

Optimization of the materials distribution in composite systems

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Abstract. The optimization of structures in macro scale is widely used nowadays. The goal of the paper is to apply optimization techniques to obtain better performance on the micro level. The presented methods open new possibilities. The structures build with the use of materials with optimal microstructure can obtain the best performance. The microstructure can be optimized taking into account loads of the macro structure. The optimization of microstructure is not easy currently, but in future, in applications where performance of the structure is very important, the presented approach may be used with success. A bio-inspired method based on the artificial immune system (AIS) is used to solve the optimization problem. Immune computing provides a great probability of finding the global optimum. The optimal topology is generated by the level set approach. Optimization (identification) of the topology and the distribution of the mass density of microstructure considered to two materials by the minimization of the fitness function which depended on the coefficients of stiffness matrices. The paper presents methodology, algorithm of optimization and numerical examples.

1. Introduction

The paper is devoted to immune optimization (identification) in multiscale problems. The structure modelled as a macrostructure with a local periodic microstructure is considered. The multiscale analysis is performed with the use of the homogenization method. The objective function evaluation with the use of the homogenization algorithm is considered.

The computational homogenization is the one of the numerical techniques which enables multiscale analysis of the structures. The detailed description of the computational homogenization in which the structures with a local periodicity are considered is presented in the paper[14]. In the local periodicity there are areas of structure with the same microstructure. The microstructures can also be built from lower scale locally periodic microstructures. The analysis of the structure taking into account the local periodicity of microstructures is the goal of the computational homogenization. Analysis in a few scales which allows to use models with at least a few orders of degrees of freedom lower than model created in one scale is the main advantage of the computational homogenization.

The material parameters for each integration point in finite elements depend on the solution of a representative volume element (RVE) in the lower scale. The RVE is a model of the microstructure which in most cases modelled as a cube or a square. Using this method voids, inclusions and other properties of microstructure can be included in the model. The boundary value problem for RVE is solved using the numerical method like FEM. The periodic displacements boundary 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 from lower to higher and higher to lower scales is needed in most cases. In the linear problem the one way transfer of results from lower to higher scales is possible. The material parameters for the higher scale are obtained on the basis of solving a few direct problems for RVE in the lower scale. The homogenized material parameters depend on average stress values in RVE obtained after applying average strains to RVE. The strain-stress relation obtained using RVE is used in the higher level model. The average strains are strains in the integration point from the higher level.

The present researches are based on the application of the artificial immune system and the finite element method to the topology optimization (identification) of microstructure RVE. This work is an extension of previous researches of Burczyński, Poteralski and Kuś concerning such optimization problems [1][2]. Recently, immunology methods have found various applications in mechanics [9][10][11].

2. Artificial immune systems

The artificial immune systems [3][4] are developed on the basis of a mechanism discovered in biological immune systems. The artificial immune systems take only a few elements from the biological immune systems. The most frequently used are the proliferation, mutation of the B-cells, memory cells, and recognition by using the B and T-cells. This algorithm is based on the Wierchoń method [8]. Difference is that the mutation operator is changed. Instead of the nonuniform mutation [5][6][7] the Gaussian mutation is used in the presented approach. At the beginning of the AIS the memory cells are created randomly. They proliferate and mutate creating B-cells. The number of clones n_c created by each memory cell is determined by the memory cells objective function value. The objective functions for B-cells are evaluated. The selection process exchanges some memory cells for better B-cells. The selection is performed on the basis of the geometrical distance between each memory cell and B-cells (measured by using design variables).

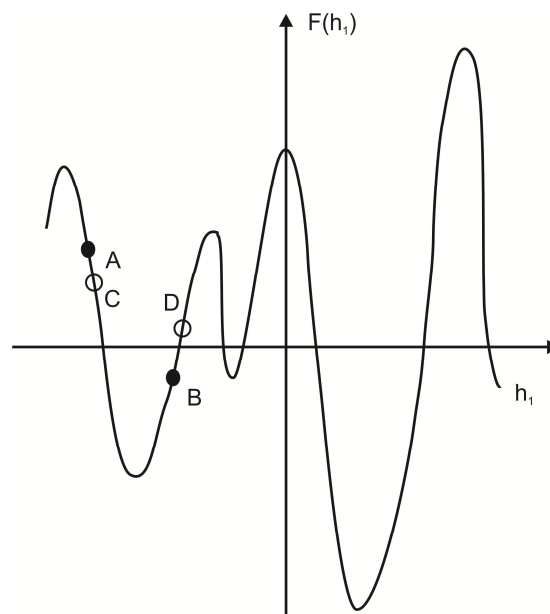


Figure 1. The idea of the selection mechanism

In the selection stage two memory cells "A" and "C" are compared and the better one (memory cell "C" - because the objective function is better) goes to next iteration.

The crowding mechanism removes similar memory cells. The similarity is also determined as the geometrical distance between memory cells. The process is iteratively repeated until the stop condition is fulfilled.

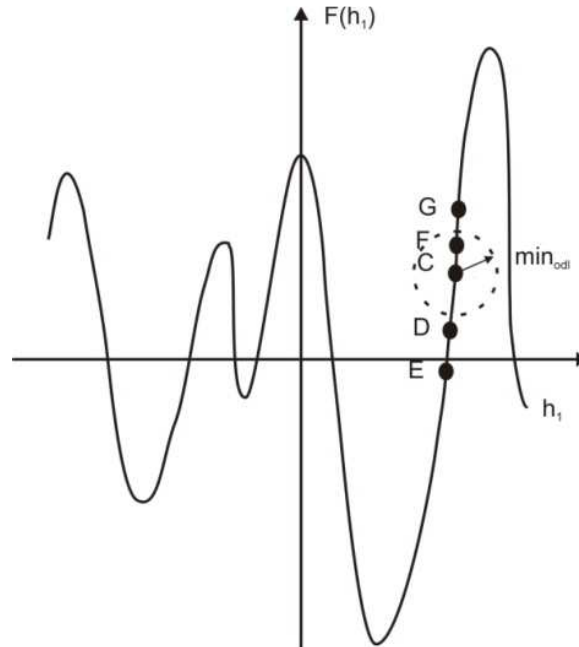


Figure 2. The idea of crowding mechanism

During the crowding mechanism for memory cell “C” only memory cell “F” is in the similarity area. The better one (memory cell “C”) stay in population and a worse (memory cell “F”) is eliminated. Finally new memory cell is generated in randomly way.

The stop condition can be expressed as the maximum number of iterations.

3. The multiscale modeling

The dependences between two or more scales is possible using the multiscale modeling (figure 3).

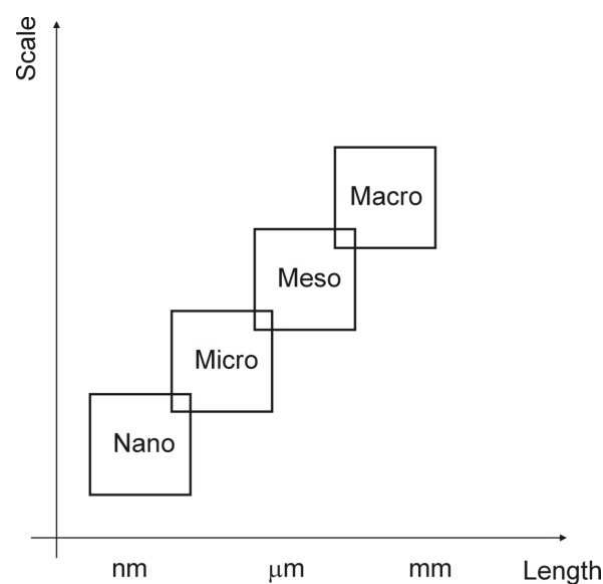


Figure 3. Multiscale modeling

Computational homogenization [12] is the one of the methods which is used in the multiscale modelling [12]. Instead of homogenous material the heterogeneous material is introduced. (figure 4).

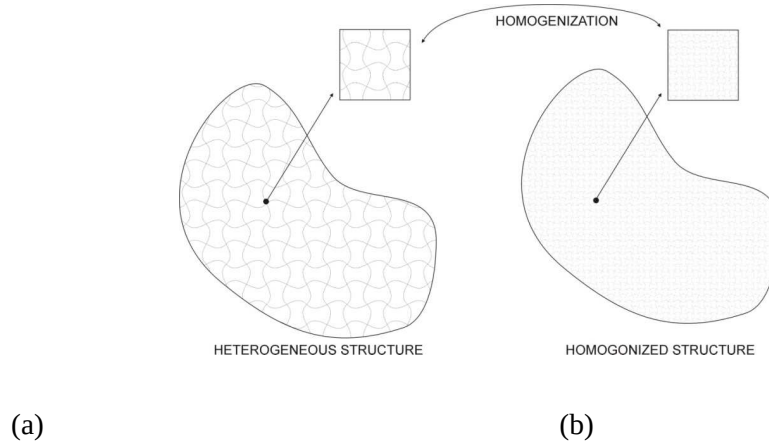


Figure 4. Homogenization of material: (a) heterogeneous structure, (b) structure after homogenization

When the microstructure is periodic the homogenization method is very useful. On the basis of a numerical solution to the boundary value problem performed in each scale is obtained using the influence between scales in the computational homogenization. Analysis of the structure in the two-scale in figure 5 is presented.

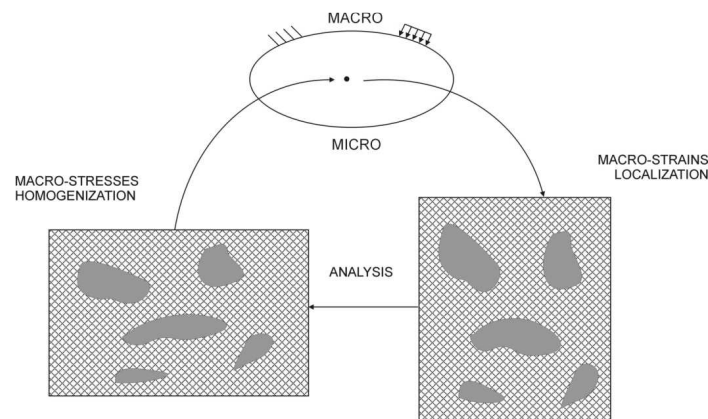


Figure 5. Two-scale computational homogenization

Using the Gauss integration point the boundary value problem for RVE could be solved. The strain values are transferred to the micromodel during the localization stage. The displacements, traction and periodic boundary conditions are applied to the microstructure. The stresses obtained after boundary value problem analysis are used to obtain homogenized average values which are transferred after the homogenized stage to the higher scale. The relationship between strains and stresses for an orthotropic elastic material are expressed as follows:

$$\sigma = C \varepsilon \quad (1)$$

$$\varepsilon = S \sigma \quad (2)$$

where:

$$\sigma = [\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23}]^T \quad (3)$$

$$\boldsymbol{\varepsilon} = [\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}]^T \quad (4)$$

are vectors of stresses and strains.

C and S are the stiffness and compliance matrices, of the orthotropic linear elastic material, respectively. They can be written as

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & sym. & & & c_{55} & 0 \\ & & & & & c_{66} \end{bmatrix} \quad (5)$$

$$S = C^{-1} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ & s_{22} & s_{23} & 0 & 0 & 0 \\ & & s_{33} & 0 & 0 & 0 \\ & & & s_{44} & 0 & 0 \\ & sym. & & & s_{55} & 0 \\ & & & & & s_{66} \end{bmatrix} \quad (6)$$

where:

$$\begin{aligned} s_{11} &= \frac{1}{E_1} & s_{22} &= \frac{1}{E_2} & s_{33} &= \frac{1}{E_3} \\ s_{44} &= \frac{1}{G_{12}} & s_{55} &= \frac{1}{G_{23}} & s_{66} &= \frac{1}{G_{13}} \\ s_{12} &= \frac{-\nu_{21}}{E_2} & s_{13} &= \frac{-\nu_{31}}{E_3} & s_{21} &= \frac{-\nu_{12}}{E_1} \\ s_{23} &= \frac{-\nu_{32}}{E_3} & s_{31} &= \frac{-\nu_{13}}{E_1} & s_{32} &= \frac{-\nu_{23}}{E_2} \end{aligned} \quad (7)$$

where E_i is Young's modulus along the axis i , G_{ij} is the shear modulus in the direction j on the plane whose normal is in the direction i , and ν_{kl} is Poisson's ratio that corresponds to contraction in the direction j when an extension is applied in the direction k .

The 9 variables are independent in the fully orthotropic elastic material [13][14] due to symmetry of the stiffness and compliance matrices.

The material coefficients can be obtained once for each microstructure in the case of linear problems. For each microstructure the six analyses should be performed to obtain the 9 independent orthotropic material coefficients. The average stresses and strains for RVE are defined as follows

$$\varepsilon_{av} = \frac{1}{|\Omega_{RVE}|} \int_{\Omega_{RVE}} \varepsilon d\Omega_{RVE} \quad (8)$$

$$\sigma_{av} = \frac{1}{|\Omega_{RVE}|} \int_{\Omega_{RVE}} \sigma d\Omega_{RVE} \quad (9)$$

where Ω_{RVE} is the area of RVE.

The constitutive relation between them has the form

$$\sigma_{av} = C^h \varepsilon_{av} \quad (10)$$

where C^h is the stiffness tensor of the equivalent homogenous material that fulfils the elastic deformation characteristic for the heterogeneous material. A detailed description of the algorithm of computational homogenization is presented in figure 6.

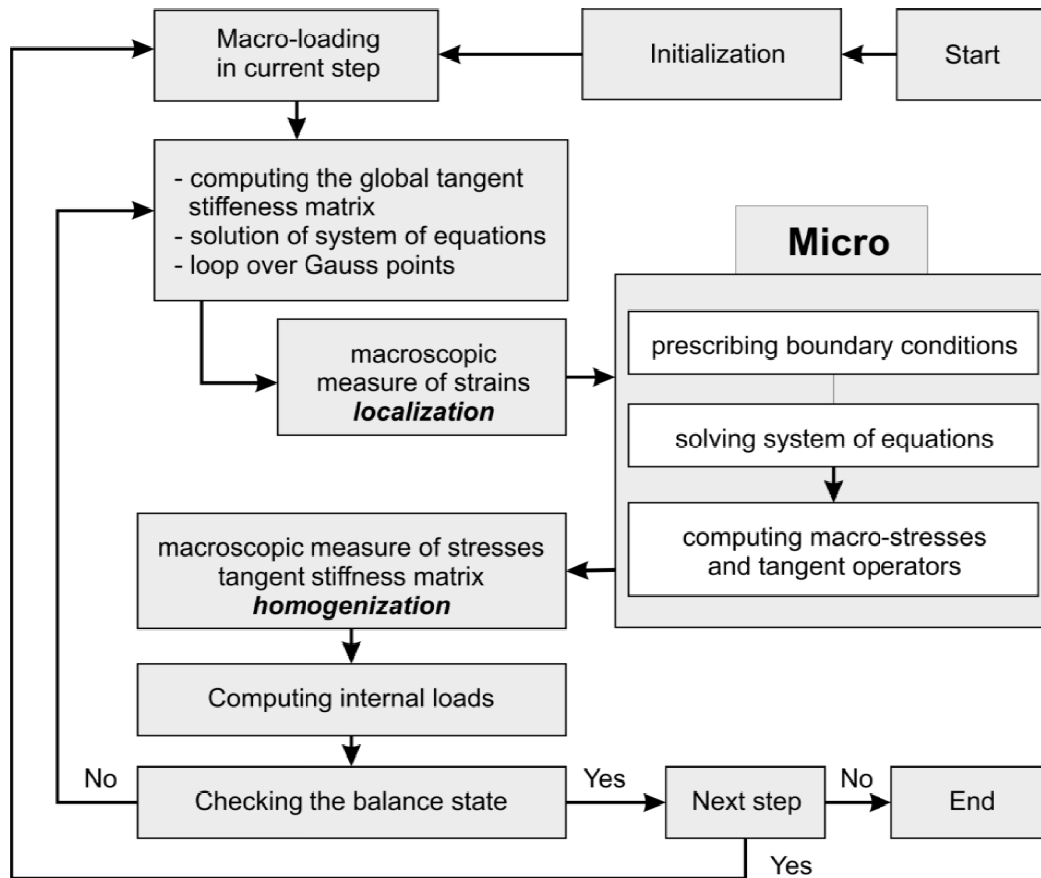


Figure 6. Computational homogenization algorithm

4. Topology optimization and parameterization

The distribution of mass density $\rho(X)$, $(X) \in \Omega_t$ in the structure is described by a hyper surface $W_\rho(X)$, $(X) \in H^3$. The hyper surface $W_\alpha(X)$, $\alpha = \rho$ is stretched under $H^d \subset E^d$, $(d=3)$ and the domain Ω_t is included in H^d , i.e. $(\Omega_t \subseteq H^d)$.

The shape of the hyper surface $W_\alpha(X)$, $\alpha = \rho$ is controlled by parameters d_j , $j=1,2,\dots,G$, which create a B-cell receptor

$$B-cell = \langle d_1, d_2, \dots, d_j, \dots, d_G \rangle \quad (11)$$

$$d_j^{\min} \leq d_j \leq d_j^{\max} \quad (12)$$

where $d_j^{\min}$, $d_j^{\max}$ - are minimum and maximum values of the parameters of B-cell receptor, respectively. Parameters of B-cell receptor are the values of the function $W_\alpha(X)$, $\alpha = \rho$ in the control points $(X)_j$ of the hyper surface, i.e. $d_j = W_\alpha[(X)_j]$, $j=0,1,2,\dots,G$.

The finite element method is applied in analysis of the structure. The domain Ω of the structure is discretized using the finite elements, $\Omega = \bigcup_{e=1}^E \Omega_e$.

The assignation of the mass density to each finite element $\Omega_e, e=1,2,...,E$ is performed by the mappings:

$$\rho_e = W_\rho \left[(X)_e \right], (X)_e \in \Omega_e, e=1,2,...,E \quad (13)$$

It means that each finite element can have different mass density.

When the value of the mass density for the e-th finite element is included in the interval $0 \leq \rho_e < \rho_{\min}$ the finite element is eliminated and the void is created, the interval $\rho_{\min} \leq \rho_e < \rho_{\max}$ the finite element remains. In the last step the Young's modulus for the e-th finite element is evaluated using the following equation

$$E_e = E_{\max} \left(\frac{\rho_e}{\rho_{\max}} \right) \quad (14)$$

where

$E_{\max}, \rho_{\max}$ - Young's modulus and mass density for the same material, respectively.

The key stage in the structural optimization is parameterization. The optimization process is not effective when the number of design variables is very large. A connection between number of finite element and design variables (parameters of B-cell receptor) leads to poor results. The better results can be obtained when the hyper surface of mass density distribution is interpolated by suitable number of values given in control points $(X)_j$. Using this approach, on the one hand, the number of design variables should be small and on the other hand should provide the good interpolation. Two different types of the interpolation procedures were applied. First the interpolation bases on neighbourhood of elements and second multinomial interpolation.

5. Numerical example

Numerical example is considered, i.e. the identification of the topology and the distribution of the mass density of microstructure considered to two materials by the minimization of the fitness function (15). The procedure described in Chapter 4 has been slightly modified, as follows: when the value of the mass density for the e-th finite element is included in the interval $0 \leq \rho_e < \rho_{\min}$ the finite element remains and has a value of mass density for material number 1 (table 3), when the value of the mass density for the e-th finite element is included in the interval $\rho_{\min} \leq \rho_e < \rho_{\max}$ the finite element also remains and has a value of mass density for material number 2 (table 3). The structures are considered in the framework of the theory of elasticity. The results of the examples are obtained by using an identification method based on the artificial immune system with the parameters included in table 1. Periodic boundary conditions are applied to the microstructure presented in the figure 7.

Table 1. The parameters of the artificial immune system

the number of memory cells	5
the number of the clones	10
crowding factor	50%
Gaussian mutation	50%

The immune process proceeds in the environment in which the structure fitness is described by the minimization of the fitness function:

$$J(\mathbf{x}) = \sum_{i=1}^n \sum_{j=1}^n \|S_{ij}(\mathbf{x}) - S_{ijref}\| \quad (15)$$

where:

S_{ij} , S_{ijref} – coefficients of compliance matrices (5).

The results of the identification process in the form of distribution of map of densities are presented in the figure 9. Geometry of the microstructure RVE in the figure 7 is presented (a, b, c =1).

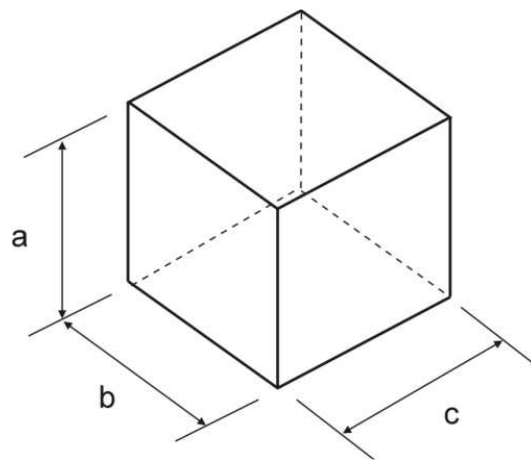


Figure 7. RVE microstructure - geometry

Material data for optimize structure in the table 2 are presented.

Table 2. Material data

material no 1 - glass		
Poisson ratio	Mass density (ρ_{max})	Young modulus
0.203076	2.5 g/cm ³	69150.9 MPa
material no 2 - epoxy		
Poisson ratio	Mass density (ρ_{max})	Young modulus
0.175124	0.55 g/cm ³	3818.47 MPa

Information about distribution of two materials in the microstructure in the table 3 is presented.

Table 3. Condition of distribution for two different materials

$\rho_e < 50\% \rho_{max}$	material no 2
$\rho_e \geq 50\% \rho_{max}$	material no 1

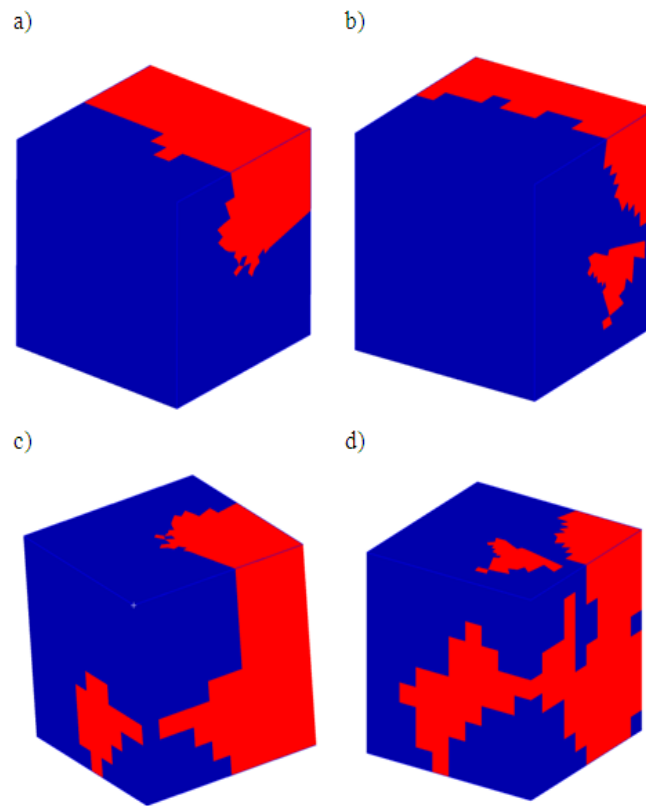


Figure 8. The results after identification process: (a), (c) the distribution of materials (Young's modules) for two different positions for the reference structure, (c) the distribution of materials (Young's modules) for two different positions for the best structure

The results of the identification for the best solution after 86 iterations, where the color red corresponds to material no. 1, and the color blue corresponds to material no. 2 are presented on the figure 8 and the table 4.

Table 4. Results of optimization

Number of iterations	Number of fitness function evaluations	Value of fitness function
86	3010	897.106018
Coefficients of compliance matrices	Reference values	Values after identifications
S_{11}	9018.59	9012.28
S_{12}	1925.6	2081.16
S_{22}	18037.4	18041.2
S_{23}	3227.03	3434.94
S_{33}	22071.2	22069.1
S_{31}	1921.72	1969.77
S_{44}	4708.77	4681.95
S_{55}	5989.53	6212.67
S_{66}	5989.53	6212.67

6. Conclusions

The paper describes the author's method of simultaneously optimization (identification) of the shape, topology and material properties of 3D structures for multiscale problem. During the optimization process the structure, which in the initial phase consisted of a homogenous material, as a result of changing material properties (change of material density) became heterogeneous material (optimization of material properties). In order to control a small number of design variables density function has been introduced describing the distribution of the material densities in a two or three-dimensional region in which the optimized mechanical structure is "submerged" (parameterization method). In this approach, design variables have values of interpolation function in appropriate distributed control points (interpolation nodes). This allows that the number of design variables is equal to the number of control points of the interpolation hyper surface and this number doesn't depend of discretization of the structure. The procedure described in this paper was used for the multiscale problem. For the multiscale modeling method of computational homogenization is used. The multiscale modeling allows one to take into account the dependences between two or more scales. The most important stage of a computational homogenization method was to develop a model of the considered structure on a lower scale, with a requirement that the size of this fragment of the structure was much smaller than the characteristic dimension of the body in a higher scale. A fragment of the structure, occurring during the computational homogenization procedure is called RVE (Representative Volume Element). Use of an artificial immune system allowed for optimal distribution of the two materials for the microstructure RVE for the objective function dependent on the parameters of the stiffness matrix. Numerical example is given and good results are obtained (figure 9) - the value of the fitness function is close to zero. Comparison between AIS, PSO and EA in another optimization problem in the paper [15][16][17][18] is presented.

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