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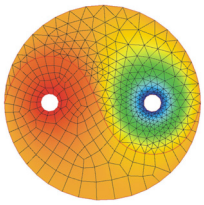

IDENTIFICATION OF STOCHASTIC MATERIAL PROPERTIES IN MULTISCALE MODELLING

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Abstract

The paper is devoted to multiscale identification of material properties in microscale. The identification process allows one to identify properties (like material constants, geometry) in microscale on the basis of measurements performed for macroscale. The presented approach assumes stochastic material properties in microscale. The identification problem is formulated as minimization of a functional which represents a distance between measured and theoretical values of displacements and strains. The Monte Carlo method combined with the finite element method is used to obtain theoretical displacements and strains values. The identification problem is solved with use of an evolutionary algorithm.

Key words identification, stochastic, multiscale, FEM

1. INTRODUCTION

The paper is devoted to identification problems in multiscale modeling in stochastic conditions. The multiscale modeling is able to take into account materials or geometrical effects which occur in microscale and obtain more precise results in macroscale analysis. The identification allows one to evaluate materials or geometrical parameters of a structure in microscale on the basis of statistical measurements in macroscale. The methodology presented in the paper takes into account stochastic nature of parameters in the microscale and the identification problem is formulated as minimization of a certain stochastic objective function. The problem is transformed into deterministic one in which a new objective functional dependent on mean values and variances is minimized with respect to moments of stochastic parameters. An approach based on evolutionary computing is presented in the minimization problem. The main advantage of the presented approach consists in the fact that a gradient of the objective functional is no needed and moreover there is a great probability of finding the global minimum. The computational homogenization is used to multiscale modelling of the structures. The problem formulation, description of optimization algorithm and a numerical example are shown in the following chapters.

2. MULTISCALE STOCHASTIC MODELLING OF STRUCTURE

The multiscale modelling incorporates two or more scales into analysis of a structure (Madej et al., 2008). One of the numerical techniques which enables multiscale analysis of physical systems is a computational homogenization. The detailed description of the computational homogenization can be found in Terada and Kikuchi (2001). In the case

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of structures with a local periodicity there are areas of the system with the same microstructure. The example of such a system is presented in figure 1. Microstructures can be also built from lower scale locally periodic microstructures. The goal of the computational homogenization is analysis of the system taking into account the local periodicity of microstructures. The main advantage of this approach is the fact that analysis in a few scales allows one to use models with at least a few orders of degrees of freedom lower than model created in one scale.

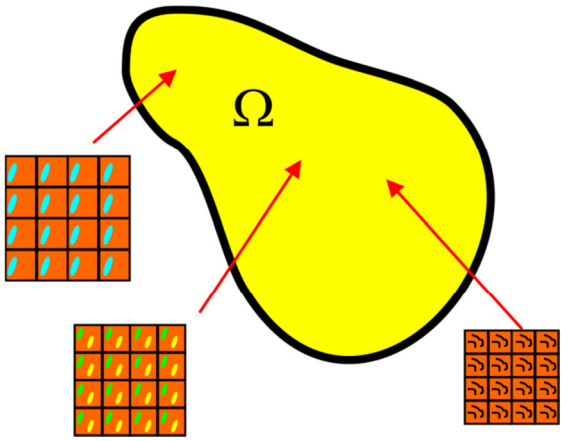

Fig. 1. *Two scale model of a material system with locally periodical microstructures.*

The material parameters for each integration point in finite elements depend on the solution of a representative volume element (RVE) in the lower scale. In most cases it is modeled as a cube (3D) or a square (2D) and it can contain voids, cracks, inclusions and other properties of microstructure. Computational methods like the Finite Element Method (FEM) (Zienkiewicz et al., 2005) or the Boundary Element Method (BEM) (Burczyński, 1995) are used to solve the boundary value problem for RVE. The periodic boundary displacement conditions are taken into account. The strains from the higher level are prescribed as additional boundary conditions. The RVE for each integration point of the higher level model must be created and stored for the next iteration steps if the nonlinear problem with plasticity is considered. The transfer of information both form lower to higher and higher to lower scales is needed in most cases. The transfer of average strains and stresses between scales is shown in figure 2.

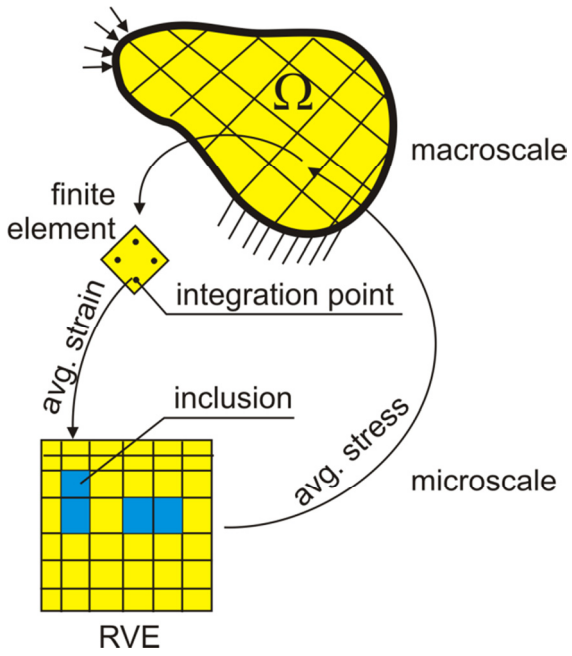

Fig. 2. *The average strain and stress transfer between scales.*

The one way transfer of results (from lower to higher scales) is possible if the linear problem is considered. The material parameters for the higher scale are obtained on the basis of solving a few direct problems for the RVE in the lower scale. The homogenized material parameters depend on average stress values in the RVE obtained after applying average strains to the RVE. The stress-strain relation is used in the higher level model. The average strains are strains in the integration point from the higher level.

Very often material and geometrical parameters of the structure in the microscale have uncertain nature. One of the most important model of uncertainty used in identification problems is based on the theory of probability and stochastic processes (Burczyński & Orantek, 2009). The multiscale analysis can be performed for structures with stochastic material or geometry which occur in the RVE.

Suppose that stochastic material and geometrical parameters of the RVE are described by random variables $X_i(\gamma), i = 1,2,..,n, \gamma \in \Gamma$, where Γ is the space of elementary events which represents all the possible simplest outcomes of a trial associated with the given random phenomenon. In the theoretical model of random phenomena the basic role is played by the probability space (Γ,F,P), where F is a σ - algebra of subset of Γ. Elements of the F are called random events and P is a probability defined on F (Papoulis, 1991). A random variable $X_i = X_i(\gamma), \gamma \in \Gamma$, defined on a sample space Γ

and measurable with respect to P, i.e. for every real number x_i, the set $\{\gamma : X_i(\gamma) < x_i\}$ is an event in F.

A random vector

$$\mathbf{X}(\gamma) = [X_1(\gamma), X_2(\gamma), ..., X_i(\gamma), ..., X_n(\gamma)] \quad (1)$$

is a function, measurable respect to P which takes every element $\gamma \in \Gamma$ into a point $\mathbf{x} \in R^n$ and has an n-dimensional Gaussian distribution of the probability density function given as follows:

$$p(x_1, x_2, ..., x_i, ...x_n) =$$

$$\frac{1}{(2\pi)^{n/2}\sqrt{|\mathbf{K}|}}\left[-\frac{1}{|\mathbf{K}|}|K_{ij}|(x_i - m_i)(x_j - m_j)\right] \quad (2)$$

$|\mathbf{K}| \neq 0$ is the determinant of the matrix covariances, $\mathbf{K}[k_{ij}], i, j = 1, 2, ..., n$, where $k_{ij} = \mathbf{E}[(X_i - m_i)(X_j - m_j)]$, $|K_{ij}|$ is the co-factor of the element k_{ij} the matrix $\mathbf{K}$ and $m_i = \mathbf{E}[X_i(\gamma)]$ is the mean value of $X_i(\gamma)$.

$\mathbf{E}[\cdot]$ indicates expectation or ensemble average.

It is assumed that random parameters are independent random variables. The joint probability density function is expressed by the probability density function of single random parameters as follows:

$$p(x_1, x_2, ..., x_i, ...x_n) = p_1(x_1)p_2(x_2)...p_i(x_i)...p_n(x_n) \quad (3)$$

where

$$p_i(x_i) = N(m_i, \sigma_i) = \frac{1}{\sigma_i\sqrt{2\pi}}\exp\left[-\frac{(x_i - m_i)^2}{2\sigma_i^2}\right] \quad (4)$$

is the probability density function of the random parameter $X_i(\gamma)$, where $\sigma_i^2 = \mathbf{E}[(X_i - m_i)]^2$ is the variance and σ_i denotes the standard deviation of $X_i(\gamma)$.

It is seen that if the random parameters $X_i(\gamma), i = 1, 2, .., n$, are random independent Gaussian variables, two moments – the mean value m_i and the standard deviation σ_i (or the variance σ_i^2) describe the probability density function of each random variable $X_i(\gamma)$.

The random vector (1) now can be replaced by a deterministic vector:

$$Y = [(m_1, \sigma_1^2), (m_2, \sigma_2^2), ..., (m_i, \sigma_i^2), ..., (m_n, \sigma_n^2)] \quad (5)$$

which is described by moments m_i and $\sigma_i^2, i = 1, 2, ..., n$.

3. MULTISCALE IDENTIFICATION PROBLEM FORMULATION IN STOCHASTIC CONDITIONS

The goal of identification in multiscale modelling is to find a vector of material and geometrical parameters **X** treated as design variables on the micro-level which minimize an objective function $J_o = J_o(\mathbf{u}, \boldsymbol{\varepsilon})$ dependent on state fields of displacements **u** and strains **ε** on the macro-level of the structure (Burczyński & Kuś, 2009). In the considered problem the vector $\mathbf{X} = \mathbf{X}(\gamma)$ contains random parameters which should be determined from experimental statistical data.

One assumes that available measurement data of random displacements $\hat{\mathbf{u}}(\mathbf{x}_k, \gamma) \equiv \hat{\mathbf{u}}_k(\gamma)$ at sensor points (figure 3) $\mathbf{x}_l, l = 1, 2, ..., K$, and strains $\hat{\varepsilon}(\mathbf{x}_l, \gamma) \equiv \hat{\varepsilon}_l(\gamma)$ at sensor points $\mathbf{x}_l, l = 1, 2, ..., L$, are characterized by the mean values $m_{\hat{\mathbf{u}}_k} = \mathbf{E}\hat{\mathbf{u}}_k(\gamma)$ and $m_{\hat{\varepsilon}_l} = \mathbf{E}\hat{\varepsilon}_l(\gamma)$ and variances $\sigma_{\mathbf{u}_k}^2 = \mathbf{E}[\hat{\mathbf{u}}_k(\gamma) - m_{\hat{\mathbf{u}}_k}]^2$ and $\sigma_{\hat{\varepsilon}_l}^2 = \mathbf{E}[\hat{\varepsilon}_l(\gamma) - m_{\hat{\varepsilon}_l}]^2$.

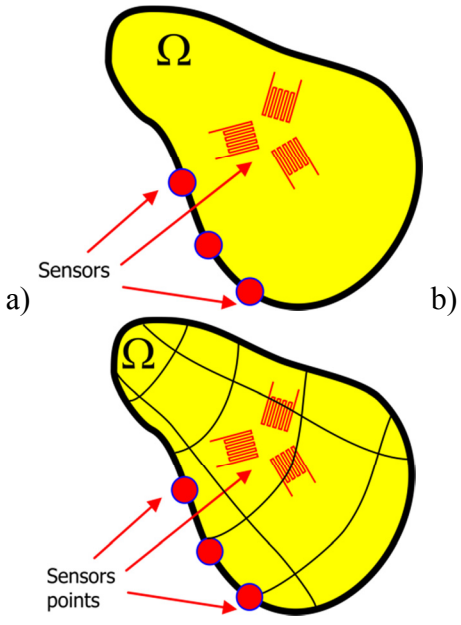

Fig. 3. *Sensors in: a) the real object and b) the computational model.*

The identification problem is solved by converting it into a constrained minimization problem. One constructs a functional which represents a distance between measured $\hat{\mathbf{u}}_k(\gamma)$ and $\hat{\varepsilon}_l(\gamma)$ and theoretical values of displacements $\mathbf{u}(\mathbf{x}_k)$ and strains $\varepsilon(\mathbf{x}_l)$:

$$J = a\sum_{k=1}^{K}\left|\mathbf{u}(\mathbf{x}_k)-\hat{\mathbf{u}}_k(\gamma)\right| + b\sum_{l=1}^{L}\left|\varepsilon(\mathbf{x}_l)-\hat{\varepsilon}_l(\gamma)\right| \quad (6)$$

where a and b are scaling coefficients.

Unknown material and geometrical parameters at the micro-level are described by random variables $\mathbf{X}(\gamma)=[X_i(\gamma)], i=1,2,...N$. It means that $J=J(\mathbf{X})$.

The problem of finding parameters $\mathbf{X}(\gamma)$ is formulated as the nonlinear stochastic programming problem which is stated as follows:

Find a vector $\mathbf{X}(\gamma)=[X_i(\gamma)], i=1,2,...n$, *which minimizes the objective functional* $J=J(\mathbf{X})$ *with imposed constraints* $x_i^- \le X_i \le x_i^+$.

where x_i^- and x_i^+ are limits of X_i.

The stochastic problem stated above can be converted into an equivalent deterministic task. The objective functional $J=J(\mathbf{X})$ can be approximated as follows:

$$J(\mathbf{X}) \approx J(m_{\mathbf{X}}) + \sum_{i=1}^{N}\left(\left.\frac{\delta J}{\delta X_i}\right|_{m_{\mathbf{X}}}\right)^2 (X_i - m_{\mathbf{X}}) = J_o(\mathbf{X}) \quad (7)$$

$J_o(\mathbf{X})$ being a linear function of normally distributed variables $X_i(\gamma)$ has also the normal distribution which is described by the mean value and variance as follows:

$$m_{J_o} = J_o(m_{\mathbf{X}}) \quad \text{and} \quad \sigma_{J_o}^2 = \sum_{i=1}^{N}\left(\left.\frac{\delta J}{\delta X_i}\right|_{m_{\mathbf{X}}}\right)^2 \sigma_{X_i}^2 \quad (8)$$

Now a new deterministic objective functional can be defined as follows:

$$I = c_1 m_{J_o} + c_2 \sigma_{J_o}^2 \quad (9)$$

where c_1 and c_2 are non-negative scaling weights indicating the relative importance for minimization of the mean m_{J_o} and the variance $\sigma_{J_o}^2$. Setting c_2=0 would mean that the mean value of m_{J_o} is to be minimized with no regard to the variance , while the choice c_1=0 would imply that one is interested in minimizing the dispersion of about an arbitrary mean value. The case c_1=c_2=1 attaches equal importance to both characteristics.

Now the problem is formulated as follows:

$$\min_{Y} I$$

$$\text{with constraints } m_i^- \le m_i \le m_i^+ \quad \text{and} \quad \sigma_i^{2-} \le \sigma_i^2 \le \sigma_i^{2+}, \quad (10)$$

where m_i^-, m_i^+ and $\sigma_i^{2-}, \sigma_i^{2+}$ are limits of mean values and variances, respectively.

Thus, the original stochastic programming problem is reduced to the nonlinear deterministic problem which can be solved using the well-know standard procedure but the main problem consists in the calculation of the derivatives $\delta J/\delta X_i$, i = 1,2,…,N. It is caused by the fact that in the general situation it is impossible to express J in the explicit form with respect to random parameters $X_i(\gamma), i=1,2,...,N$. The problem of finding derivatives $\delta J/\delta X_i$ can be solved using the idea of stochastic shape sensitivity analysis (Burczyński, 1995a).

In the present paper the problem of minimization of the objective functional is solved using the evolutionary algorithms (Burczyński et al., 2006).

If one assumes that

$$c_1 a = \frac{a_1}{|m_{\hat{\mathbf{u}}}|} \quad \text{and} \quad c_1 b = \frac{b_1}{|m_{\hat{\varepsilon}}|}$$
$$c_2 a^2 = \frac{a_2}{|\sigma_{\hat{\mathbf{u}}}^2|} \quad \text{and} \quad c_2 b^2 = \frac{b_2}{|\sigma_{\hat{\varepsilon}}^2|} \quad (11)$$

where a_1, a_2, b_1 and b_2 are new scaling coefficients then the deterministic objective function I can be expressed as follows:

$$I = a_1\sum_{k=1}^{K}\left|\frac{m_{u_k}-m_{\hat{u}_k}}{m_{\hat{u}_k}}\right| + a_2\sum_{k=1}^{K}\left|\frac{\sigma_{u_k}^2-\sigma_{\hat{u}_k}^2}{\sigma_{\hat{u}_k}^2}\right| +$$
$$b_1\sum_{l=1}^{L}\left|\frac{m_{\varepsilon_l}-m_{\hat{\varepsilon}_l}}{m_{\hat{\varepsilon}_l}}\right| + b_2\sum_{l=1}^{L}\left|\frac{\sigma_{\varepsilon_l}^2-\sigma_{\hat{\varepsilon}_l}^2}{\sigma_{\hat{\varepsilon}_l}^2}\right| \quad (12)$$

The objective functional (12) incorporates the differences of mean values and variances of displacements and/or strains obtained from numerical analysis and measurements. The mean values and variances for the numerical analysis can be obtained by solving direct problem with use of computational stochastic methods as the stochastic finite element method (Kleiber & Hien, 1992) or the stochastic

boundary element method (Burczyński & Skrzypczyk, 1999).

In the paper averaged material properties for the RVE are obtained with use of the homogenization method based on the stochastic FEM analysis. The Monte Carlo (MC) based FEM method is applied. The main disadvantage of the MC is a large number of FEM computations needed to obtain stochastic results. The material properties of the composite are randomly generated with the prescribed mean value and variance. The Muller-Box randomization is used to create random material properties. The homogenization method is used for each set of material properties in MC method. The results obtained in each run of MC method are collected and used to present stochastic results of analysis. The presented approach is very time consuming. The multiscale analysis can be performed in parallel way. The averaged material properties are obtained on the basis of 6 independent FEM analyses of RVE (for 3D case). This step can be easy parallelized with speedup close to linear. The MC method also can be parallelized, the multiscale analyses can be performed for each set of material parameters. The stochastic FEM analysis can be also shorten significantly by using other stochastic methods like perturbation method (Kaminski & Kleiber, 2000; Sakata & Ashida, 2011).

4. THE EVOLUTIONARY ALGORITHMS

To minimize the objective functional I (12) the evolutionary algorithm is used in the paper as optimization method (Kuś & Burczyński, 2010; Kuś et al., 2011). The flowchart of the evolutionary algorithm is presented in figure 4. The evolutionary algorithm operates on a population of chromosomes. The design variables are coded into each chromosome, and each chromosome is a potential solution of the optimization problem. The initial population of chromosomes is created in the random way in the first step of the evolutionary algorithm. Then the objective functional values for all chromosomes are calculated. In the next step changes of chromosome genes values are performed by using evolutionary operators. The new generation is performed on the basis of the offspring population created during the selection process. The algorithm iterates until the end condition is fulfilled (expressed e.g. as a maximum number of iterations).

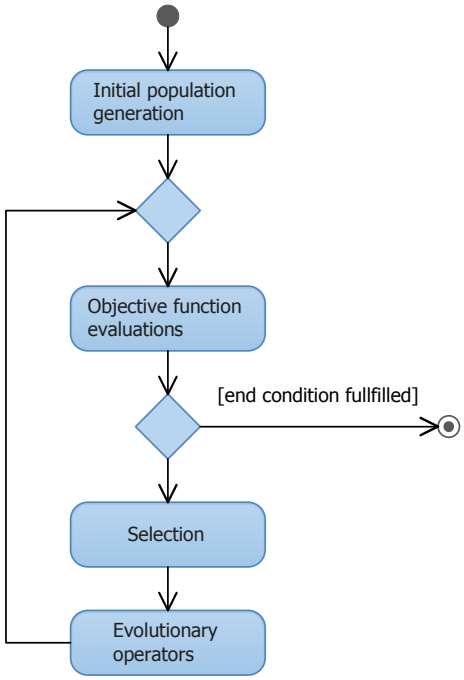

Fig. 4. *The flowchart of the evolutionary algorithm.*

6. NUMERICAL EXAMPLE OF IDENTIFICATION OF MICROSTRUCTURE MATERIAL PROPERTIES

As an example of identification of random parameters the two scale structure is considered (figure 5).The microstructure is built from two materials with stochastic parameters: Young's moduli $E_1(\gamma)$ and $E_2(\gamma)$ and Poison's ratios $\nu_1(\gamma)$ and $\nu_2(\gamma)$, respectively.

The mean values of Young's moduli $m_{E_i}, i=1,2$ and Poisson's ratios $m_{\nu_i}, i=1,2$ are considered to be known and the Poisson's variances $\sigma^2_{\nu_i}, i=1,2$ are also known (see table 1). The goal of the identification is to find variances of Young's moduli $E_1(\gamma)$ and $E_2(\gamma)$:

$$Y=[\sigma^2_{E_1},\sigma^2_{E_2}] \tag{13}$$

with constraints

$$\sigma^{2-}_{E_i} \le \sigma^2_{E_i} \le \sigma^{2+}_{E_i}, i=1,2$$

where limits of variances are given as follows:

$$\sigma^{2-}_{E_1}=0.0025\ [MPa]^2;\ \sigma^{2+}_{E_1}=2.2500\ [MPa]^2$$

and

$$\sigma^{2-}_{E_2}=0.25\ [MPa]^2;\ \sigma^{2+}_{E_2}=225.00\ [MPa]^2$$

Table 1. *The material properties for the microscale*

Material parameter	Value
Young's modulus mean value m_{E_1}	3.4 [*MPa*]
Young's modulus mean value m_{E_2}	72.0 [*MPa*]
Poisson's ratio mean value m_{ν_1}	0.18
Poisson's ratio mean value m_{ν_2}	0.20
Poisson's ratio variance $\sigma^2_{\nu_1}$	0.000625
Poisson's ratio variance $\sigma^2_{\nu_2}$	0.000625

The identification is performed on the basis of stochastic values of displacements for the macro model. The number of displacements sensor point was K=70 and displacements were measured in two directions on the lower part of the macromodel. The objective function described by (12) was applied with parameters $a_1=a_2=1$, $b_1=b_2=0$. The stochastic direct problem was solved by using MC FEM. The MSC.Nastran was applied for single FEM analysis in micro or macro-scales. The homogenization procedure was parallelized in presented approach.

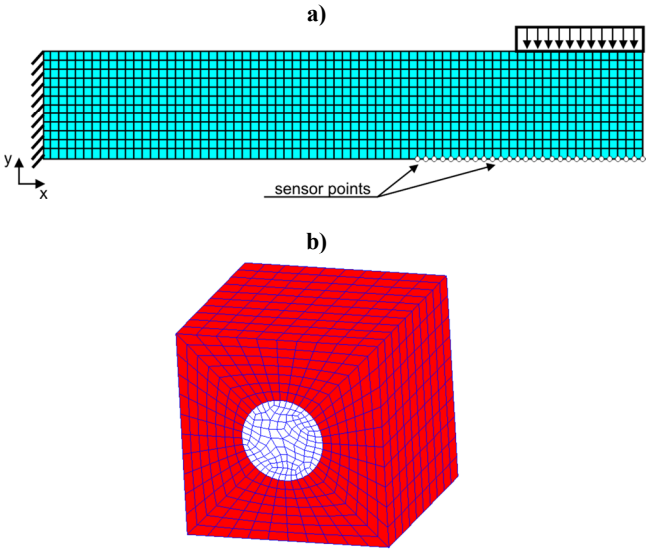

Fig. 5. *a) The macro model with sensor points and boundary conditions, b) the micromodel with two materials*

The minimization of the functional I (12) with respect to Y (13) was performed with use of the described evolutionary algorithm. The simple crossover combined with the Gaussian mutation and the uniform mutation and the ranking selection were used. The parameters of the evolutionary algorithm are shown in table 2. The operators and their probabilities were chosen on the basis of previous numerical experiments based on mathematical test functions and test engineering problems.

Table 2. *The evolutionary algorithm parameters*

Parameter	Value
Number of genes	2
Number of chromosomes	10
Probability of Gaussian mutation and simple crossover	0.9
Probability of uniform mutation	0.1
Ranking selection pressure	0.8

The statistical measured displacements were numerically simulated for the testing purposes. The exact results were known before identification process.

The results of identification after 10 iterations of the evolutionary algorithm are presented in Table 3. The obtained variances of Young's moduli are close to the actual ones. The change of properties of material number 2 had bigger influence on the displacements in the macroscale, the result obtained for this material are closer to actual one.

The number of identified parameters influences the number of genes and iterations of the evolutionary algorithm. The cost of computations will be higher in case of increasing number of identified parameters.

Table 3. *The results of identification*

Parameter	Actual value	Obtained value
Young's modulus variance $\sigma^2_{E_1}$	0.25 $[MPa]^2$	0.14 $[MPa]^2$
Young's modulus variance $\sigma^2_{E_2}$	25.0 $[MPa]^2$	25.7 $[MPa]^2$

7. CONCLUSIONS

The methodology of identification of stochastic parameters of the micromodel on the base of statistical measurements performed for the macroscale was presented in the paper. The problem was solved by

using the Monte Carlo FEM. The numerical example of identification was presented and proved proposed methodology. The identification of full set of random number parameters is planned in the future research. The main drawback of presented method is very slow stochastic direct problem solving. The authors plan to incorporate more efficient methods for obtaining direct problem solutions and parallelization of MC method.

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IDENTYFIKACJA STOCHASTYCZNYCH PARAMETRÓW MATERIAŁOWYCH W MODELOWANIU WIELOSKALOWYM

Streszczenie

Artykuł jest poświęcony zagadnieniom identyfikacji parametrów modelu w skali mikro w ujęciu wieloskalowym. Pozwala to uwzględnić wpływ parametrów materiałowych oraz geometrycznych w skali mikro na rozwiązania w skali makro. Rozwiązanie zagadnienia identyfikacji umożliwia określenie parametrów struktury w skali mikro na podstawie pomiarów przeprowadzonych dla skali makro. Przedstawiona w pracy metodologia oparta jest na założeniu, że parametry w skali mikro mają naturę stochastyczną i można je wyznaczyć dysponując wynikami statystycznych pomiarów eksperymentalnych przemieszczeń i odkształceń w skali makro. Zagadnienie sprowadzono do minimalizacji różnicy między charakterystykami probabilistycznymi przemieszczeń i odkształceń obliczonych dla modelu stochastycznego oraz obiektu rzeczywistego. W tym celu zastosowano koncepcję homogenizacji komputerowej, metodę Monte Carlo oraz algorytm ewolucyjny. Opracowaną koncepcję identyfikacji w warunkach stochastycznych zweryfikowano pozytywnie na przykładzie numerycznym.

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