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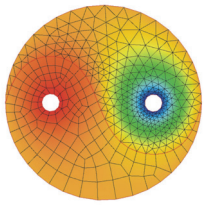

PARALLEL IDENTIFICATION OF VOIDS IN A MICROSTRUCTURE USING THE BOUNDARY ELEMENT METHOD AND THE BIOINSPIRED ALGORITHM

WACŁAW KUŚ*, RADOSŁAW GÓRSKI

Silesian University of Technology, Institute of Computational Mechanics and Engineering, Konarskiego 18A, 44-100 Gliwice, Poland
**Corresponding author: waclaw.kus@polsl.pl*

Abstract

The problem of identification of the size of a void in a microscale on the basis of the homogenized material parameters is studied in this work. A three-dimensional unit-cell model of a porous microstructure is modelled and analyzed by the boundary element method (BEM). The method is very accurate and for the considered problem requires discretization only the outer boundary of models. The algorithm used for identification is characterized by a hierarchical structure which allows for parallel computing on three different levels. The parallel algorithm is used for evolutionary computations. The solution of boundary value problems by the BEM and the determination of effective material properties by numerical homogenization method are also parallelized. The computation of the compliance matrix for a porous microstructure is shown. The matrix is used to formulate the objective function in identification problem in which the size of a void is searched. The scalability tests of the algorithm are performed using a server consisting of eight floating point units. As a result of using the hierarchical structure of the identification algorithm and the BEM, a significant computation speedup and the accuracy are achieved.

Key words: parallel computing, bioinspired algorithms, identification, boundary element method, micromechanics, numerical homogenization

1. INTRODUCTION

The bioinspired algorithms are very efficient optimization tools for single and multimodal objective functional problems (Michalewicz, 1996). The main drawback of these algorithms is a large number (hundreds or thousands) of objective function evaluations. The time needed for an evaluation of a single objective function depends on a boundary value problem usually solved by numerical methods, like the finite element method (FEM) or the boundary element method (BEM). The overall wall time of identification can be shortened when the parallel algorithms are used (Kuś & Burczyński, 2008).

Apart from the analytical models and experimental testing, numerical simulations play today an important role in the prediction of a behaviour of new materials of a complex structure. A recent increase in a computational power gives a possibility of studying different materials using a numerical homogenization approach. Since the direct modelling and analysis of most of engineering structures made of heterogeneous materials is computationally very demanding, the numerical homogenization methods can be performed instead. By using this technique, a complex microstructure may be represented for instance by means of a representative volume element (RVE) or a unit cell and can be

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modelled and analyzed on two or more different scales.

Because the main emphasis in this work is put on parallel bioinspired computations assisting numerical homogenization, analytical homogenization procedures are out of the scope of this paper and will not be discussed. Among the numerical homogenization methods, the FEM and the BEM are the most frequently used. The studies in the literature concern the homogenization of different materials of complex microstructures, for example composite materials, cellular materials, heterogeneous tissue scaffolds and other. Fang et al. (2005) for instance have studied homogenization of porous tissue scaffolds by the FEM and by two other approaches. They computed the effective mechanical properties of different scaffolds materials and pore shapes. Düster et al. (2012) have shown a new approach for the numerical homogenization of heterogeneous and cellular materials using the finite cell method. The important feature of the method is a possibility of discretizing of complicated microstructures in a fully automatic way. Chen and Liu (2005) have analysed composites reinforced by spherical particles or short fibres by the advanced BEM. Difficulties in dealing with nearly-singular integrals during modelling of composites with closely packed fillers have been resolved by new and improved techniques. Araujo et al. (2010) have modelled and analysed three-dimensional composite microstructures by the BEM and the parallel algorithm. Multiscale analysis by coupling the molecular statics and the BEM is presented by Burczyński et al. (2010a). Optimization of macro models analyzed by the FEM using parallel algorithms is shown by Kuś and Burczyński (2008). Identification of material parameters of a bone by using a multiscale modelling and a distributed parallel evolutionary algorithm is presented by Burczyński et al. (2010b).

In the present paper the identification of voids in microstructures modelled by the BEM is presented. In order to speed up the computations, the identification problem is solved by the parallel hierarchical algorithm. In order to solve the problem, the developed system is build of three programs, i.e. an evolutionary algorithm (an optimization tool), a computational homogenization module (evaluation of objective function) and the BEM program (a boundary value problem solver). Three-dimensional unit-cell models (which play the role of a RVE) of microstructures with voids are considered. The numerical homogenization of an orthotropic material is shown for which the homogenized properties are determined. The properties are used to formulate the objective function depending on the quantities of a macro and micro model in order to identify the size of a void in the unit cell model of the material. As a result, the parameters defining voids in the material on a microscale are determined on the basis of orthotropic parameters in a macroscale.

2. COMPUTATIONAL HOMOGENIZATION BASED ON THE BEM

In this section, the idea of a numerical homogenization is described within the framework of a linear elastic material characterized by a periodic microstructure containing voids. It is assumed that the material is macroscopically orthotropic and that a macro model of a structure made of this material is subjected to small deformations. The porous microstructure is modelled and analyzed by the BEM. Boundary integral equations for a general three-dimensional (3D) isotropic body are shown. The stress-strain relationships for an orthotropic material are presented. As a result of the numerical homogenization by the BEM, the macroscopic homogenized properties of the material are determined on the basis of analysis of the unit cell models in a micro scale.

First, consider a 3D body (a macro model) made of a homogeneous, isotropic and linear elastic material. The external boundary of the body is denoted by Γ. The body is statically loaded along the boundary Γ by boundary tractions t_j, displacements of the body are denoted by u_j.

Assuming that the body forces does not act on the body, the relation between the loading of the body and its displacements can be expressed by the boundary integral equation (known as the Somigliana identity) in the following form (Gao & Davies, 2002):

$$c_{ij}(x')u_j(x') + \int_\Gamma T_{ij}(x',x)\,u_j(x)\,\mathrm{d}\Gamma(x) = \int_\Gamma U_{ij}(x',x)\,t_j(x)\,\mathrm{d}\Gamma(x) \qquad (1)$$

where x' is a collocation point, for which the above integral equation is applied, x is a point on the external boundary Γ, a constant c_{ij} depends on the position of the point x', U_{ij} and T_{ij} are fundamental solutions of elastostatics. The summation convention is used in the equation (the indices for a 3D problem are $i,j = 1,2,3$).

Numerical BEM equations are obtained after discretization of the boundary integral equation (1), which is successively applied for all collocation points. In the developed computer program the outer boundary of the body is divided into 8-node quadratic boundary elements. Along the external boundary the variations of coordinates, displacements and tractions are interpolated using quadratic shape functions. The resulting BEM equations can be expressed in the following matrix form:

$$\mathbf{H}\,\mathbf{u} = \mathbf{G}\,\mathbf{t} \tag{2}$$

where **u** and **t** are displacement and traction vectors, respectively, **H** and **G** are coefficient matrices dependent on the boundary integrals of fundamental solutions and shape functions, and their elements are integrated numerically using the Gauss quadratures.

Consider now a heterogeneous material with a periodic microstructure with voids in the form of rectangular prisms. A unit cell of this material (a micro model) representing its porous microstructure contains a single rectangular prism of arbitrary side lengths (i.e. a_1, a_2, a_3) as shown in figure 1. Because there are three mutually perpendicular symmetry planes with respect to the void aligned along the x_1, x_2 and x_3 axes, the material in a macro scale is referred to as orthotropic.

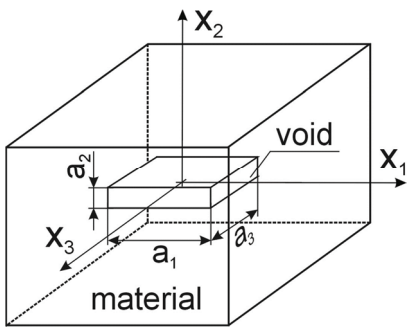

Fig. 1. *A unit cell model of an orthotropic material*

If a material has a non-regular and non-uniform microstructure, the representative volume elements (RVE) representing a microstructure of this material should be rather used than the unit cell models. More comprehensive definitions of the RVE can be found elsewhere, for instance in Kouznetsova (2002). In the RVE or the unit cell analysis, representative sections (volumes) of a material are analyzed in order to calculate the homogenized properties. The coupling of the macro and micro levels is based on the averaging theorems. Thus, the relation between strains and stresses is formulated in an average sense in order to determine the homogenized (the effective) macroscopic properties.

The mechanical properties of a linear elastic material are characterized by the compliance matrix **S** or by the stiffness matrix **C**. The means for obtaining the elements of the compliance matrix **S** for an orthotropic material by using the numerical homogenization concept and the BEM are presented below.

Using the engineering notation, the strain-stress relationships for an orthotropic material have the following form (Kollár & Springer, 2003):

$$\begin{Bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{12} & S_{22} & S_{23} & 0 & 0 & 0 \\ S_{13} & S_{23} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{66} \end{bmatrix} \begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{13} \\ \tau_{12} \end{Bmatrix} \tag{3}$$

where the compliance matrix **S** has 12 nonzero elements, but only 9 are independent, ε_1, ε_2, ε_3 and γ_{23}, γ_{13}, γ_{12} are engineering strains, σ_1, σ_2, σ_3 and τ_{23}, τ_{13}, τ_{12} are engineering stresses. The walls of the unit cell in figure 1 align with the x_1, x_2 and x_3 axes, in which the strains and stresses in equation (3) are defined. For the considered orthotropic material in a macro scale, the compliance matrix is specified in the coordinate system defined by these axes, which are perpendicular to the three symmetry planes. The compliance matrix **S** is symmetrical for an elastic material ($S_{ij} = S_{ji}$) and it is the inverse of the stiffness matrix ($\mathbf{S} = \mathbf{C}^{-1}$).

In order to compute the elements of the compliance matrix, 6 numerical tests are performed using the unit cell in figure 1, i.e. 3 tensile tests and 3 shear tests. In this work, homogeneous static boundary conditions are applied. The unit tractions are prescribed to the unit cell models. For instance, for the tensile test in the x_1 direction only the traction in this direction (σ_1 stress) is prescribed and the remaining are zero. When the first stress state is applied, then the resulting strains are obtained from the strain-stress relationships for an orthotropic material and the first column of the compliance matrix in equation (3) is determined. Repeating an analysis five more times for the remaining unit stress vectors allows determining all columns of the compliance matrix. In order to determine the homogenized macroscopic properties represented by this matrix, the

relation between strains and stresses is formulated in an average sense. The average strains are computed on the basis of displacements obtained from the BEM analysis by their integration over the boundaries of the models. These strains provide the relevant terms in the compliance matrix **S** and thus the effective properties.

3. FORMULATION OF IDENTIFICATION PROBLEM

The identification problem consists in finding the side lengths a_1, a_2, a_3 of the void in the unit cell model in figure 1 by minimization the following functional F dependent on the elements of the compliance matrix:

$$F = \sum_{i=1}^{n} \left| s_i - \hat{s}_i \right| \tag{4}$$

where s_i are computed homogenized material properties, i.e. the elements of the compliance matrix $s_i = \{S_{11}, S_{22}, S_{33}, S_{12}, S_{13}, S_{23}, S_{44}, S_{55}, S_{66}\}$, $\hat{s}_i$ are reference homogenized material properties related to a macromodel (e.g. from experiments), n is a number of independent material parameters for an orthotropic material ($n = 9$ in this case).

The identification problem is solved by the evolutionary algorithm, in which a population of chromosomes are processed in each iteration. The design variables (the side lengths a_1, a_2, a_3) are coded in genes of each chromosome which is a potential solution of the problem. At the beginning, the initial population of chromosomes is generated randomly. Then the values of the objective function (fitness function) for all chromosomes are calculated. The fitness function defined by equation (4) is obtained by solving six boundary value problems with the use of the BEM and the homogenization procedure. In the next step, the randomly chosen chromosomes and their genes are modified by using evolutionary operators. The new generation is created on the basis of the offspring population during the selection process. The loop of the algorithm is repeated until the end condition is fulfilled (expressed e.g. as a maximum number of iterations).

In order to improve the evolutionary process of the algorithm and speed up the computations, the island (also called distributed) version of the evolutionary algorithm is proposed in the present work. It uses few subpopulations of chromosomes which evolve separately. The chromosomes between subpopulations can be exchanged during a migration phase. Another improvement concerns the evaluation of fitness function. The developed algorithm uses a database containing an information about evaluated chromosomes and their fitness function. It prevents from the evaluation of fitness function for chromosomes which have the same genes. If this is the case, the value from the database is used. The procedure saves much time because solving of a boundary value problem is usually the most expensive operation in terms of time during the evolutionary process.

Identification problems belong to a class of ill-defined problems and the uniqueness of the solution is not guaranteed. The same value of the objective function may be obtained for different number and other parameters of voids.

4. PARALLELIZATION OF IDENTIFICATION ALGORITHM

The aim of parallelization of the identification algorithm is to obtain the results as fast as possible. Two factors are taken into account in the parallelization strategy: wall time of computations and memory consumption. The memory usage by the algorithm is important because the methods used in the paper increase memory requirements. The physical memory installed in a server should be taken into account during parallelization of the algorithm to prevent swapping memory to disk which may lead to much longer wall time of computations. In the considered process of identification solving of a boundary value problem is the most time consuming task. The parallelization of the identification algorithm can be performed on at least three levels as shown in figure 2. On each level different program of the developed system consisting of three modules is applied, i.e. on the first level the evolutionary algorithm, on the second the computational homogenization procedure and on the third the BEM program for the solution of a boundary value problem (parallel system of equations solver - PSS). The parameter nLx is a number of threads used by a program on level x. The parallelization is hierarchical and the total number of parallel threads is equal to the multiplication of the parameters nLx for all three levels.

The parallelization of the evolutionary algorithms is quite easy (Kuś & Burczyński, 2008). The efficiency of using a parallel algorithm is high especially for problems for which evaluation of a fitness function is long (from seconds to hours or in some cases days). The maximum number of parallel

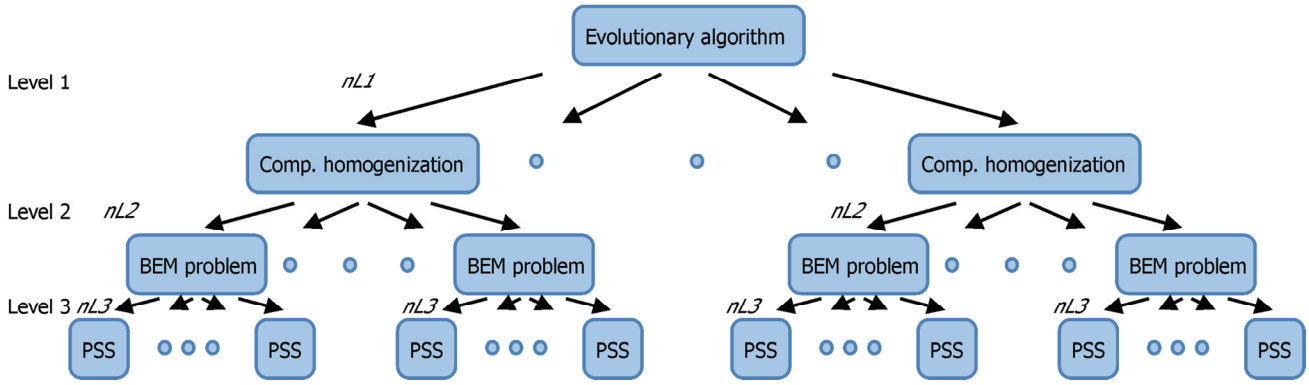

Fig. 2. A hierarchical parallel structure of identification algorithm

threads *nL1* is equal to the total number of chromosomes. The parallel evolutionary algorithms that use the floating point representation operate on small populations of chromosomes, for example 10, 20, 50. The parallelization increases the memory requirements for computations. The memory amount is a sum of memory requirements for the evaluation of a fitness function for each chromosome. The memory consumption is *nL1* times larger than in the case of a sequential algorithm. The parallelization on level 2 is related with the parallel computational homogenization. The homogenization procedure consists of boundary value problems solved in a parallel way and sequential algorithm which computes homogenized material properties. The maximum number of parallel tasks is 6 for a 3D problem. The homogenization procedure runs 6 BEM analyses therefore the number of parallel tasks should be 1, 2, 3 or 6 in order to use all cores equally. The boundary value problem is solved with the use of the BEM on third level of parallelization. Several steps of the BEM algorithm can be parallelized. The most important is parallelization of solving of the system of equations. In the BEM the full matrices are created thus the standard algorithms like LAPACK can be used in order to solve a system of algebraic numerical equations. The parallel approach is realized with the use of an Intel MKL library.

***Table 1.** Homogenized properties of the reference material*

Material parameter	S_{11}	S_{12}	S_{13}	S_{22}	S_{23}	S_{33}	S_{44}	S_{55}	S_{66}
Value [GPa^{-1}]	1.076	-0.318	-0.319	1.050	-0.317	1.057	2.729	2.780	2.763

5. NUMERICAL TESTS

A geometry of the considered RVE is presented in figure 1. The unit cell size is 1×1×1 mm. The constraints on design variables, i.e. the side lengths a_1, a_2, a_3, are imposed and each is within the range of 0.05 to 0.85 mm. For each test the prescribed traction to a wall of the unit cell is p = 1 MPa. The linear elastic material properties of the microstructure are as follows: Young's modulus E = 1.0 GPa and Poisson's ratio ν = 0.3. Each outer wall of the unit cell and inner wall of the void is divided into 16 quadratic boundary elements, resulting in 192 elements for the whole model. The orthotropic properties of the reference material are shown in table 1. The elements of the reference compliance matrix were obtained for an actual void and its side lengths shown in table 2.

The parameters of the evolutionary algorithm are as follows: number of genes is 3, number of chromosomes is 20, number of iterations is 50, probability of simple crossover with Gaussian mutation is 90%, probability of uniform mutation is 10%. The results of identification and an error with respect to the actual void are shown in table 2. The corresponding value of the objective function is F = 0.027 GPa^{-1}.

***Table 2.** Actual and found void side lengths*

Void parameter	Actual	Found	Error %
a_1	0.200	0.217	8.5
a_2	0.400	0.346	13.5
a_3	0.300	0.319	6.3

The tests were performed with the use of a server Dell PowerEdge R515. The server contains two processors AMD Opteron 6272, each with 16 cores (8 floating point units). In all tests, parameters of the evolutionary algorithm are the same as in the previ-

ous example. The maximum value of the *nL1* parameter is 18 (which corresponds to a maximal number of chromosomes evaluated in each iteration of the evolutionary algorithm). The times of identification for all tests are presented in table 3. The speedup is computed in a reference to results for the test 1. The parallelization on the level 3 (tests 1-6) is not efficient due to a partial parallelization of the BEM algorithm. The parallel evolutionary algorithm and the homogenization procedure are characterized by a similar efficiency (tests 7-16). The maximum number of parallel evolutionary algorithm threads is 18, the homogenization allows 6 parallel threads, the total number of cores which may be used in computations is equal to 108. In the future the authors plan to use a cluster with more number of cores to check the scalability of the presented approach.

Table 3. *Times of identification for different number of tasks*

Test	*nL1*	*nL2*	*nL3*	Number of threads	Time [s]	Speedup
1	1	1	1	1	21 220	1
2	1	1	2	2	18 136	1.17
3	1	1	4	4	17 983	1.18
4	1	1	8	8	17 112	1.24
5	1	1	16	16	16 449	1.29
6	1	2	1	2	11 937	1.78
7	2	1	1	2	12 039	1.76
8	2	2	1	4	6 861	3.09
9	1	6	1	6	5 975	3.55
10	6	1	1	6	5 802	3.66
11	2	6	1	12	3 426	6.19
12	16	1	1	16	3 213	6.60
13	8	2	1	16	2 806	7.56
15	3	6	1	18	2 549	8.32
16	6	3	1	18	2 539	8.36

6. CONCLUSIONS

The identification of the size of a pore in a micro scale model on the basis of parameters in a macro scale is considered in this work. A three-dimensional unit-cell model of a porous material is modelled and analyzed by the boundary element method (BEM). The main advantage of using the BEM in analysis is its high accuracy and that it requires discretization only the outer boundary of the considered models. The advantages are valuable and can be exploited in more complex problems dealing for instance with numerical homogenization and optimization or identification. In order to solve the problem, the hierarchical parallelization of the algorithms was developed. In numerical examples, parameters defining geometry of a void were successfully identified. The results of numerical tests with wall time measurements for different number of cores are shown. The time of computations is reduced from about 6 hours to about 40 minutes when one core and the parallel approach is applied, respectively.

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RÓWNOLEGŁA IDENTYFIKACJA PUSTEK W MIKROSTRUKTURZE Z WYKORZYSTANIEM METODY ELEMENTÓW BRZEGOWYCH ORAZ ALGORYTMU INSPIROWANEGO BIOLOGICZNIE

Streszczenie

W pracy przedstawiono zagadnienie identyfikacji rozmiaru pustki w skali mikro, na podstawie zhomogenizowanych parametrów materiałowych. Trójwymiarowy model komórki jednostkowej mikrostruktury porowatej modelowany i analizowany jest metodą elementów brzegowych (MEB). Metoda jest bardzo dokładna i dla rozważanego zadania wymaga jedynie dyskretyzacji zewnętrznego brzegu modeli. Zastosowany algorytm do identyfikacji charakteryzuje się hierarchiczną budową pozwalającą prowadzić obliczenia w sposób równoległy na trzech różnych poziomach. Wykorzystano równoległy algorytm do obliczeń ewolucyjnych. Zrównoleglono także rozwiązywanie zadań brzegowych za pomocą MEB oraz wyznaczanie zastępczych własności materiałowych metodą numerycznej homogenizacji. Pokazano sposób wyznaczania macierzy podatności mikrostruktury porowatej. Macierz jest wykorzystana do sformułowania funkcji celu w zagadnieniu identyfikacji, w którym poszukiwany jest rozmiar pustki. Przeprowadzono testy skalowalności algorytmu z użyciem serwera zawierającego osiem jednostek zmiennoprzecinkowych. Jako rezultat zastosowania algorytmu o budowie hierarchicznej oraz MEB uzyskano znaczne przyśpieszenie i dokładność obliczeń.

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