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# ADAPTIVE MODELLING OF MICROSCOPIC HETEROGENEOUS MEDIUM UNDERGOING LARGE DEFORMATION

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*Summary* In this paper we propose an algorithm for numerical modelling of the hyperelastic heterogeneous medium. Its microstructure changes with increasing deformation, depending on the spatial position in terms of the macroscopic deformation. The homogenized stiffness coefficients and the averaged stresses associated with the updated Lagrangian formulation are approximated over the macroscopic domain according to the local deformation. A concept of the so-called macroelements is introduced, each macroelement is related to a subdomain. Problems of the modelling error and of the adaptive approximation refinement are discussed. Numerical examples for materials with incompressible, or rigid inclusions are introduced to demonstrate performance of the method.

## INTRODUCTION

The problem of computing large deformation in heterogeneous media is characterized by macroscopically non-uniform change of microstructure, thereby depending on the spatial position. Starting with perfect periodic distribution of inhomogeneities (e.g. inclusions) in the reference state, due to nonuniform deformation the material becomes functionally graded. This phenomenon tightly couples the sequence of the macroscopic and the local microscopic problems, that result from the two-scale homogenization method applied to the incremental formulation. This difficulty has been addressed in [4], where the microscopic cell problems are solved for each macroscopic element using parallel computational tools. Another approach, cited therein, is based on creating the database of pre-computed homogenized coefficients. In [3] an approximation scheme for the homogenized coefficients is proposed which allows for significant reduction of computational cost related to the local cell problems. Here we extend the approach by adaptive refinement of the approximation, which is controlled by the “modelling error” indicator, cf. [1].

## HOMOGENIZED PROBLEM AND LOCAL CELL PROBLEMS

The two-scale homogenization procedure is applied to the finite deformation problem linearized using the updated Lagrangian formulation. We consider microstructures formed by hyperelastic incompressible matrix and incompressible inclusions. Such material yields the decomposition of the microscopic representative cell $Y \in \mathbb{R}^d$, $Y = \overline{Y_m \cup Y_c}$, where $Y_c$ is the inclusion. The following local cell problems are solved to compute the corrector functions $\chi_i^{kl} \in H^1_\#(Y_m)^d$ for displacements and $\tilde{\pi}^{kl} \in L^2(Y_m)$ for the pressure nonuniformity (the difference between the pressure in $Y_m$ and the uniform pressure in $Y_c$)

$$\tilde{a}_{Y_m}(\chi^{kl} - \Pi^{kl}, v) - (\tilde{\pi}^{kl}, \mathrm{div}_y v)_{Y_m} = 0 \quad \forall v \in H^1_\#(Y_m)^d \, , \tag{1}$$

$$(q, \mathrm{div}_y \chi^{kl} - \mathrm{div}_y \Pi^{kl})_{Y_m} = 0 \quad \forall q \in L_2(Y_m) \, , \tag{2}$$

where $\Pi_i^{kl} = \delta_{ik} y_l$, the bilinear form $\tilde{a}_{Y_m}(u,v) = \int_{Y_m} \left( D^{\mathrm{eff}}_{ijkl} + \tau^{\mathrm{eff}}_{lj}\delta_{ki} + J\tilde{p}\,\delta_{il}\delta_{jk} \right) \partial^y_l u_k \, \partial^y_j v_i \, J^{-1} dy$ is defined in terms of the tangent modulus, the Kirchhoff stress and the pressure nonuniformity, $\tilde{p}(y) = p(y) - \bar{p}$ for $y \in Y_m$ and $\bar{p}$ is the pressure in $Y_c$. The correctors determine the homogenized stiffness coefficients $Q_{ijkl} = |Y|^{-1} \, \tilde{a}_{Y_m}(\chi^{kl} - \Pi^{kl}, \chi^{ij} - \Pi^{ij}) + \bar{p}\delta_{il}\delta_{jk}$, which constitute the bilinear form of the macroscopic subproblem: given the external load functional $L(v)$, the temporary averaged stress functional $\mathcal{S}(v)$ and the out-of-incompressibility functional $Z(q)$, find the displacement and pressure incremental fields $\delta u \in V(\Omega)$ and $\delta\bar{p} \in L^2(\Omega)$, respectively, for which

$$\mathcal{B}(\delta u, v) - (\delta\bar{p}, \mathrm{div}_x v)_\Omega = L(v) - \mathcal{S}(v) \, , \quad \forall v \in V(\Omega) \tag{3}$$

$$(q, \mathrm{div}_x \delta u)_\Omega = Z(q) \, , \quad \forall q \in L^2(\Omega) \tag{4}$$

where $\mathcal{B}(\delta u, v) = \int_\Omega Q_{ijkl} \partial^x_l \delta u_k \, \partial^x_j v_i \, dx$, and $\mathcal{S}(v) = \int_\Omega |Y|^{-1} \int_Y \tau_{ij} J^{-1} \, dy \, \partial^x_j v_i \, dx$. In order to recover the homogenized coefficients in $\Omega$, we use the approximation scheme, as briefly introduced below.

## ALGORITHM FOR SOLVING THE 2-SCALE NONLINEAR PROBLEM

Given the temporary (deformed) reference macroscopic configuration $\Omega$, the approximation scheme $\mathbb{F}$ for the homogenized coefficients and a new load represented by $L(v)$ in (3), the following 2 step algorithm applies:

1. Using the macroscopic deformation update $\mathbb{F}$, if necessary, then compute the approximation of $Q_{ijkl}$ and that of the averaged stresses for each macroscopic (integration) point of $\Omega$;

2. Solve (3)–(4) for $\delta u(x)$ and $\delta\bar{p}(x)$; update $\Omega$ and the macroscopic deformation gradients; if the “convergence”is not achieved, return to step 1.

### Approximation of the homogenized coefficients

We now explain the step 1. The approximation scheme $\mathbb{F}$ is represented by the so-called "macroelements" $M_k$ defined in the deformation space, each one associated with (disconnected) subdomain $\Omega_k \subset \Omega$. For 2D problems $M_k$ is a box with vertices $\boldsymbol{f}_i$, $i = 1, \ldots, m (= 8)$ and one "central" point $^*\boldsymbol{F}$, which characterizes the deformation in $\Omega_k$:

$$M_k(^*\boldsymbol{F}, \{\boldsymbol{f}_j\}_{j=0}^m) = \{\boldsymbol{F} \,|\, \exists \boldsymbol{f} \in \mathrm{conv}\{\boldsymbol{f}_j\}_{j=0}^m \;:\; \boldsymbol{F} = \boldsymbol{f}\, {}^*\boldsymbol{F}\}\;, \tag{5}$$

so that the deformation gradients $\boldsymbol{F}(x) \in M_k$, $x \in \Omega_k$, up to the rigid body rotation. Each $\boldsymbol{f}_j\, {}^*\boldsymbol{F}$ determines a fictitious microstructural configuration $(Y, p)$, for which (1)–(2) must be solved and which alternatively should be updated using macroscopic strains and the corrector functions. Using the sensitivity analysis of homogenized coefficients and stresses w.r.t. the macroscopic deformation, cf. [2], an interpolation scheme is defined over any simplex $S_k^I$, $I \subset \{1, \ldots, m\}$ embedded in $M_k$; this is the tool for constructing the approximation scheme $\mathbb{F}\{M_k\}$.

### Adaptive approximation refinement strategy

Obviously, the quality of the solutions to (3)–(4) depends on the approximation scheme outlined above, which introduces the modelling error. We suggest a concept of adaptive refinement of $\mathbb{F}$ to use as few computations of the microscopic cell problems as possible. Given the set $\{M_k\}_{k=1}^N$, consider two different schemes $\mathbb{F}^i\{M_k\}_{k=1}^N$, $i = 0, 1$. For these we obtain the corresponding functionals $\mathcal{B}^i(u, v)$ and $\mathcal{S}^i(v)$. The macroscopic solution $\delta u^0$, $\delta \bar{p}^0$ is known only for $i = 0$. The upper and lower bounds of difference in the solution $\|\delta u^1 - \delta u^0\|_{\mathcal{B}^1}$ can be computed using the residual function, cf. [1], $\mathcal{R}_{\delta u^0}(u) \equiv -\Delta\mathcal{B}(\delta u^0, u) - \Delta\mathcal{S}(u)$, defined by subtracting $\mathcal{B}^1 - \mathcal{B}^0$ and $\mathcal{S}^1 - \mathcal{S}^0$. The error evaluated over $\Omega_k$ serves as the indicator for refinement of the macroelement $M_k$. In the paper we discuss also the influence of the macroscopic modelling error on the microscopic responses. In Fig. 1 we illustrate the adaptive algorithm: finite extension of the clamped strip considered, material with incompressible inclusions; subdomains for 2 and 4 macroelements, respectively, displayed with different colours. The maxima of norms for variation of deformation within the subdomains are: 0.185 for 1 subdomain, 0.159 for 2 subdomains and 0.083 for 4 subdomains.

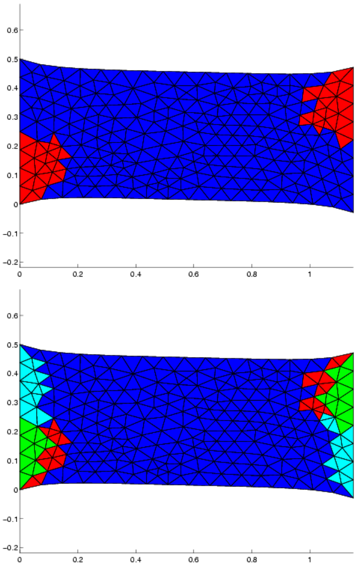

Fig. 1: Macroscopic subdomains for 2 and 4 macroelements.

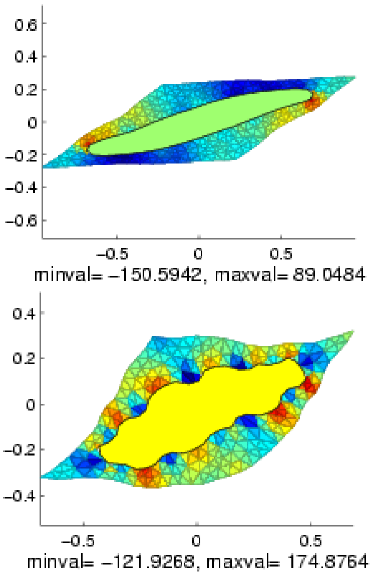


Fig. 2: Microstructures for smooth muscle modelling.

## CONCLUSIONS

The adaptive approximation scheme for homogenized coefficients was employed in the large deformation analysis of hyperelastic heterogeneous materials. The strategy for modelling refinement is based on error indication associated with two different approximations of stiffnesses and stresses. For enhancement of the computational speed parallel computing tools can be used. Further modifications of the approach for functionally graded materials are possible, which may allow for applications e.g. in muscle tissue modelling, see Fig. 2. (The research has been supported by the project LN00B084 of The New Technologies Research Centre, UWB, Plzeň.)

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