

Topological optimization of microstructure by means of bio-inspired methods

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1. Abstract

Optimization of structures in the 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 approach opens 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. Optimization of the microstructure is not easy currently, but in the future, the presented approach may be used with success when performance of the structure is very important. 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. It is developed on the basis of a mechanism discovered in biological immune systems. An immune system is a complex system which contains distributed groups of specialized cells and organs. The main purpose of the immune system is to recognize and destroy pathogens - funguses, viruses, bacteria and improper functioning cells. The artificial immune system takes only a few elements from the biological immune systems. Mutation of the B cells, proliferation, memory cells, and recognition by using the B and T cells are used the most frequently.

The unknown global optimum is represented by the searched pathogen. The memory cells contain design variables and proliferate during the optimization process. The B cells created from memory cells undergo the mutation. The B cells evaluate and better ones exchange memory cells. The optimal topology is generated by the level set approach. The crowding mechanism is used - the diverse between memory cells is forced. A new memory cell is randomly created and substitutes the old one, if two memory cells have similar design variables. The crowding mechanism allows finding not only the global optimum but also other local ones. Additional the Gaussian mutation is used in this approach. The paper presents methodology, algorithm of optimization and numerical examples.

2. Keywords: topology optimization, artificial immune system, multiscale modeling

3. Introduction

Shape and topology optimization have been an active research area for some time. Recently, several innovative approaches for topology optimization have been developed. Perhaps one of the simplest optimization method is the method based on removing inefficient material from a structure. This method is named Evolutionary Structural Optimization [26]. However, this method is not based on the application of the evolutionary algorithm but on different rejection criteria for removing material which depends on the types of design constraints.

One of the most famous structural optimization approaches is the approach based on material homogenization method [4][5] and it has been applied to various optimization problems. The homogenization design method assumes the introduction of the periodic microstructures of a particular shape into the finite elements of the discretized domain. The size and the orientation of the microstructures in the elements determine the density and the structural characteristics of the material in the elements. An optimization process consisting in application of the mathematical programming techniques leads to the minimization of the structure compliance by changing the orientation and size of the microstructures. As a result the optimization process composite structures emerge.

Another approach to the structural optimization is based on generating inside a domain a new void (so-called bubble) on the basis of special criteria and next on performing simultaneous shape and topology optimization. This approach was originated by Eschenauer and Schumacher [17]. Coupling of this approach, the boundary elements and the genetic algorithms was considered by Burczyński and Kokot [6]. From the mathematical point of view this approach is based on replacing a one-connected domain with a multi-connected domain.

Another interesting approach assumes the discretization of the domain into binary material/void elements introduced by Anagnostou at al [1]. This approach was developed by Kirkpatrick at al [18], who proposed finding the optimal material configuration within the design domain by using simulated annealing. Jensen and Sandgren [22], proposed the application of the genetic algorithm in order to solve similar optimization problems. This approach has been developed by Chapman [16].

One of the most interesting recent approaches to the structural optimization problem is method named Multi-GA System introduced by Woon at al [25] which assumes the application of two simultaneously and parallel running genetic algorithms. The first external genetic algorithm is used to define the optimum shape of the structure

through operating on the external boundary while the second internal is used to optimize the internal topology. This method does not require the application of the post-processing or additional algorithms to generate smooth boundaries.

The present approach is based on the application of the artificial immune system and the finite element method to topology optimization of the microstructure. This work is an extension of previous researches of Burczyński, Poteralski and Kuś concerning such optimization problems [8][10][11][21]. Recently, computational immune methods have found various applications in mechanics. The main advantage of the artificial immune system is the fact that this approach does not need any information about the gradient of the fitness function and gives a strong probability of finding the global optimum. The fitness function is calculated for each B-cell in each iteration by solving a boundary-value problem by means of the finite element method (FEM). In order to solve the optimization problem the fitness function, design variables and constraints are formulated.

The description of artificial immune systems is presented in Section 4. Section 5 contains computational homogenization methodology in multiscale modeling. Parameterization in the topology optimization problem is described in Section 7. Computational implementation of the presented approach is considered in Section 8. Conclusion remarks are described in Section 9.

4. Artificial immune systems

The artificial immune systems (AIS) are developed on the basis of a mechanism discovered in biological immune systems [20]. An immune system is a complex system which contains distributed groups of specialized cells and organs. The main purpose of the immune system is to recognize and destroy pathogens - fungi, viruses, bacteria and improper functioning cells. The lymphocytes cells play a very important role in the immune system. The lymphocytes are divided into several groups of cells. There are two main groups B and T cells, both contains some subgroups (like B-T dependent or B-T independent). The B cells contain antibodies, which could neutralize pathogens and are also used to recognize pathogens. There is a big diversity between antibodies of the B cells, allowing recognition and neutralization of many different pathogens. The B cells are produced in the bone marrow in long bones. A B cell undergoes a mutation process to achieve big diversity of antibodies. The T cells mature in thymus, only T cells recognizing non self cells are released to the lymphatic and the blood systems. There are also other cells like macrophages with presenting properties, the pathogens are processed by a cell and presented by using MHC (Major Histocompatibility Complex) proteins. The recognition of a pathogen (Fig. 1a) is performed in a few steps. First, the B cells or macrophages present the pathogen to a T cell using MHC (Fig. 1b), the T cell decides if the presented antigen is a pathogen. The T cell gives a chemical signal to B cells to release antibodies. A part of stimulated B cells goes to a lymph node and proliferate (clone) (Fig. 1c). A part of the B cells changes into memory cells, the rest of them secrete antibodies into blood. The secondary response of the immunology system in the presence of known pathogens is faster because of memory cells. The memory cells created during primary response, proliferate and the antibodies are secreted to blood (Fig. 1d). The antibodies bind to pathogens and neutralize them. Other cells like macrophages destroy pathogens (Fig. 1e). The number of lymphocytes in the organism changes, while the presence of pathogens increases, but after attacks a part of the lymphocytes is removed from the organism.

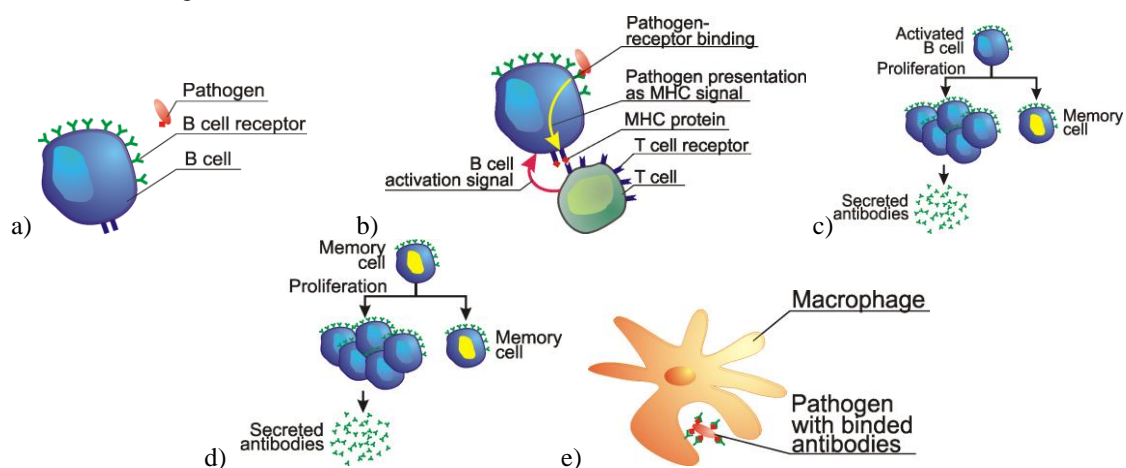


Figure 1: An immune system, a) a B cell and pathogen, b) the recognition of pathogen using B and T cells, c) the proliferation of activated B cells, d) the proliferation of a memory cell – secondary response, e) pathogen absorption by a macrophage

The artificial immune systems [2], [13], [14] take only a few elements from the biological immune systems. The most frequently used are the mutation of the B cells, proliferation, memory cells, and recognition by using the B and T cells. The artificial immune systems have been used to optimization problems in [15], classification and also computer viruses recognition in [2]. The cloning algorithm presented by von Zuben and de Castro uses some mechanisms similar to biological immune systems to global optimization problems. The unknown global optimum is the searched pathogen. The memory cells contain design variables and proliferate during the optimization process. The B cells created from memory cells undergo mutation. The B cells evaluate and better ones exchange memory cells. In Wierzchoń [24] version of Clonalg the crowding mechanism is used - the diverse between memory cells is forced. A new memory cell is randomly created and substitutes the old one, if two memory cells have similar design variables. The crowding mechanism allows finding not only the global optimum but also other local ones. The presented approach is based on the Wierzchoń [24] algorithm, but the mutation operator is changed. The Gaussian mutation is used instead of the nonuniform mutation in the presented approach. The Fig. 2 presents the flowchart of an artificial immune system. The memory cells are created randomly. They proliferate and mutate creating B cells. The number of clones 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). 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. The stop condition can be expressed as the maximum number of iterations.

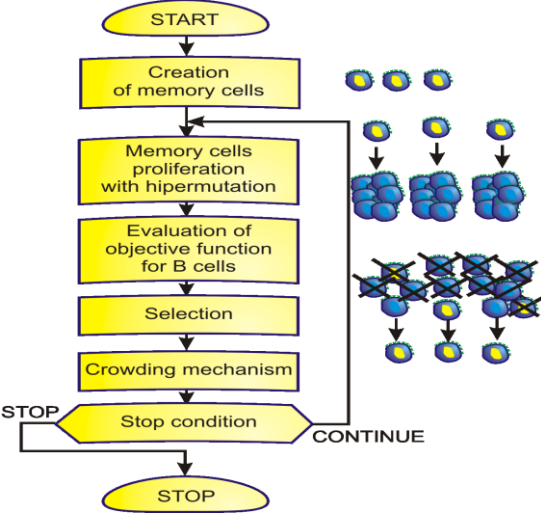


Figure 2: The flowchart of an artificial immune system

5. Computational methodology in multiscale modeling

The multiscale modeling allows one to take into account the dependences between two or more scales (Fig. 3).

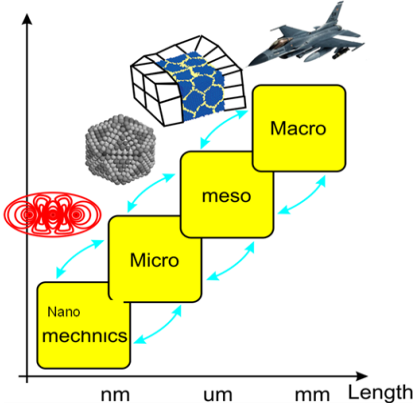


Figure 3: Multiscale modeling

One of the methods used in the multiscale modeling is the computational homogenization [19]. A heterogeneous material is replaced with a homogenous one (Fig. 4).

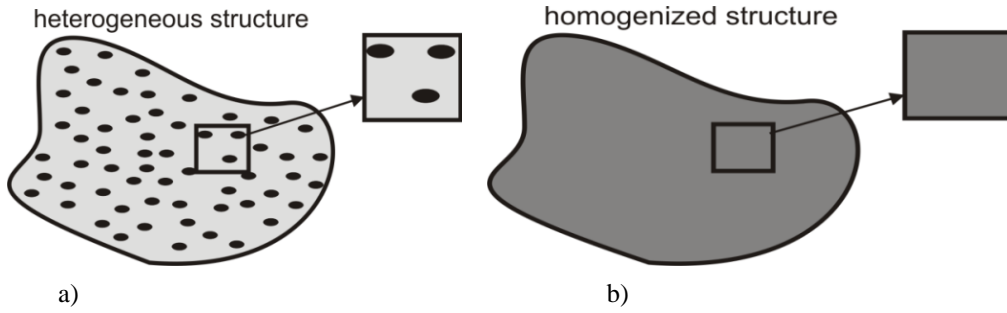


Figure 4: Homogenization of material: a) heterogeneous structure, b) structure after homogenization

The homogenization is useful when the microstructure is periodic. The influence between scales in the computational homogenization is obtained on the basis of a numerical solution to the boundary value problem performed in each scale. The two-scale analysis of the structure is shown in Fig. 5.

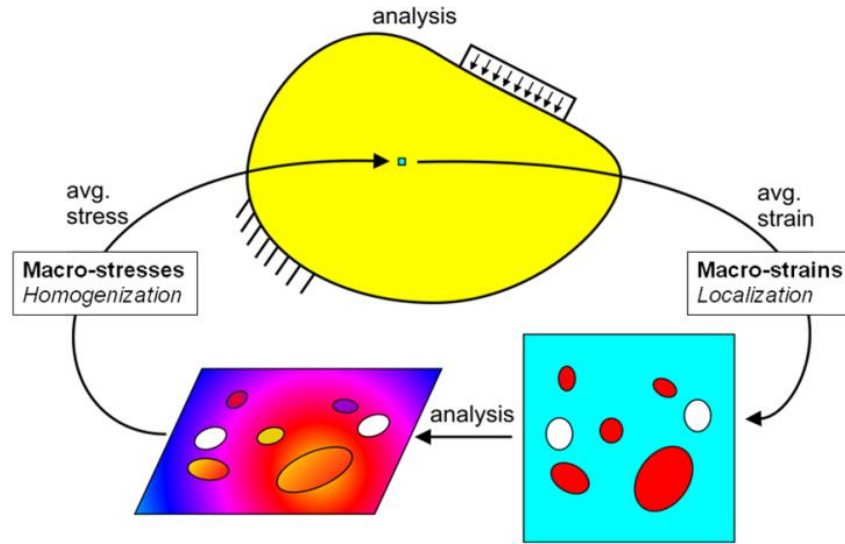


Figure 5: Two-scale computational homogenization

The boundary value problem for the Representative Volume Element (RVE) is solved for each Gauss integration point. The strain values are transferred to the micromodel during the localization stage. The traction, displacements or 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 stresses and strains for an orthotropic elastic material are expressed as follows:

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

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

where:

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

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

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 .

Due to symmetry of the stiffness and compliance matrices, the 9 variables are independent in the fully orthotropic elastic material [3][23].

The material coefficients in the case of linear problems can be obtained once for each microstructure. The six analyses should be performed for each microstructure to obtain the 9 independent orthotropic material coefficients. The average strains and stresses 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 Fig. 6.

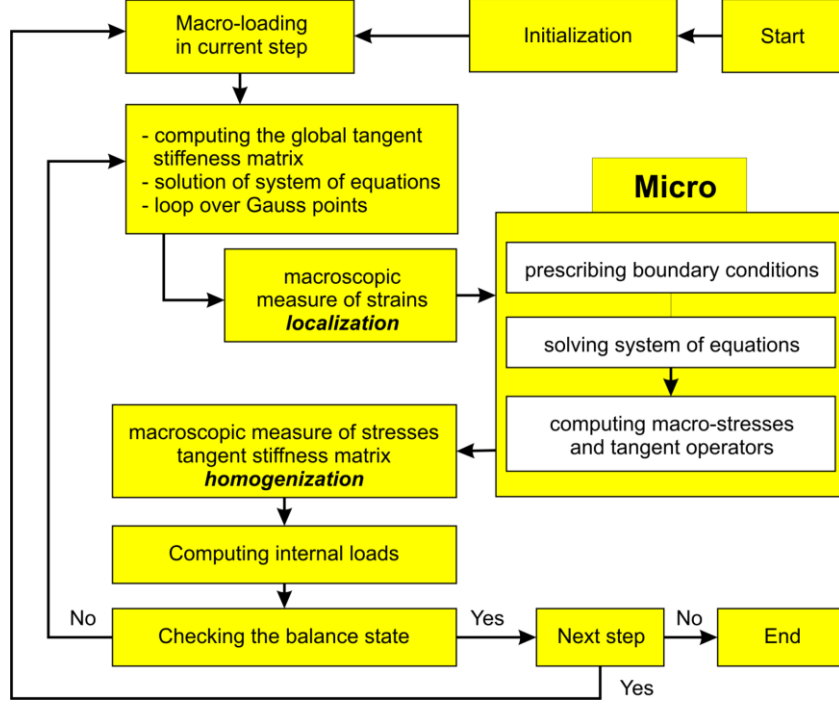


Figure 6: Computational homogenization algorithm

7. Parameterization in topology optimization

The distribution of a mass density $\rho(X)$, $(X) \in \Omega_t$ in the micro-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 Ω_e , $e=1,2,\dots,E$ is performed by the mappings:

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

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 next 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}, ρ_{\max} - Young's modulus and mass density for the same material, respectively,

Parameterization is the key stage in topology optimization. The great number of design variables causes that the optimization process is not effective. A connection between design variables (parameters of B-cell receptor) and number of finite element 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 $(X)_j$. This number, on the one hand, should provide the good interpolation, and on the other hand the number of design variables should be small. Two different types of the interpolation procedures were applied [7][9][12]. First the multinomial interpolation the second one interpolation bases on neighbourhood of elements.

8. Numerical example

Topology optimization in the form of the distribution of the mass density of the microstructure is considered for two materials by minimization of the fitness function (15). The procedure described in Section 7 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 microstructures are considered in the framework of the theory of elasticity. The results of the examples are obtained by using an optimization method based on the artificial immune system with the parameters included in Tab 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:

$$J = \left| \frac{2c_{11}}{c_{22}} - 1 \right| \quad (15)$$

where:

c_{11}, c_{22} – coefficients of stiffness matrices (5).

Optimal structure for which the stiffness in one direction (c_{22}) was two times higher than the stiffness in the second direction (c_{11}) was searched.

Results of the optimization process in the form of distribution of map of densities are presented in the Fig. 9.

Geometry of the microstructure RVE in the figure 7 is presented (a, b, c =1).

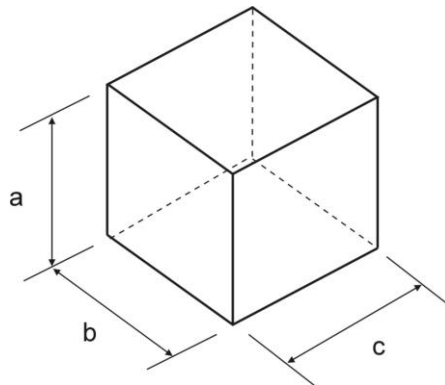


Figure 7: RVE microstructure - geometry

Material data for optimize structure are presented in Table 2.

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 is presented in Table 3.

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

Results of optimization for the best solution after 40 iterations are presented on the Figure 9 and Table 4. The color red corresponds to material no. 1, and the color blue corresponds to material no. 2.

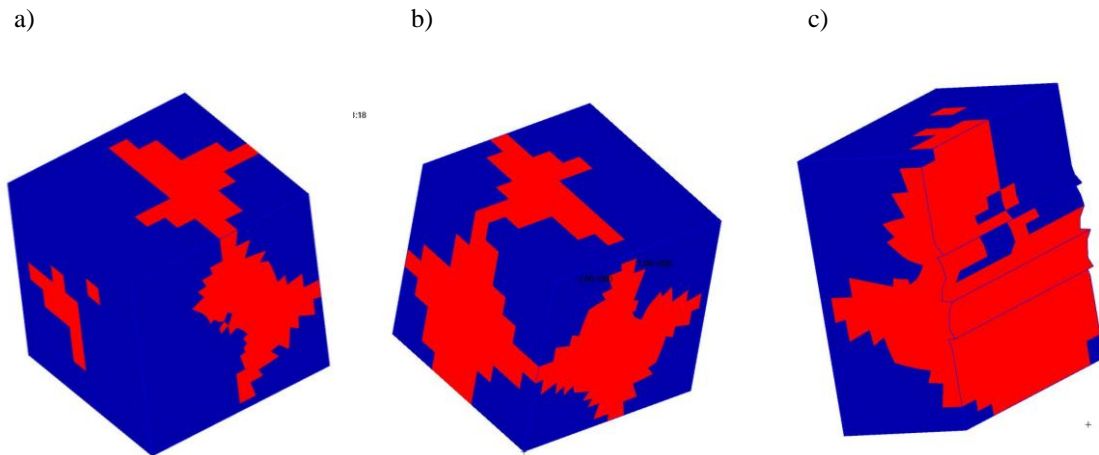


Figure 9: Results after optimization process: a), b), c) the best structure obtained after optimization process, a), b) the distribution of materials (Young's modulus) for two different positions, c) the distribution of materials (Young's modulus) inside the domain

Number of iterations	Number of fitness functions evaluations	Value of the fitness function
40	1400	0.000011

History of the fitness function for the best B-cell in particular iterations is presented in Figure 10.

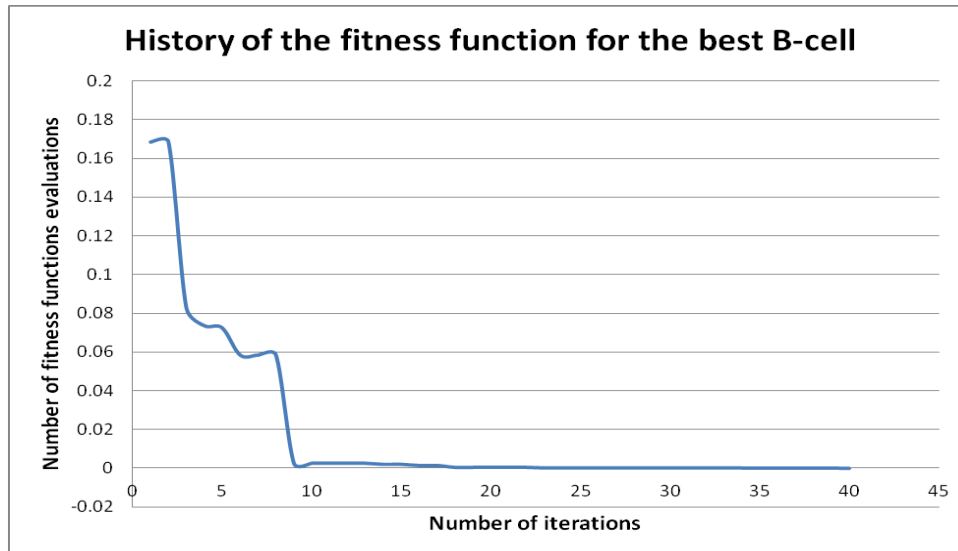


Figure 10: History of the fitness function for the best B-cell

9. Conclusions

Topology optimization based on seeking the best distribution of the mass density of the microstructure was considered for two materials. The examined problem was solved as a minimization task using the artificial immune system, FEM and the computational homogenization for the fully orthotropic elastic material with 9 independent material parameters. The proposed approach can be used for the more number of different materials and creation of voids can be also adopted.

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