\right\}, \tag{12}$$

where Γ_u is the part of the boundary with the prescribed Dirichlet boundary conditions.

The above problem is a single step in an incremental algorithm. The homogenized coefficients $\hat{\mathcal{Q}}_{ijkl}$ as well as $\hat{\mathcal{S}}_{ij}$ must be recovered almost everywhere in Ω,

which means, in practice, at each Gauss quadrature point of the finite element approximation of (10). In contrast to linear deformation models, this is the crucial point of the whole coupled micro-macro computing in our nonlinear case; after computing the macroscopic strain field, using $\Delta \boldsymbol{u}^0$, the local microscopic configurations must be updated and the corrector functions must be recomputed by solving (5), (6), individually for each Gauss quadrature point in Ω wherein the "macro-strains" vary nonuniformly. In [4] the method of approximation for $\hat{\mathcal{Q}}_{ijkl}$ and $\hat{\mathcal{S}}_{ij}$ was suggested which was aimed at reducing the number of the microscopic problems to be solved. In this article the parallel algorithm for reducing the computational time is presented.

3. Updating scheme $t \longrightarrow t + \Delta t$

The macroscopic configuration Ω is simply updated by the increment of the macroscopic displacement Δu^0 resulting from (10)

$$\Omega^{(t+\Delta t)} := \Omega^{(t)} + \{\Delta \boldsymbol{u}^0\}. \tag{13}$$

At the microscopic level the updating scheme is not so straightforward. We need to evaluate the increments of the microscopic displacement $\Delta \boldsymbol{u}^*$ and the pressure Δp^0. These increments depend on the characteristic response functions $\boldsymbol{\chi}$ and $\boldsymbol{\pi}$ and on the macroscopic deformation $\partial_j^x \Delta u_i^0$

$$\Delta u_i^* := (\Pi_i^{rs} - \chi_i^{rs})\, \partial_s^x \Delta u_r^0(\boldsymbol{x}), \quad \Delta p^0 := -\pi^{rs}\, \partial_s^x \Delta u_r^0. \tag{14}$$

After that we are able to update the microscopic configuration Y and the total deformation gradient $\boldsymbol{F}$ as

$$Y^{(t+\Delta t)} := Y^{(t)} + \{\Delta \boldsymbol{u}^*\}, \quad f_{ij} := \delta_{ij} + \partial_j^y \Delta u_i^*, \quad F_{ij} := f_{ik} F_{kj}. \tag{15}$$

This updating scheme does not lead to the equilibrium state, either the equilibrium equation or the pressure constitutive relation,

$$\frac{\partial \sigma_{ij}^{(t)}}{\partial^{(t)} y_j} = 0 \quad \text{or} \quad p^{(t)} = -\gamma (J^{(t)} - 1), \tag{16}$$

is not satisfied. As a consequence, we need to perform several iteration steps to achieve the equilibrium state. The (pseudo)time t is associated with load steps, it is not the real time.

The problem of computing the deformation in the macroscopic domain is solved iteratively using three nested loops. In the toplevel loop the load steps are applied, the medium loop is needed to achieve the macroscopic equilibrium, while the innermost loop leads to the local microscopic equilibrium for a fixed macroscopic deformation. The whole algorithm is shown in Fig. 2.

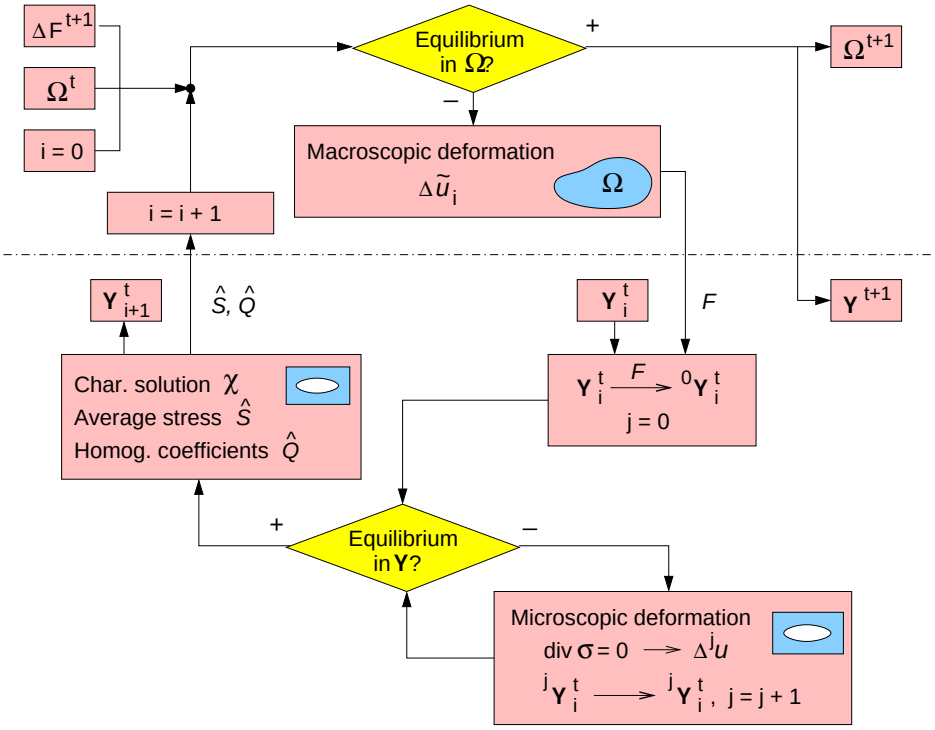

Fig. 2: *ULF macro–micro algorithm.*

4. Parallel strategy

It is evident that the complexity of this algorithm is considerable. In order to reduce a computational time the parallel computation strategy is employed. We take one computational node (master node) that works on the macroscopic problem while the other nodes (slaves) solve the microscopic problems demanded by the master. Master node sends to the slave nodes the deformation gradients in the appropriate macroscopic quadrature points and receives the homogenized coefficients and the average stress in these points, see Figures 3, 4.

For the parallel computation we use a Linux cluster communicating via the MPI message passing library. The computational algorithm is well parallelized and the speed-up is almost linear.

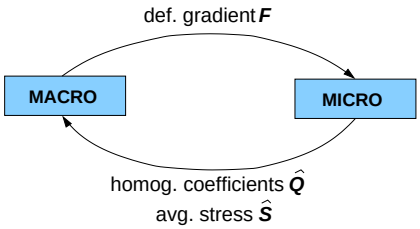

Fig. 3: *Parallel communication.*

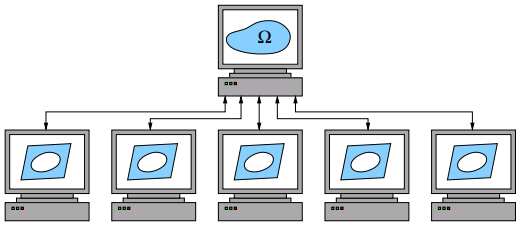

Fig. 4: *Parallel distribution.*

5. Numerical example

In Fig. 5 we can see a deformation of the macroscopic structure as well as the deformed microstructures in two selected macroscopic points. Also the efficiency and the speed-up of the parallel algorithm is shown.

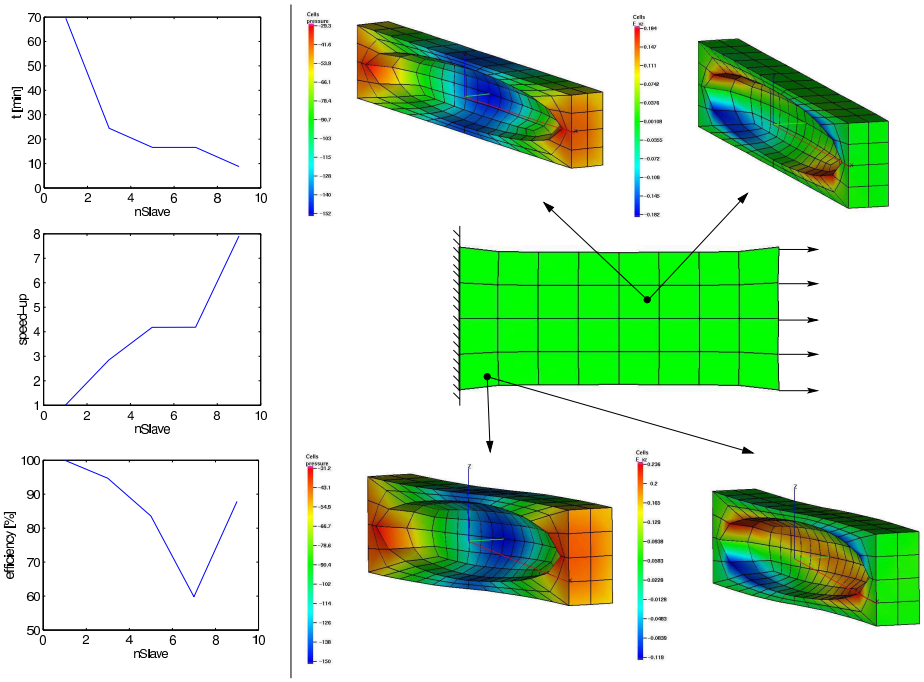

Fig. 5: *Efficiency, speed-up; pressure field and shear deformation.*

References

[1] D. Cioranescu, P. Donato: *An introduction to homogenization*. Oxford Lecture Series in Mathematics and its Applications 17, Oxford University Press, Oxford 1999.

[2] M.A. Crisfield: *Non-linear finite element analysis of solid and structures*. John Wiley & Sons Ltd, Chichester, vol. II., 1997.

[3] G.A. Holzapfel: *Nonlinear solid mechanics – a continuum approach for engineering*. John Wiley & Sons Ltd, Chichester, England, 2000.

[4] E. Rohan: *Mathematical modelling of soft tissues*. Habilitation thesis, University of West Bohemia, Plzeň 2002.

[5] E. Rohan: *Sensitivity strategies in modelling heterogenous media undergoing finite deformation*. Math. and Computers in Simul., 61, 261–270.

[6] E. Sanchez-Palencia: *Non-homogeneous media and vibration theory*. Lecture Notes in Physics 127. Springer, Berlin, 1980.