Publishing House
A K A P I T

COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów

Vol. 13, 2013, No. 2

NUMERICAL ASPECTS OF COMPUTATIONAL HOMOGENIZATION

MARTA SERAFIN*, WITOLD CECOT

Cracow University of Technology, ul. Warszawska 24, 31-155 Kraków
**Corresponding author: mserafin@L5.pk.edu.pl*

Abstract

Computational homogenization enables replacement of a heterogeneous domain by an equivalent body with effective material parameters. Approach that we use is based on two-scale micro/macro analysis. In the micro-scale heterogeneous properties are collected in so-called representative volume elements (RVE), which are small enough to satisfy separation scale condition, but also large enough to contain all information about material heterogeneity. In the macro-scale the material is assumed as a homogeneous with the effective material parameters obtained during RVE analysis. The coupling between both scales is provided at the selected macro-level points, which are associated to independent RVE. Then, approximation of solution in the whole domain is performed. Even though such a homogenization significantly reduces the time of computation, the efficiency and accuracy of the analysis are still not trivial issues. In the micro-level it is required to guarantee accurate representation of heterogeneity and at both scales the optimal number of degrees of freedom should be used.

The paper presents application of one of the most efficient numerical techniques, i.e. automatic hp-adaptive FEM that enables a user to obtain error-controlled results in rather short time; assessment of homogenization error, that is crucial for determination of parts of the body, where homogenization cannot be used and the hp-mixed FEM discretization details.

Key words: homogenization, representative volume element, adaptive finite element method, mixed FEM

1. INTRODUCTION

Even though numerical homogenization speeds up solution of real-life problems for heterogeneous materials the time of computation may be very large, especially if nonlinearity is accounted for. Therefore, we discuss in this paper certain numerical aspects that should increase efficiency of computational homogenization (Feyel, 2003; Gitman, 2006; Kouznetsova et al., 2004) without loosing its accuracy.

Numerical analysis is performed by the automatic *hp*-adaptive version of FEM (Demkowicz et al., 2002). It is well known that the method gives the fastest convergence for linear problems. We have confirmed that one may expect the same situation for inelastic problems (Serafin and Cecot, 2012) and it may be used both at the micro and macro-levels.

Since stresses are of primary interest we decided to use the mixed FEM, in which stresses are approximated directly, rather than by derivatives of displacements. The stability of this approach is a difficult task (Arnold et al., 2007) but efficient and stable *hp*-mixed FEM is possible if appropriate weak formulation and shape functions are used.

In order to increase reliability of the results the error of homogenization is estimated (Cecot et al., 2012). We propose assessment of homogenization error by additional analyses in selected subdomains with boundary conditions determined by the homogenized solution. Residuum of the differential equa-

 ISSN 1641-8581

tion for heterogeneous body may also be used as another criterion for detection of subdomains with large discrepancy between the exact and homogenized solutions.

2. ADAPTIVE FINITE ELEMENT METHOD

In this paper automatic *hp*-adaptive finite element method, proposed by Demkowicz et al. (2002), is used for numerical analysis. Its main adventage is exponential convergence, superior to *h* and *p* adaptation techniques, where only algebraic convergence may be obtained.

This automatic mesh adaptation was successfully used for various linear problems. Its key point is an appropriate strategy of anisotropic *h*, *p* or *hp* mesh refinement. The strategy proposed by Demkowicz et al. (2002) is based on the interpolation error estimate, which is a good upper bound of the best approximation error that in turn, for coercive problems by the Cea's lemma, is the upper bound for the actual approximation error. The aforementioned interpolation error is estimated making use of a fine mesh solution ($\mathbf{u}_{h/2,p+1}$), denoted here for the sake of brevity by $\mathbf{u}$ that serves as a substitute for the exact solution. Such an "exact" solution is interpolated locally by the possible new *hp*-refined meshes. The difference between $\mathbf{u}$ and its interpolant approximates the interpolation error and the optimal anisotropic mesh refinement is determined in such a way that the reduction of the interpolation error per number of additional degrees of freedom is maximal. It means that for the coarse mesh the optimal (*h*, *p* or *hp*) refinement is determined by maximizing the following expression

$$\omega = \frac{|\mathbf{u}-\Pi_{hp}\,\mathbf{u}|^2_{H^1} - |\mathbf{u}-\Pi_{hp,new}\,\mathbf{u}|^2_{H^1}}{N_0 - N_C} \quad \text{and}$$

$$\omega(M_{hp,opt}) = \max_{M_{hp,new}} \omega(M_{hp,new}) \qquad (1)$$

with additional assumption that the mesh is one-irregular, where $M_{hp,new}$, $M_{hp,opt}$ denote arbitrary and the optimal new meshes, respectively; $\Pi_{hp}\,\mathbf{u}$, $\Pi_{hp,new}\,\mathbf{u}$ denote H^1 projection-based interpolants on the current and optimal meshes, respectively; N_0, N_C are the numbers of degrees of freedom in optimal and current meshes. The maximization is performed by search over a suitable subset of all possible *hp* refinements for every coarse mesh element.

Thus, the algorithm of adaptation approach starts with the solution of the problem on the current (coarse) mesh ($\mathbf{u}_{h/2,p+1}$). Then, the refinement in both *h* and *p* is performed and the optimal mesh is selected by maximization of the function ω defined by equation (1). For large problems computation of the fine mesh solution may be time-consuming. However, only partially convergent solution obtained by e.g. a fast two-grid solver may be used to guide the optimal *hp*-refinement.

In this paper convergence of *hp* adaptation strategy for elastic-plastic problems is examined for two-scale modeling and some modifications of the algorithm are proposed. According to literature (Barthold et al., 1998; Cecot, 2007; Gallimard, 1996), inelastic deformations should be accounted for in a special way in a-posteriori error estimates in order to obtain appropriate stress approximation accuracy. Additional *h*-refinement is proposed along elastic-plastic interface, which is a place of lower solution regularity. Such an algorithm is called here modified (automatic) *hp*-refinement.

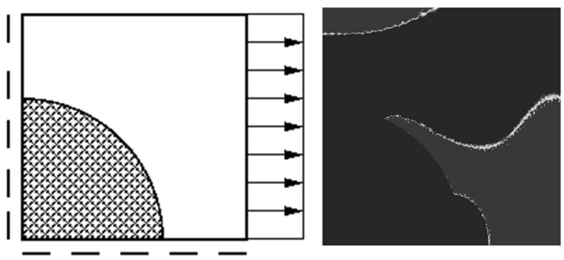

Fig. 1. *RVE. Boundary conditions, elastic and plastic zones. No-penetration boundary conditions were assumed on the left and bottom sides. Zero and constant loading (220 MPa) were applied at the top and right edges.*

Table 1. *Material parameters.*

Material parameters	inclusion	matrix
Young modulus (GPa)	300	100
Poisson ratio	0.3	0.3
Yield strength (MPa)	300	200
Hardening coefficient (GPa)	30	10

To verify the efficiency of automatic *hp*-adaptive FEM for inelastic problems RVE with cylinder-like inclusion was analyzed. A quarter of the domain was considered (figure 1). Both materials underwent elastic-plastic deformations. More precisely plane strain problem with the Mises yield condition, normality rule with kinematic hardening and boundary conditions, specified in figure 1, are considered. Material parameters are collected in table 1. After additional *h*-refinements of elements, which contained both elastic and plastic parts, elastic-plastic zone was successfully detected. Comparison of meshes obtained by original and modified *hp* algorithm is shown in figure 2. Convergence history is presented in figure 3. On the basis of this and other, not presented here, examples one may conclude that the original automatic *hp* algorithm works well for inelastic problems, even though elastic-plastic interface is not detected in accurate way.

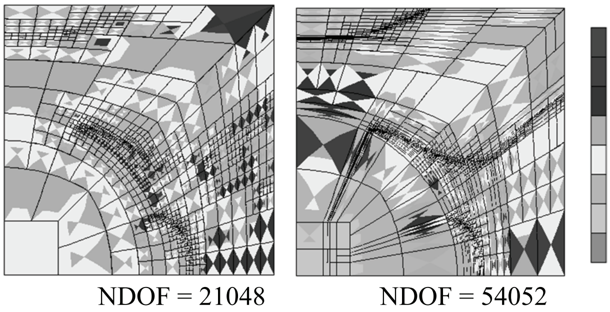

Fig. 2. RVE. Mesh after 40 steps of original and 20 steps of modified hp-refinements (grey scale indicates order of approximation).

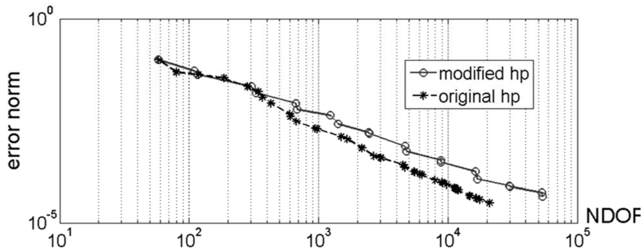

Fig. 3. RVE. Convergence of error norm.

3. MIXED FINITE ELEMENT METHOD

Mixed method enables independent approximation of at least two fields. Such approximation of stresses is useful in multiscale computations, where homogenization is based on evaluation of stress in the micro-scale. However, stable mixed finite elements for solid mechanics are very difficult to construct. They have to provide symmetry of stress tensor and continuity of only traction across interelement boundaries, rather than all the stress components. One may use a modified Hellinger-Reissner principle, in which stress tensor symmetry is enforced in a weak way (Arnold et al., 2007; Qiu & Demkowicz, 2009).

The problem has the following form: *find* $\boldsymbol{\sigma} \in H_t(\mathrm{div}, \Omega, M)$, $\mathbf{u} \in L^2(\Omega, V)$ *and* $\mathbf{p} \in L^2(\Omega, K)$ *such that:*

$$\begin{cases} \int_\Omega \boldsymbol{\tau}:\mathbf{C}^{-1}\boldsymbol{\sigma}\, d\Omega + \int_\Omega \mathrm{div}\boldsymbol{\tau}\cdot\mathbf{u}\, d\Omega + \int_\Omega \boldsymbol{\tau}\cdot\mathbf{p}\, d\Omega = \int_{\partial\Omega} \boldsymbol{\tau}\mathbf{n}\cdot\hat{\mathbf{u}}\, ds \\ \int_\Omega \mathbf{v}\cdot\mathrm{div}\boldsymbol{\sigma}\, d\Omega = -\int_\Omega \mathbf{v}\cdot\mathbf{b}\, d\Omega \\ \int_\Omega \mathbf{q}\cdot\boldsymbol{\sigma}\, d\Omega = 0 \end{cases} \quad (2)$$

$$\forall\boldsymbol{\tau} \in H_0(\mathrm{div}, \Omega, M),\ \forall\mathbf{v} \in L^2(\Omega, V),\ \forall\mathbf{q} \in L^2(\Omega, K)$$

where M is the space of second order, but not necessary symmetric tensors, K is the space of skew-symmetric tensors.

The example of a tensor shape function that enables obtaining continuous tractions at every point of element interfaces may have the following form

$$\boldsymbol{\sigma}^x = \begin{bmatrix} x_{,\xi}y_{,\eta} & y_{,\xi}y_{,\eta} \\ -x_{,\xi}x_{,\eta} & -y_{,\xi}x_{,\eta} \end{bmatrix} / \det\mathbf{J} \quad (3)$$

where ξ and η denote coordinates of master element, x and y are coordinates of physical element, **J** stands for Jacobi matrix of transformation between those elements.

One may also use formula obtained by Piola transformation that gives the following stress shape function possessing the same properties

$$\boldsymbol{\sigma}^x = \begin{bmatrix} x_{,\xi} & y_{,\xi} \\ 0 & 0 \end{bmatrix} / \det\mathbf{J} \quad (4)$$

The main difference between both formulas is in definition of degrees of freedom (traction in normal/tangent or x/y directions). Comparison of traction components continuity of approximation by equations (3) and (4) is shown in figure 4.

The RVE with square-like inclusion in plane strain state was considered as a benchmark for the proposed mixed approximation. A quarter of the domain was taken into account (figure 5) with appropriate boundary conditions. Deformations were only in elastic range. In this example inclusion was much weaker than the matrix (Young modulus: 0.002GPa and 200GPa, respectively; Poisson ratio for both materials: 0.3). Simulation of tension was performed and this way effective material parameters were computed. Convergence of effective Young modulus obtained by classical FEM (displacement formulation) and mixed method (displacement-stress formulation) is compared in figure 6. One may observe, that if we use both methods with small number of degrees of freedom we are able to evaluate effective value with a good accuracy as an average of both solutions.

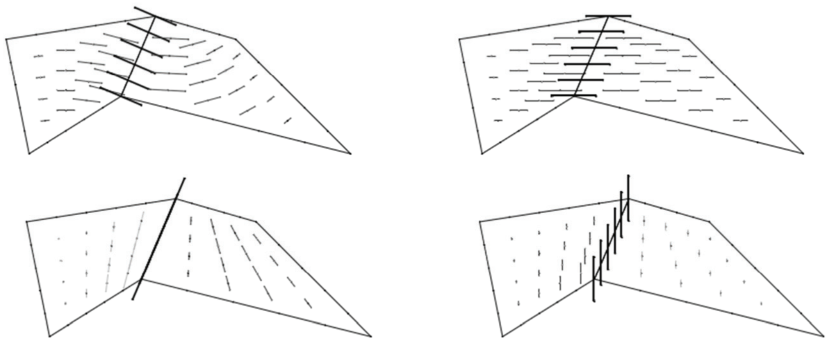

Fig. 4. Traction components continuity. The arrows along the common edge denote tractions evaluated for stress fields of adjacent elements along this edge.

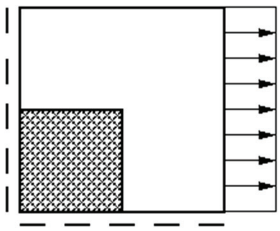

Fig. 5. RVE. Boundary conditions. No-penetration boundary conditions were assumed on the left and bottom sides. Zero and constant loading were applied at the top and right edges.

mation analysis of macrostructures. In that method the adaptation zones that correspond to regions with high strain-gradients, are identified based on a post-processing step on the homogenized solution. Subsequently, for critical zones, exact microstructural representation is introduced, without intermediate models.

Here, other possibilities of modeling error estimation are presented, since this issue is essential for reliability of the results. One is based on the solution of heterogeneous problem in selected subdomains with boundary conditions assumed on the basis of homogenized solution. Such an error estimate consists of a few steps:

1) compute the homogenized solution $\mathbf{u}_0$ in domain Ω,
2) select a part of the body, where the error should be estimated and consider heterogeneous material in this subdomain,
3) solve the boundary value problem for cut-off heterogeneous subdomain **A** with boundary conditions resulted from homogenized solution; obtain the solution $\mathbf{u}_I$ and consider it in a smaller truncated part of the selected heterogeneous domain **B**,
4) estimate the error between solution $\mathbf{u}_I$ and homogenized one $\mathbf{u}_0$ in subdomain **B**.

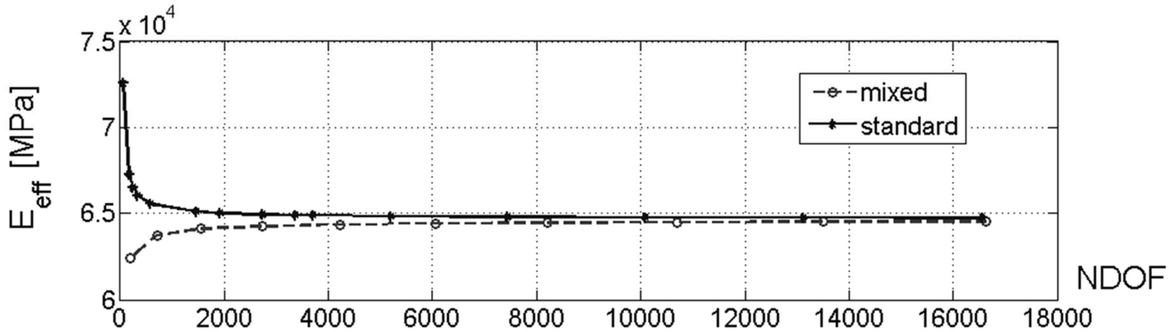

Fig. 6. Effective Young modulus.

4. MODELING ERROR ESTIMATION

Replacement of a heterogeneous body by a homogenized one with effective material parameters introduces an error, related to incomplete information about the microstructure. Thus, it may happen that the homogenization should not be used for certain part of the domain. A global explicit estimate using the homogenized (coarse) elasticity tensor and the actual fine-scale elasticity tensor was proposed by Zohdi et al. (1996). However, it is not able to capture local error. A scale adaptation strategy developed by Temizer and Wriggers (2011) was used to account for loss of accuracy for the finite defor-

Another possibility is based on residuum, by analogy to the explicit residual error indicator for FEM solution (Babuska & Miller, 1987; Babuska & Rheinboldt, 1978). The proposed algorithm of homogenization error estimation may be stated in the following way:

1) compute effective material parameters for homogenized domain,

2) solve homogenized problem with effective properties to obtain $\mathbf{u}_0$,
3) compute residuum R of equilibrium equation $\mathbf{R} = \mathrm{div}\boldsymbol{\sigma}_0 + \mathbf{X}$ for heterogeneous body in each macro-scale finite element, where $\mathbf{X}$ denotes body forces, $\boldsymbol{\sigma}_0$ stands for stress tensor (in fact, $\mathbf{R}$ is a distribution; its norm, which we are interested in, may be bounded by the norms of regular part of $\mathbf{R}$ and jumps of the first derivatives of the solution),
4) compute jumps of tractions at interfaces of finite elements ($\mathbf{J}_\mathbf{i}^\mathbf{e} = \mathbf{t}_\mathbf{i}^+ - \mathbf{t}_\mathbf{i}^-$ on $\partial\omega_k$) and material components ($\mathbf{J}_\mathbf{i}^\mathbf{m} = \mathbf{t}_\mathbf{i}^{\mathrm{m}1} - \mathbf{t}_\mathbf{i}^{\mathrm{m}2}$ on $\partial\omega_m \subset \partial\omega_k$), where $\partial\omega_k$ denotes common edge of adjacent elements and $\partial\omega_m$ stands for material (m1, m2) interfaces,
5) wherever $\eta_R = h\|\mathrm{R}\|_0 + h^{1/2}\|\mathbf{J}^\mathbf{e}\|_0 + h^{1/2}\|\mathbf{J}^\mathbf{m}\|_0$ is large, homogenization should not be used.

The L-shaped domain in plane strain state was considered to perform numerical tests. The metal matrix was reinforced by cylinder-like inclusions, distributed uniformly. Assumed boundary conditions, as well as material distribution, are shown in figure 7.

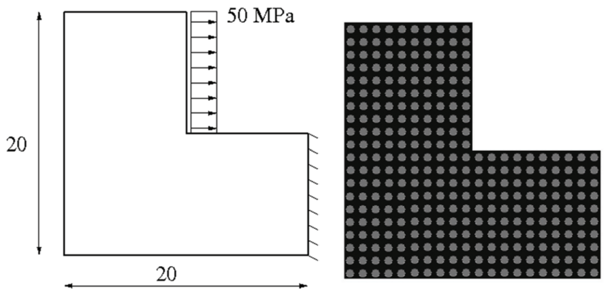

Fig. 7. L-shaped domain. Boundary conditions and material distribution.

A part of the domain (reentrant corner of L-shaped domain – figure 8) was selected and estimation by subdomain solutions was used. Estimated error for displacements is as follows

$$\frac{\|\boldsymbol{u} - \boldsymbol{u}_0\|_{0,B}}{\|\boldsymbol{u}_0\|_{0,B}} \approx 0{,}13\%$$

The residual modeling error estimate was also used for this example. Residuum in each macro-element of homogenized body was calculated and error indicators were evaluated. Assumed admissible error enables selection of subdomains, which should not be homogenized (figure 9). Automatic *hp* refinements enables obtaining a mesh that captures all the details of heterogeneity in selected subdomains.

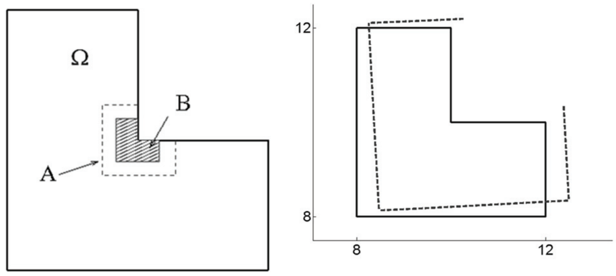

*Fig. 8. L-shaped domain. Boundary displacements for cut-off heterogeneous domain **A** resulted from homogenized solution.*

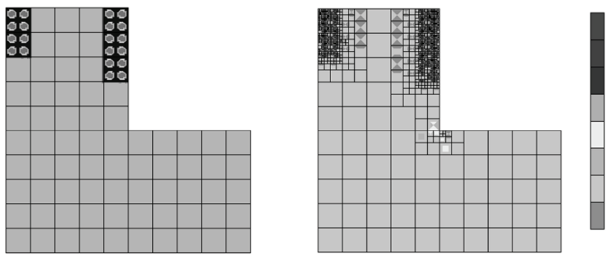

Fig. 9. L-shaped domain with homogeneous and heterogeneous subdomains. New material distribution after excluding, on the basis of residual error estimate, two subdomains from homogenization and appropriate FE mesh (gray scale indicates order of approximation).

5. CONCLUSIONS

The paper presents application of two efficient numerical techniques, i.e. automatic *hp* mesh adaptation and mixed approximation for inelastic two-scale analysis. Prospects of both approaches were positively verified by solution of selected numerical examples. In order to obtain reliable results the error introduced by homogenization was estimated giving information about quality of the results. Numerical improvements of computational homogenization, presented in this paper, will be used in further applications of the approach in modeling of elastic-plastic composites

Acknowledgment. This research was supported by the National Science Center under grant 2011/01/B/ST6/07312.

REFERENCES

Arnold, D.N., Falk, R., Winther, R., 2007, Mixed finite element methods for linear elasticity with weakly imposed symmetry, *Mathematics of Computations*, 76, 1699-1723.

Babuska, I., Miller, A., 1987, A feedback finite element method with a posteriori error estimation. Part 1, *Comp. Meth. Appl. Mech. Engng*, 61, 1-40.

Babuska, I., Rheinboldt, W.C., 1978, Error estimates for adaptive finite element computations, *Int. J. Num. Meth. Engng*, 12, 1597-1615.

Barthold, F., Schmidt, M., Stein, E., 1998, Error indicators and mesh refinements for finite-element-computations of elastoplastic deformations, *Computational Mechanics*, 22, 225-238.

Cecot, W., 2007, Adaptive FEM analysis of selected elastic-visco-plastic problems, *Comp. Meth. Appl. Mech. Engng*, 196, 3859-3870.

Cecot, W., Serafin, M., Klimczak, M., 2012, Reliability of computational homogenization, *International US-Poland Workshop: Multiscale Computational Modeling of Cementitious Materials*, ISBN 978-83-7242-667-3, 183-194.

Demkowicz, L., Rachowicz, W., Devloo, Ph., 2002, A fully automatic hp-adaptivity, *Journal of Scientific Computing*, 17, 127-155.

Feyel, F., 2003, A multilevel finite element method (FE^2) to describe the response of highly non-linear structures using generalized continua, *Comput. Methods Appl. Mech. Engrg.*, 192, 3233-3244.

Gallimard, L., Ladeveze, P., Pelle, J.P., 1996, Error estimation and adaptivity in elastoplasticity, *Int. J. Numer. Meth. Engng*, 39, 189-217.

Gitman, I., 2006, *Representative Volumes and Multi-scale Modelling of Quasi-brittle Materials,* PhD thesis, Delft University of Technology.

Kouznetsova, V., Geers, M., Brekelmans, W., 2004, Size of a representative volume element in a second-order computational homogenization framework, *International Journal for Multiscale Computational Engineering*, 2, 575-598.

Qiu, W., Demkowicz, L., 2009, Mixed hp-finite element method for linear elasticity with weakly imposed symmetry, *Comp. Meth. Appl. Mech. Engng*, 198, 3682-3701.

Serafin, M., Cecot, W., 2012, Self hp-adaptive FEM for elastic-plastic problems, *International Journal for Numerical Methods in Engineering* (submitted).

Zohdi, T.I., Oden, J.T., Rodin, G.J., 1996, Hierarchical modeling of heterogeneous bodies, *Comput. Methods Appl. Mech. Engrg.*, 138, 273-298.

Temizer, I., Wriggers, P., 2011, An adaptive multiscale resolution strategy for the finite deformation analysis of microheterogeneous structures, *Comput. Methods Appl. Mech. Engrg.*, 200, 2639-2661.

NUMERYCZNE ASPEKTY HOMOGENIZACJI OBLICZENIOWEJ

Streszczenie

Homogenizacja komputerowa pozwala na zastąpienie materiału niejednorodnego przez ośrodek jednorodny z efektywnymi parametrami materiałowymi. Podejście to bazuje na analizie w dwóch skalach – mikro i makro. W skali mikro rozważa się materiał niejednorodny w tzw. reprezentatywnym elemencie objętościowym (RVE), który jest na tyle mały, żeby zapewnić separację skal, równocześnie na tyle duży, aby informacje o wszystkich niejednorodnościach zostały w nim zawarte. W skali makro zakłada się materiał jednorodny z efektywnymi parametrami materiałowymi otrzymanymi z analizy RVE. Transfer informacji między skalami dokonywany jest w wybranych punktach skali makro, powiązanymi z niezależnymi RVE. Następnie dokonywana jest aproksymacja rozwiązania w skali makro. W ten sposób redukowany jest czas obliczeń, jednak należy zagwarantować poprawność uzyskanych wyników. W skali mikro niezbędne jest dokładne odzwierciedlenie mikrostruktury, a w obu skalach optymalnej liczby stopni swobody.

W pracy zastosowano dwie efektywne techniki numeryczne, t.j. hp-adaptacyjną wersję metody elementów skończonych, która pozwala na uzyskanie wiarygodnych wyników w stosunkowo krótkim czasie oraz sformułowanie wielopolowe pozwalające uzyskać możliwie dokładną aproksymację naprężeń, będących głównym celem obliczeń. W publikacji zawarto również możliwości oszacowania błędu homogenizacji, niezbędnego do wyznaczenia obszarów, w których homogenizacja nie powinna być stosowana ze względu na zbyt duży błąd.

Received: September 20, 2012
Received in a revised form: October 31, 2012
Accepted: November 9, 201