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Comparison of Two Methods for Numerical Upscaling

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The main objective of this paper is to compare two discretization-based homogenization methods. A local numerical homogenization and a multiscale finite element method (MsFEM) are first briefly presented and next numerically tested. In the case of MsFEM, a new shape function construction is also presented. Extensive comparison of both techniques constitutes the main part of this study. Novelty of this research is to combine aforementioned methods with mesh adaptivity at the coarse mesh level and the application of the higher-order approximation.

Key words: local numerical homogenization, multiscale FEM, multigrid homogenization.

1. Introduction

Even though computational resources continuously become more powerful, yet they are still limited in many practical applications. Moreover, a solution, if feasible, to a huge problem provides enormous amount of data. These two contradictory facts can be found in the context of heterogeneous materials modeling. On the one hand, we may be unable to exactly demonstrate small inclusions in terms of FEM and, therefore, solve a problem for such a fine discretization. On the other hand, we may be even unwilling to analyze, e.g., displacements of every single inclusion. Nevertheless, occurrence of such inclusions influences the global response of the material and it has to be accounted for in reliable analyses.

Various homogenization methods are used in order to make modeling of heterogeneous materials feasible. Typically, two scales of analysis are considered: macro and microscale. Aforementioned approaches are used as upscaling methods that deliver solution at the macro level.

In this paper, we compare two discretization-based methods: a local numerical homogenization and a multiscale finite element method (MsFEM). Their principles are very similar. First, a coarse mesh is generated. Then, all of its

elements are independently refined in order to comply with the microstructure. Subsequently, the effective stiffness matrices of macro elements are computed. Finally, a locally homogenized problem is solved. Our enhancement to both homogenization methods is an application of automatic adaptivity at both scales. The analyses are carried out in *hp3d* code.

2. Local numerical homogenization

This method has been proposed for flash imprint lithography purposes initially. Its mathematical formulation and numerical results can be found in [1]. Later on, the method was used for modeling of visco-elastic materials [2].

The effective stiffness matrix $\mathbf{K}_H$ is computed in such a way that the difference between the coarse and fine mesh solutions was minimized. Given symmetric fine mesh stiffness matrices assembled into $\mathbf{K}_h$, a non-zero fine mesh load vector $\mathbf{f}_h$, interpolation matrix $\mathbf{A}$, a positive-definite symmetric weight matrix $\mathbf{B}$, and a dimensionless small parameter $\varepsilon > 0$, we search for a symmetric matrix $\mathbf{K}_H^{\dagger}$ (pseudoinverse of the coarse element stiffness matrix $\mathbf{K}_H$) minimizing E, where

$$E\left(\mathbf{K}_H^{\dagger}\right) = \frac{1}{2}\left\|\left(\mathbf{K}_h^{\dagger} - \mathbf{A}\mathbf{K}_H^{\dagger}\mathbf{A}^T\right)\mathbf{f}_h\right\|_{\mathbf{B}}^2 + \frac{\varepsilon}{2}\left\|\mathbf{K}_h^{\dagger} - \mathbf{A}\mathbf{K}_H^{\dagger}\mathbf{A}^T\right\|_{F,\mathbf{B}}^2 \|\mathbf{f}_h\|_2^2 \tag{2.1}$$

and

$$\|\mathbf{x}\|_2 = \sqrt{trace(\mathbf{x}^T\mathbf{x})}$$

denotes Euclidean norm,

$$\|\mathbf{x}\|_{\mathbf{B}} = \sqrt{trace(\mathbf{x}^T\mathbf{B}\mathbf{x})}$$

denotes a Euclidean norm weighted with the matrix $\mathbf{B}$,

$$\|\mathbf{X}\|_{\mathbf{F},\mathbf{B}} = \sqrt{trace(\mathbf{X}^T\mathbf{B}\mathbf{X})}$$

denotes a Frobenius norm weighted with the matrix $\mathbf{B}$, and $\mathbf{x}$ and $\mathbf{X}$ are arbitrary vector and matrix, respectively.

Problem (2.1) with symmetry condition implied on $\mathbf{K}_H^{\dagger}$ is reduced to the Lyapunov equation solution. The matrix $\mathbf{A}$ is computed on the basis of L_2 projection of coarse mesh shape functions onto the fine mesh shape functions space. The vector $\mathbf{f}_h$ is not usually given explicitly. This vector is evaluated on the basis of the trial coarse mesh solution. Algorithms for Moore-Penrose pseudoinverse can be found, e.g., in [3].

Until now, we have used local numerical homogenization only with a linear approximation at both scales. The specifics of the Moore-Penrose pseudoinverse have limited the application of higher-order functions.

3. Multiscale finite element method

The MsFEM is equivalent to multigrid homogenization [4–6]. It is based on special shape functions. Standard ones are modified in order to account for the microstructure heterogeneity. Problem can be formulated in a weak form as follows.

Find $\mathbf{\Phi}(\mathbf{x}) \in V_0 + \widehat{\mathbf{\Psi}}$ such that

$$\int_{\Omega} \boldsymbol{\sigma}(\mathbf{\Phi}) : \boldsymbol{\varepsilon}(\mathbf{v}) \mathrm{d}\Omega = \int_{\Omega} \mathbf{v} \cdot Reg[\operatorname{div} \boldsymbol{\sigma}(\mathbf{\Psi})] \mathrm{d}\Omega \qquad \forall \mathbf{v} \in V_0, \tag{3.1}$$

where $\mathbf{\Psi}$ is a coarse mesh vector-valued shape function, $\mathbf{\Phi}$ is its interpolant, *Reg* denotes regular part of the derivative, and $\mathbf{\Omega}$ stands for the coarse element domain.

The degrees of freedom (DOFs) of the discrete solution to (3.1), obtained for every coarse mesh shape function, are the column of the inter-grid operator $\mathbf{I}_{M \times N}$, where M denotes the number of the coarse element DOFs and N is the number of the fine mesh DOFs. If restriction operator $\mathbf{R} = \mathbf{I}^T$, coarse mesh quantities can be computed as $\mathbf{K}_H = \mathbf{I}^T \mathbf{K}_h \mathbf{I}$ and $\mathbf{f}_H = \mathbf{I}^T \mathbf{f}_h$.

We have used the MsFEM with arbitrary higher-order shape functions at both scales. Selected standard and modified coarse mesh shape functions for a $1 \times 1 \times 1$ cube (Fig. 1) are shown in Fig. 2. Heterogeneity is represented by a small $0.5 \times 0.5 \times 0.5$ cube. Poisson's ratio is the same for both materials and is equal to 0.3, whereas the Young modulus for the blue "matrix" is equal to *1e6*, and for the inclusion is equal to *1e7*.

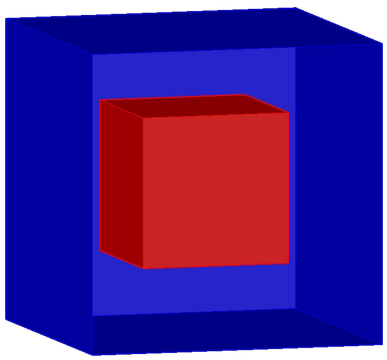


Fig. 1. Inclusion.

At both scales, the third-order Peano shape functions were used. The fine mesh consists of 512 elements.

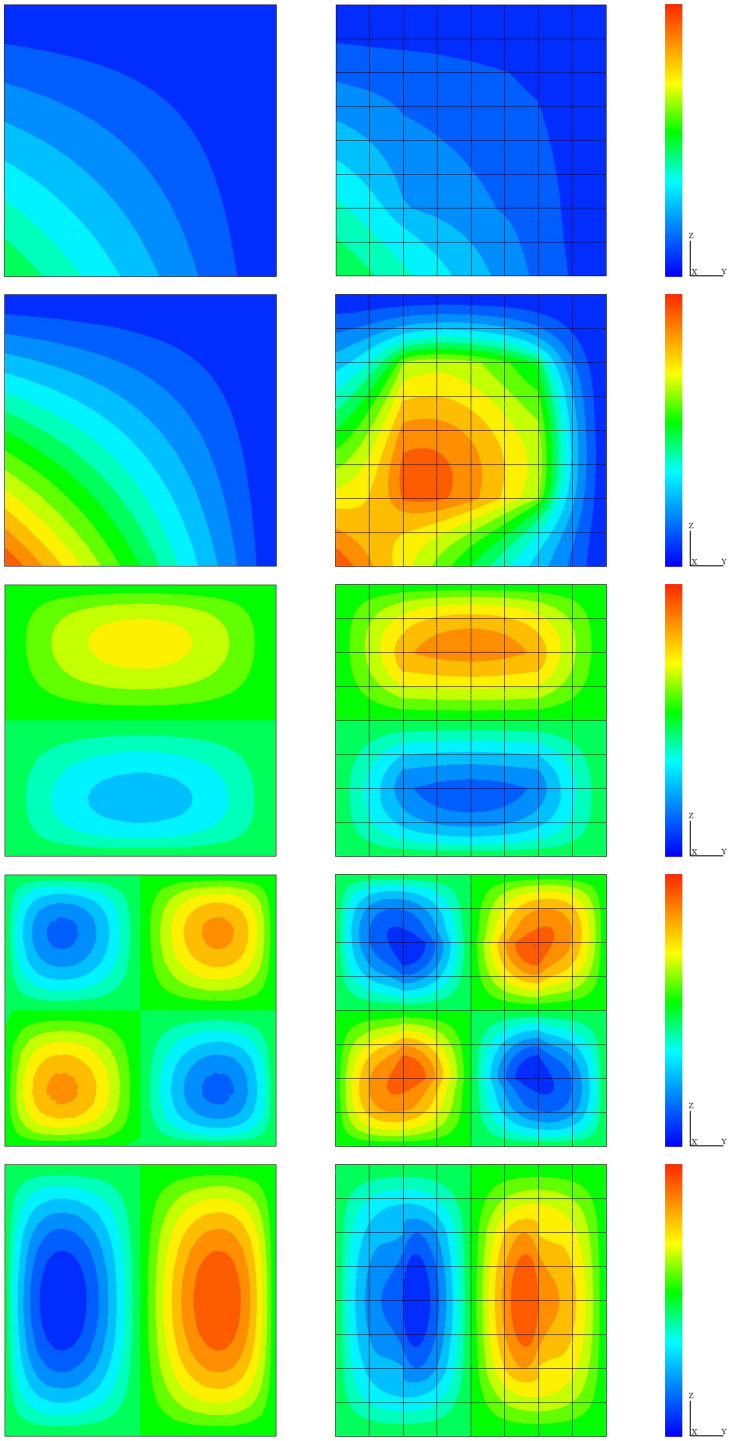


FIG. 2. Selected standard (left) and modified (right) coarse mesh shape functions.

4. Numerical results

In order to compare a local numerical homogenization with the MsFEM, the analysis of the Fichera corner is presented. The corner is a cube defined by two opposite points $(-1, -1, -1)$ and $(1, 1, 1)$ with the cuboidal part between $(0, 0, 0)$ and $(1, 1, 1)$ removed. The three faces meeting at point $(0, 0, 0)$ are fixed. The remaining ones are subjected to a load of intensity 100 acting along x-axis. Non-periodic distribution of inclusions is shown in Fig. 3. It is to resemble functionally graded material. Poisson's ratio is equal to 0.3 for both materials. Young's modulus equals *1e6* for the matrix and *2e6* for the inclusions.

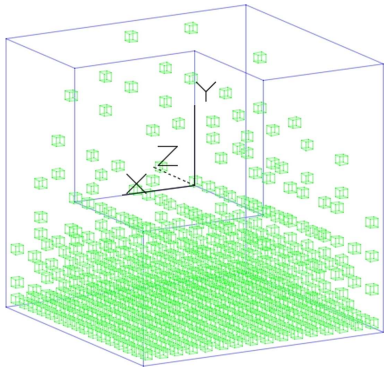


Fig. 3. Distribution of inclusions in Fichera corner.

Linear approximation was used initially at coarse and fine mesh levels for both homogenization methods. A coarse mesh was h-adaptively refined [7] to account for the global singularity. The direct solution obtained with about 100 000 DOFs (linear approximation) was used to validate the homogenized solutions.

4.1. Results for local numerical homogenization

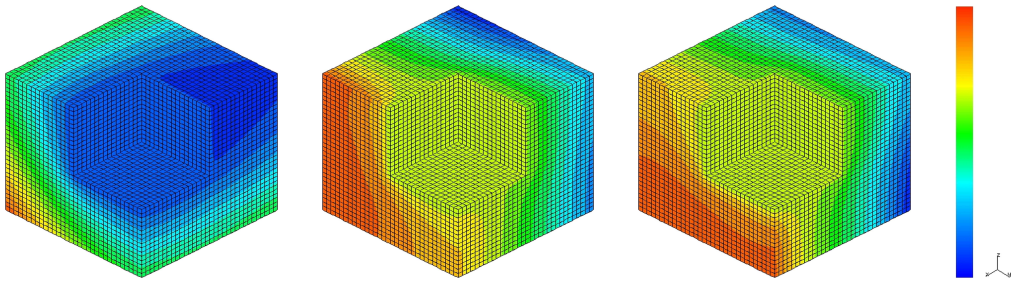
Displacement maps for $p = 1$ at both scales are shown in Fig. 4. The number of DOFs at the coarse mesh level is equal to about 500.

4.2. Results for MsFEM

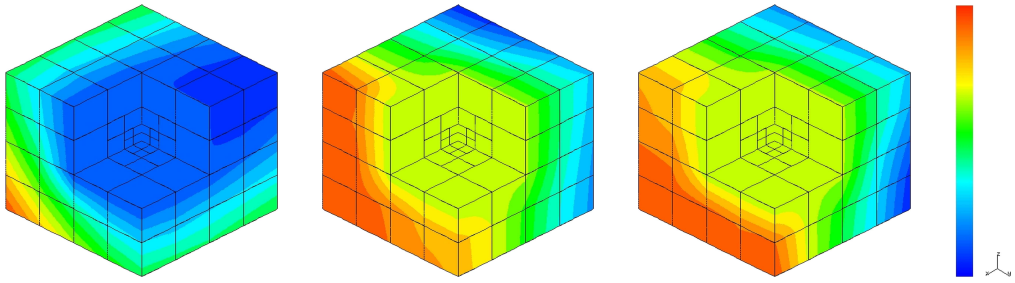
Displacement maps for $p = 1$ at both scales are shown in Fig. 5.

In order to improve the MsFEM results, we increased the approximation order at the coarse mesh scale to $p = 2$ (Fig. 6). The number of DOFs at the coarse mesh level is equal to nearly 4000.

Displacements along the segment between points $(-1, -1, -1)$ and $(0, 0, 0)$ are shown in Fig. 7. The fine mesh solution is marked with blue and the MsFEM solution with red.

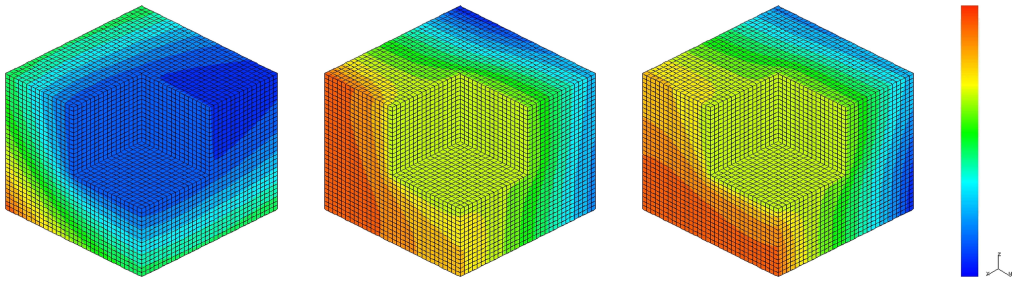


$u_x \in [-2.96e-4,\ 3.50e-3]$ $u_y \in [-1.37e-3,\ 7.28e-4]$ $u_z \in [-1.37e-3,\ 7.28e-4]$

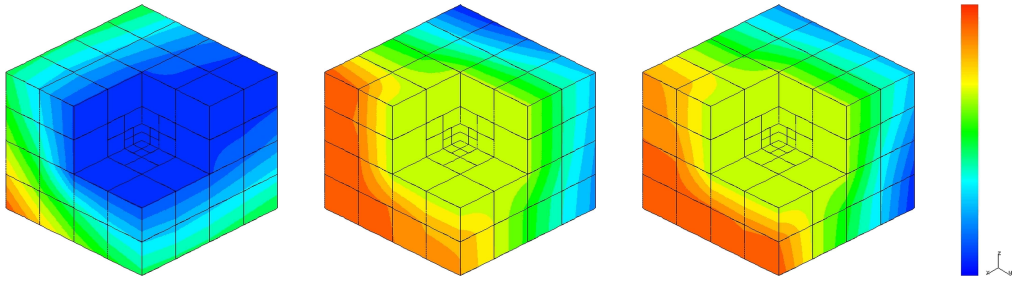


$U_x \in [-2.43e-4,\ 3.09e-3]$ $U_y \in [-1.21e-3,\ 6.18e-4]$ $U_z \in [-1.22e-3,\ 6.18e-4]$

FIG. 4. Maps of displacements – local numerical homogenization ($p_{\mathrm{MACRO}} = +1$, $p_{\mathrm{MICRO}} = 1$, top row) and the reference solution (bottom row).

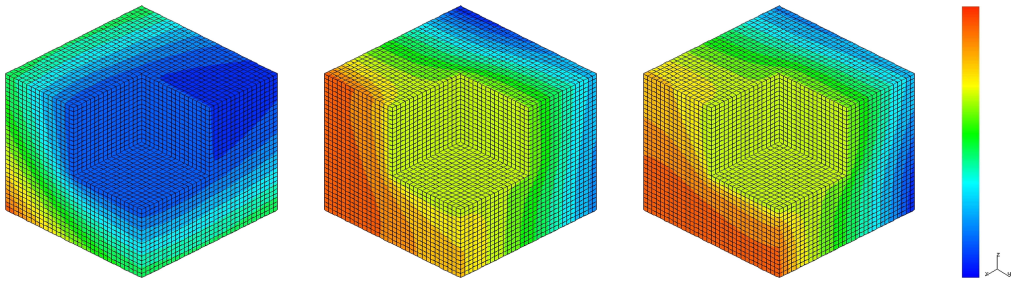


$u_x \in [-2.96e-4,\ 3.50e-3]$ $u_y \in [-1.37e-3,\ 7.28e-4]$ $u_z \in [-1.37e-3,\ 7.28e-4]$

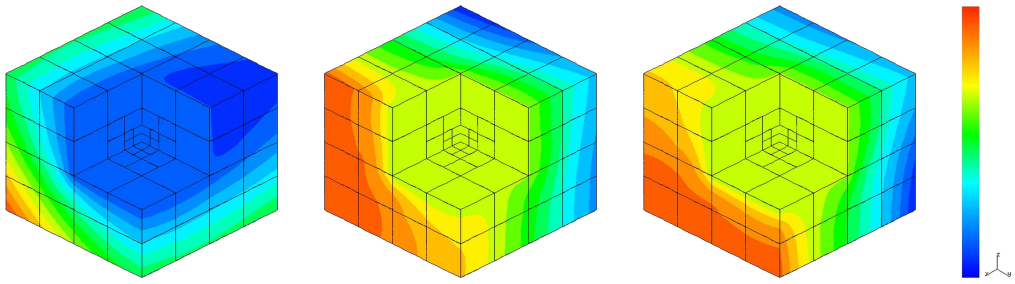


$U_x \in [-2.10e-4,\ 2.99e-3]$ $U_y \in [-1.16e-3,\ 5.76e-4]$ $U_z \in [-1.16e-3,\ 5.76e-4]$

FIG. 5. Maps of displacements – MsFEM ($p_{\mathrm{MACRO}} = 1$, $p_{\mathrm{MICRO}} = 1$, top row) and the reference solution (bottom row).



$u_x \in [-2.96e-4,\ 3.50e-3]$ $u_y \in [-1.37e-3,\ 7.28e-4]$ $u_z \in [-1.37e-3,\ 7.28e-4]$



$U_x \in [-2.88e-4,\ 3.44e-3]$ $U_y \in [-1.34e-3,\ 7.13e-4]$ $U_z \in [-1.34e-3,\ 7.13e-4]$

FIG. 6. Maps of displacements – MsFEM ($p_{\mathrm{MACRO}} = 2$, $p_{\mathrm{MICRO}} = 1$, top row) and the reference solution (bottom row).

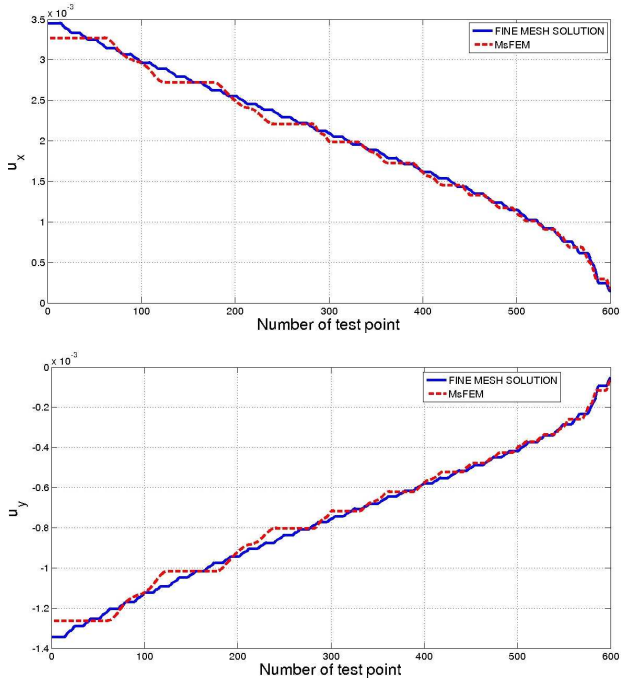


FIG. 7. Displacements along the segment – components u_x (top) and u_y (bottom).

5. Conclusions

The presented results illustrate applicability of both homogenization methods to difficult problems with singularities at both analysis levels. A reasonable reduction of DOFs number was obtained without introducing large error to the solution. Both methods were implemented in *hp*-adaptive code [7]. However, only the MsFEM is capable of dealing with higher-order approximation at any of the scales. Due to the specifics of the Moore-Penrose pseudoinverse, local numerical homogenization cannot cope with higher-order functions. Practical application to nonlinear problems also shows the superiority of the MsFEM, since the evaluation of effective stiffness matrices is load independent, which is contrary to the local homogenization in which these computations have to be repeated for the updated load vector.

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