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EFFICIENT COMPUTATIONAL ALGORITHM FOR SOLVING TWO-SCALE PROBLEMS OF LARGE DEFORMING HETEROGENEOUS PERIODIC STRUCTURES

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Abstract: *We propose an efficient computational algorithm for solving coupled two-scale problems of large deforming heterogeneous hyperelastic media with periodic structure. Our algorithm is based on clustering points in the deformation space and the approximating material coefficients with the help of the sensitivity analysis method. The effectiveness of the proposed approach is compared with the standard FE^2 computational scheme in a simple 2D example.*

Keywords: Homogenization, hyperelasticity, model order reduction, finite element method.

1. Introduction

We consider a heterogeneous hyperelastic medium with a periodic structure subjected to large deformations. The updated Lagrangian formulation and the two-scale homogenization method are employed to get the coupled macro-micro system of equations, which must be solved in an iterative loop. The standard two-scale finite element approach for nonlinear problems leads to the FE^2 computational strategy, see e.g. Schröder (2014); Lukeš (2023), where the local microscopic problems are computed at all quadrature points of the macroscopic domain. This strategy is very computationally demanding and difficult to use in practical applications. In this paper, we propose using the K-means clustering algorithm, employed e.g., in Benaimeche et al. (2022), and sensitivity analysis techniques, see Rohan (2003), to reduce the number of local problems that need to be solved during macroscopic iterations and loading steps. We demonstrate the proposed approach in 2D numerical simulations, where we measure the computational time and observe the error induced by the approximation.

2. Two-scale model of hyperelastic structures

We use the neo-Hookean hyperelastic material model to describe the nonlinear behavior of compressible heterogeneous structures. The Cauchy stress in such a structure can be expressed as

$$\boldsymbol{\sigma} = K(J-1) + \mu J^{-5/3}\,(\boldsymbol{b} - \mathrm{tr}(\boldsymbol{b})/3\boldsymbol{I}), \tag{1}$$

where, μ is the shear modulus, K is the bulk modulus, $\boldsymbol{F}$ is the deformation gradient, $J = \det(\boldsymbol{F})$, $\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^T$, and $\boldsymbol{I} = (\delta_{ij})$ is the Kronecker symbol. The constitutive equation (1), together with the equilibrium equation (∇ is the gradient operator and $\boldsymbol{f}$ stands for external forces)

$$-\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f} \tag{2}$$

define the nonlinear problem that is linearized using the updated Lagrangian formulation. The linearized incremental form of the problem is treated by the homogenization procedure, which results in the coupled

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system of macroscopic and microscopic equations. At the macroscopic level, we must solve the following equilibrium equation for the unknown macroscopic displacement increments $\delta \boldsymbol{u}^0$

$$\int_\Omega \boldsymbol{\mathcal{A}} \nabla_x \delta \boldsymbol{u}^0 : \nabla_x \boldsymbol{v} = L^{new}(\boldsymbol{v}) - \int_\Omega \boldsymbol{\mathcal{S}} : \nabla_x \boldsymbol{v}, \qquad \text{for all } \boldsymbol{v} \in \boldsymbol{V}_0(\Omega). \tag{3}$$

L^{new} involves all forces applied in the current loading step, $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{S}}$ are the homogenized coefficients arising from the solution of a microscopic subproblem, $\boldsymbol{V}_0(\Omega)$ is the set of admissible functions that are equal to zero on the Dirichlet boundary of Ω, and ∇_x denotes the gradient operator with respect to the macroscopic scale x.

For a given macroscopic deformation $\boldsymbol{F}(x)$, we solve the local problem at the deformed locally periodic reference cell $Y(x)$ (see Lukeš (2023)) to find the characteristic responses $\boldsymbol{\chi}$:

$$\int_{Y(x)} \mathbb{A} \nabla_y (\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}) : \nabla_y \boldsymbol{v} = 0, \qquad \text{for all } \boldsymbol{v} \in \boldsymbol{H}^1_\#(Y). \tag{4}$$

By $\boldsymbol{H}^1_\#(Y)$ we denote the functional space of $Y(x)$ locally periodic functions, $\Pi^{ij}_k = y_j \delta_{ik}$, and $\mathbb{A}$ is the fourth-order tangential stiffness tensor (Truesdell rate of the Kirchhoff stress). The microscopic configuration $Y(x)$ is updated at each iteration step using the macroscopic (incremental) deformation $\nabla_x \delta \boldsymbol{u}^0$ and the microscopic response $\boldsymbol{\chi}^{ij}$ as: $Y^{new}(x) = Y^{old}(x) + (\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}) \frac{\partial \delta u^0_i}{\partial x_j}$.

The homogenized stiffness coefficients $\boldsymbol{\mathcal{A}}$ and the averaged Cauchy stress $\boldsymbol{\mathcal{S}}$ are given by

$$\boldsymbol{\mathcal{A}} = \frac{1}{|Y|} \int_Y \mathbb{A} \nabla_y (\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}) \nabla_y (\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}), \quad \boldsymbol{\mathcal{S}} = \frac{1}{|Y|} \int_Y \boldsymbol{\sigma}. \tag{5}$$

3. Approximation of homogenized coefficients

Solving the nonlinear macroscopic problem by the finite element method requires knowing the tangent modulus and stress tensors at all quadrature points $\hat{x}$ of Ω at each iteration step. To avoid the computational bottleneck of the FE^2 approach, we propose the following algorithm reducing the number of computed local subproblems. In the first step, the polar decomposition of the macroscopic deformation $\boldsymbol{F}(\hat{x}) = \hat{\boldsymbol{R}}\hat{\boldsymbol{U}}$ is employed to decompose the deformation into the rotation tensor $\boldsymbol{R}$ and the symmetric stretch tensor $\boldsymbol{U}$. Then, $\hat{\boldsymbol{U}}$ is used to express the symmetric strain tensor $\hat{\boldsymbol{e}} = \hat{\boldsymbol{U}} - \boldsymbol{I}$, which components represent a point in the 3 (for 2D) or 6 (for 3D) dimensional space of deformations. Using the K-means clustering method, see Lloyd (1982) for details, we can find a minimal number of sets $O^k = \{\hat{\boldsymbol{e}} : |\hat{\boldsymbol{e}} - \mathring{\boldsymbol{e}}^k| < \rho\}$, such that $\bigcup_k O^k$ includes all strains $\hat{\boldsymbol{e}}$, where $\mathring{\boldsymbol{e}}^k$ is the mean value (center) of points in O^k, and ρ is a given parameter. Now, instead of solving the local microscopic subproblems (4) for all macroscopic deformations $\boldsymbol{F}(\hat{x})$, we solve the subproblems only for a reduced number of deformations $\mathring{\boldsymbol{F}} = \mathring{\boldsymbol{e}}^k + \boldsymbol{I}$ to get the homogenized coefficients $\mathring{\boldsymbol{\mathcal{A}}}$ and $\mathring{\boldsymbol{\mathcal{S}}}$. The choice of the ρ parameter affects the number of sets O^k (we call them centroids) and the accuracy of the resulting approximation. The centroids are constructed on the fly during the macroscopic iterations when newly appeared deformations $\hat{\boldsymbol{e}}$ cannot be covered by the existing centroids.

Approximation of the homogenized coefficients in the quadrature points $\hat{x}$ is made with the help of the sensitivity analysis technique as suggested in Rohan (2003). The coefficient sensitivities $\delta\mathring{\boldsymbol{\mathcal{A}}}$, $\delta\mathring{\boldsymbol{\mathcal{S}}}$ with respect to deformations can be evaluated using the already computed characteristic responses $\boldsymbol{\chi}$, see Rohan (2003), so there is no need to solve any additional microscopic problem. The following approximation scheme for the homogenized coefficients is used

$$\boldsymbol{\mathcal{A}}(\hat{x}) \approx \hat{\boldsymbol{R}}^T \left(\sum_i \left(\mathring{\boldsymbol{\mathcal{A}}}^i + \delta\mathring{\boldsymbol{\mathcal{A}}}^i(\hat{\boldsymbol{g}}^i) \right) w_i \right) \hat{\boldsymbol{R}}, \qquad \boldsymbol{\mathcal{S}}(\hat{x}) \approx \hat{\boldsymbol{R}}^T \sum_i \left(\mathring{\boldsymbol{\mathcal{S}}}^i + \delta\mathring{\boldsymbol{\mathcal{S}}}^i(\hat{\boldsymbol{g}}^i) \right) w_i, \tag{6}$$

where the summation is performed for all centroids to which $\hat{\boldsymbol{e}}$ belongs, $\hat{\boldsymbol{g}}^i$ is the relative strain of $\hat{\boldsymbol{e}}$ with respect to $\mathring{\boldsymbol{e}}^i$, and w_i are the weights reflecting the distance $|\hat{\boldsymbol{e}} - \mathring{\boldsymbol{e}}^i|$, $\sum_i w_i = 1$.

4. Numerical simulation

The suggested reduction strategy is demonstrated in a simple 2D example. We consider a rectangular macroscopic domain of shape 0.4×0.25 m fixed on its left edge and displaced on the right edge as depicted in

Fig. 1 left. The total prescribed displacement $\bar{\boldsymbol{u}} = [0.05, -0.05]^T$ m is applied uniformly in six loading steps. The microscopic periodic unit cell Y consisting of two hyperelastic parts, see Fig. 1 right, is defined by the following material parameters: $K = 1\,000$ Pa, $\mu = 100$ Pa in Y_1 and $K = 1\,000$ Pa, $\mu = 10$ Pa in Y_2.

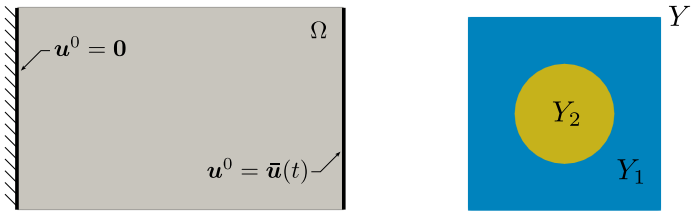

Fig. 1: Macroscopic domain Ω and the applied boundary conditions (left), periodic cell $Y = Y_1 \cup Y_2$ (initial configuration, right).

The deformed macroscopic sample and the deformed microscopic cells in selected macroscopic points are shown in Fig. 2. To be able to measure the approximation error of the proposed algorithm, we choose three quadrature points of the macroscopic domain, labelled in Fig. 2 left by symbol $\circ$, in which the extra local problems are solved, and the exact values of the homogenized coefficients are evaluated.

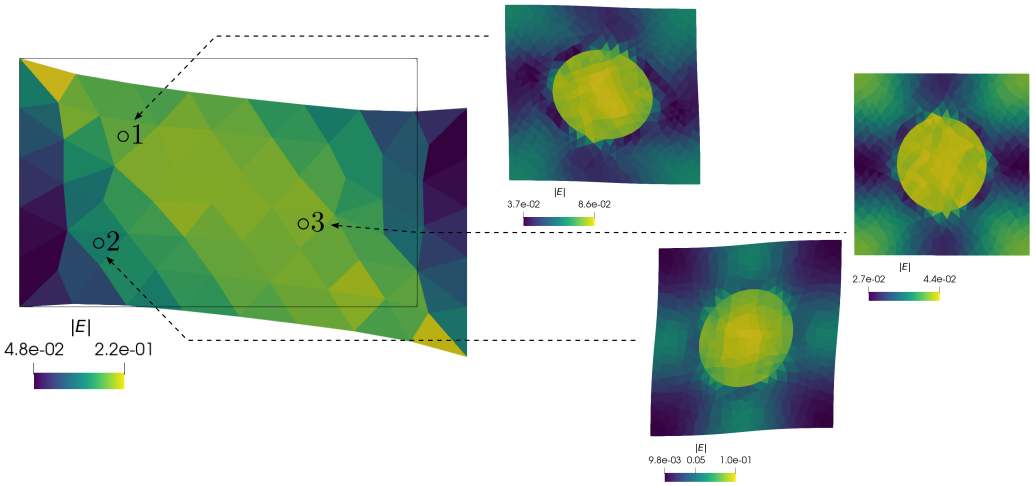

Fig. 2: Deformed macroscopic domain (left), deformed microscopic configurations at the macroscopic checkpoints (right).

The coefficient components $\mathcal{A}_{1111}$, $\mathcal{S}_{11}$ are compared for different parameters ρ in Fig. 3. We label the exact values by superscript ^{exact} and the approximated values by ^{approx}.

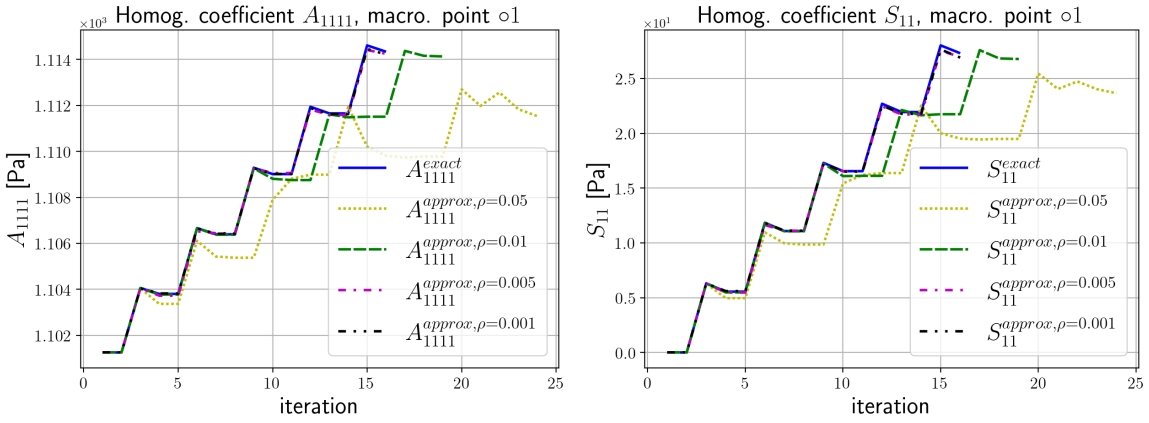

Fig. 3: Comparison of components $\mathcal{A}_{1111}$, $\mathcal{S}_{11}$ calculated for $\rho = 0.05, 0.01, 0.005, 0.001$ with the exact solution.

The efficiency of our new algorithm is apparent from Fig. 4, where we compare the computation time of the coupled two-scale simulations and the number of solved local microproblems for various ρ with the full FE^2 simulation without any reduction (denoted by "No approx"). The computation time of the full simulation is less than the reduced simulation for $\rho = 0.001$ in our case. This result occurs because the computation time of our simple 2D local problem is very small, and it is comparable to the time required to evaluate the sensitivities and for the approximation of the coefficients. For more complex geometries at the microscopic level and for 3D problems, the solution time of (4) will grow much more than the overhead associated with sensitivity analysis and approximation.

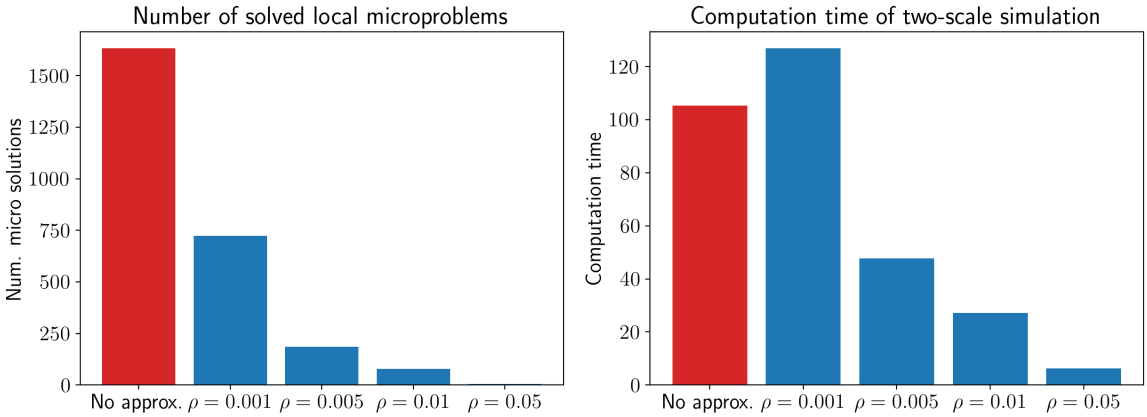

Fig. 4: Number of solved local microproblems (left), computation time of the simulation (right).

The two-scale numerical simulation has been implemented in SfePy (Simple Finite Elements in Python), see Cimrman (2023), which allows to solve the local problems efficiently using parallel computing on multiple cores or processors.

5. Conclusion

The proposed algorithm can efficiently reduce the computational complexity of the coupled two-scale problems arising from the homogenization of heterogeneous structures undergoing large deformations. The problem reduction efficiency can be controlled by the parameter ρ, which, for a particular application, should be chosen in such a way as to minimize the number of centroids associated with sets O^k while keeping the approximation error below the given limit. In the case of the presented 2D simulation, for $\rho = 0.005$, we achieve less than half the computational time with a relative error of the order of 10^3.

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