Publishing House
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów

Vol. 9, 2009, No. 2

PARALLEL EVOLUTIONARY OPTIMIZATION IN MULTISCALE PROBLEMS

WACŁAW KUŚ[1], TADEUSZ BURCZYŃSKI[1,2]

[1] *Department for Strength of Materials and Computational Mechanics, Silesian University of Technology, Konarskiego 18a, 44-100 Gliwice, Poland*
[2] *Institute of Computer Modelling, Artificial Intelligence Section, Cracow University of Technology, Warszawska 24, 31-155 Kraków, Poland*
Corresponding Author: waclaw.kus@polsl.pl (W. Kuś)

Abstract

The paper is devoted to optimization in multiscale problems. The composite modelled as a macrostructure with a local periodic microstructure is considered. The multiscale analysis is performed with the use of the homogenization method. The parallel evolutionary algorithm used in computations allows to shorten wall time of optimization. The fitness function evaluation with the use of the parallel homogenization algorithm is considered. The paper contains a description of the parallel evolutionary algorithm, the homogenization method, the optimization formulation and numerical examples.

Key words: optimization, parallel evolutionary algorithm, multiscale analysis, computational homogenization

1. INTRODUCTION

The multiscale modelling of materials [9,11] and structures is an important area of research allowing designing new materials and products with better quality, strength and performance parameters. The multiscale approach allows to create reliable models taking into account products and material properties and topology in different length scales. The multiscale models can be analysed using many approaches. The bridging and homogenization methods are most popular [8]. The bridging consists in connecting of scales on some boundaries. This method is especially important if some phenomenon occurs in a small part of the structure and should be taken into account. The example of the bridging method is connection between an atomic model and a continuum model discretized by the finite element method (FEM) for problems with the crack initialization and propagation. The area near the crack is modelled using the discreet atomic model and the rest of the structure is analysed by means of finite elements [12]. The two main approaches – mathematical and computational homogenization are used for analysing models with a locally periodical microstructure. The mathematical homogenization method is widely used in analyses of laminates. The micromodels have to be analysed for each local microstructure when the computational homogenization is used. The computational homogenization allows to consider complicated microstructure with nonlinearities like the elasto-plastic material, the contact with friction, wear or phase changes in the micromodel. The computational homogenization is used in the paper; the description of this method is presented in section 2.

The optimization in multiscale modelling allows to find structures with better performance or strength in one scale with respect to design variables in an-

 ISSN 1641-8581

other scale. Problems considered in the paper tackle optimization of microstructure parameters on the base of an objective functional based on the macro-model. The design variables describe the micro-model. The problem formulation is shown in section 3. The paper is extension of previous own work published in [3]. The new elements are connected with the use of the parallel homogenization and numerical tests of parallel algorithms.

The analysis methods of multiscale models can be used in the optimization algorithm. The global optimization algorithms based on bioinspired algorithms are widely used in optimization and identification problems in the field of solid mechanics. The most important advantages of bioinspired algorithms are their robustness, great probability of finding the global optimum and easy adaptation to new problems. The main disadvantage is long computation time due to the need of solving hundreds or thousands direct problems during optimization. The computations can be performed faster by using parallel multi-subpopulation approaches presented in section 4.

Optimization performed with the use of the evolutionary algorithm and multiscale FEM models is used to prepare numerical examples presented in section 5. The study of parallelization of optimization and homogenization algorithm is shown in section 5.2.

2. COMPUTATIONAL HOMOGENIZATION IN MULTISCALE MODELLING

One of the numerical techniques which enables multiscale analysis of structures is a computational homogenisation. The detailed description of the computational homogenization can be found in [5,7]. The structures with local periodicity are considered. The local periodicity means there are areas of a structure with the same microstructure. The example of such a structure is presented in figure 1a. The microstructures can also be build from lower scale locally periodic microstructures like in figure 1b. The goal of the computational homogenization is analysis of the structure taking into account a local periodicity of microstructures. The main advantage of the computational homogenization is 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.

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, voids, inclusions and other properties of microstructure can be included in the model. The RVE is in most cases modelled as a cube or a square. The numerical method like FEM is used to solve the boundary value problem for RVE. 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 form lower to higher and higher to lower scales is needed in most cases. The one way transfer of results (from lower to higher scales) is possible if the linear problem is considered. The transfer of average strains and stresses between scales is shown in figure 2.

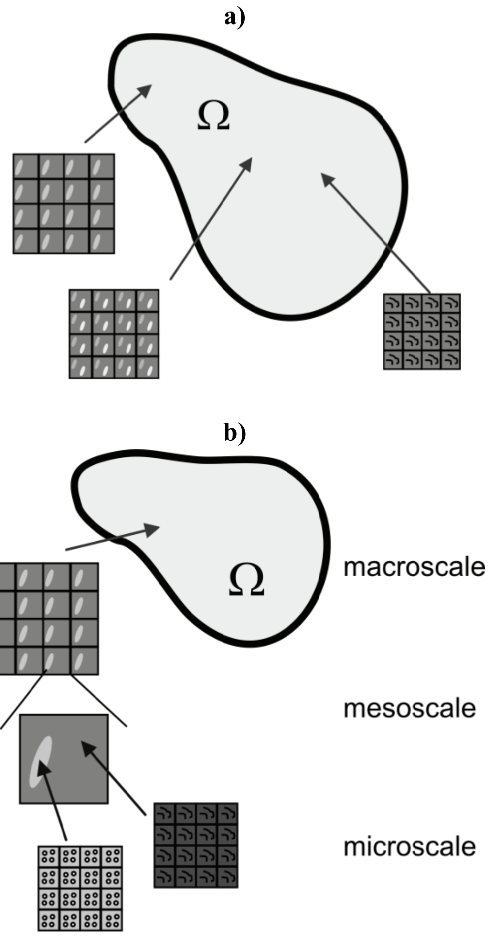

Fig. 1. *a) Two scale model of a structure with locally periodical microstructures, b) three-scales model of a structure.*

The material parameters for the higher scale are obtained on the basis of a few direct analysis 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

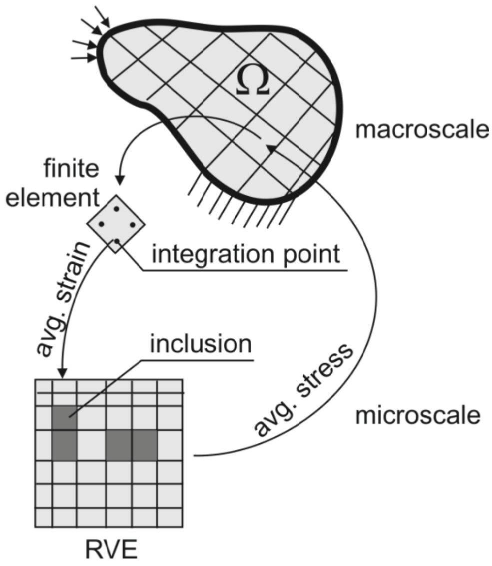

Fig. 2. *The average strain and stress transfer between scales.*

stress-strain 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 homogenization for linear 2D problems is considered in paper. The micromodel is solved for prescribed strains 3 times (strain applied in two axes and shear strain). The results obtained from micromodel analyses are used to build anisotropic material properties for macromodel. The macromodel is computed once. The homogenization algorithm can be easy parallelized when micromodels are analysed. The three analyses can be performed in the parallel way without data exchange. The speedups obtained using such a parallelization highly depend on the ratio between the time needed to compute micromodel and macromodel problems. The study of optimization with the use of parallel analysis is shown in section 5.

3. THE PROBLEM FORMULATION

The goal of optimization in multiscale modeling is to find a vector (chromosome) **ch** of material or geometrical parameters (design variables) on the micro-level (RVE) which minimizes an objective function $J_o=J_o(\mathbf{u},\boldsymbol{\varepsilon},\boldsymbol{\sigma})$ dependent on state fields of displacements **u**, strains **ε** and stresses **σ** on the macro-level of the structure

$$\min_{\mathbf{ch}} J_o \tag{1}$$

where

$$\mathbf{ch} = [x_1, x_2, ..., x_n] \tag{2}$$

x_i are design variables (genes) with imposed constraints

$$\begin{aligned} &x_i^{\min} \le x_i \le x_i^{\max}, \quad && i = 1,2,..,n \\ &J_\alpha(\mathbf{u},\varepsilon,\sigma) \le 0, \quad && \alpha = 1,2,..,A \end{aligned} \tag{3}$$

The chromosome **ch** defines material properties and/or shape of the microstructure components. Genes stored in **ch** , describe the micromodel material in the first case. The Young's moduli, Poisson's coefficients, friction coefficients and parameters of the elastoplastic curve can be determined using presented approach. The vector of parameters used in the paper contain real values therefore the material parameters can be directly obtained from **ch** . The other possibility is shape optimization of microstructure components. The shape of the fibers in the RVE is described by using NURBS curves. The NURBS are build on a top of a polygon with control points as points on the lines ends. The coordinates of control points are used as design variables (genes). The vector of parameters can directly reflect these variables like in the first case. The both groups of problems can be combined allowing shape and material optimization and identification.

4. THE PARALLEL EVOLUTIONARY ALGORITHM

The evolutionary algorithms [10] are well known and applied in many areas of optimization and identification problems [1]. The algorithms are based on biological evolution of species and belong to the bioinspired algorithms group. The algorithms operate on a population of chromosomes. The chromosome contains genes – design parameters. Each chromosome is equivalent to one solutions of the identification problem. The quality of solution is described using a fitness function. The fitness function is built on the base of the objective function and introduced constraints.

The main disadvantage of serial evolutionary algorithms is the long time needed for computation. The distributed evolutionary algorithm (DEA) [2,6] allows shortening computations. The DEA works similarly to a few evolutionary algorithms operating in a parallel way. The DEA uses a few subpopulations instead of one population. A migration mechanism exchanges chromosomes between subpopulations. The evolutionary algorithms exchange chromosomes during the migration phase between subpopulations. When DEA is used the number of fitness function evaluations can be lower in comparison with serial evolutionary algorithms. DEA works in the parallel manner, usually.

The flowchart of the distributed evolutionary algorithm for one subpopulation is presented in figure 3. The starting subpopulation of chromosomes is created randomly. The evolutionary operators change chromosomes and the fitness function value for each chromosome is computed. The migration exchanges a part of chromosomes between subpopulations. The selection decides which chromosomes will be in the new population. The selection is done randomly, but the fitter chromosomes have bigger probability to be in the new population. The selection is performed on chromosomes changed by operators and immigrants. The next iteration is performed if a stop condition is not fulfilled. The stop condition can be expressed as a maximum number of iterations.

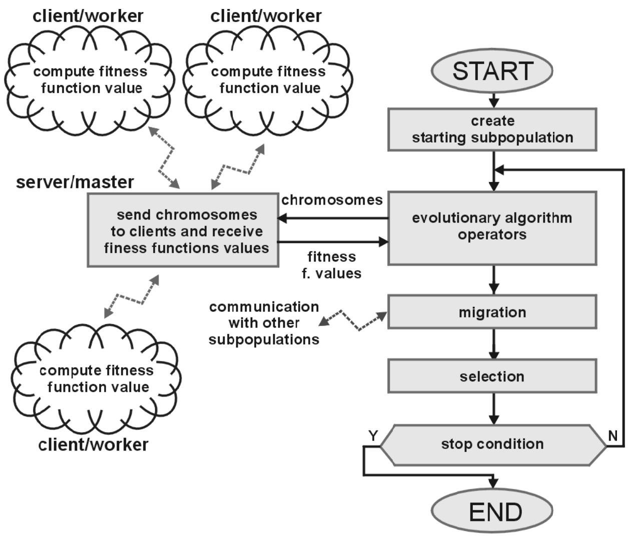

Fig. 3. The flowchart of the parallel evolutionary algorithm.

5. THE NUMERICAL EXAMPLE

5.1. Shape optimization

The numerical example of evolutionary optimization [3] for a 2D structure made from the composite is considered (figure 4a). The optimization criterion is to minimize the maximal reduced displacement of the structure. The objective function is evaluated for each chromosome. The shape of the fibre is coded into chromosomes. Coordinates of the NURBS control polygon points play the role of genes (figure 4b). The simple crossover and the Gaussian mutation are applied in the optimization process.

A representative volume element (RVE) is used as the microstructure. The periodic boundary conditions are applied (the periodicity of displacements is used). Numerical results of optimization are shown in figure 5. The best microstructure after the first generation is shown in figure 5a, and after optimization in figure 5b.

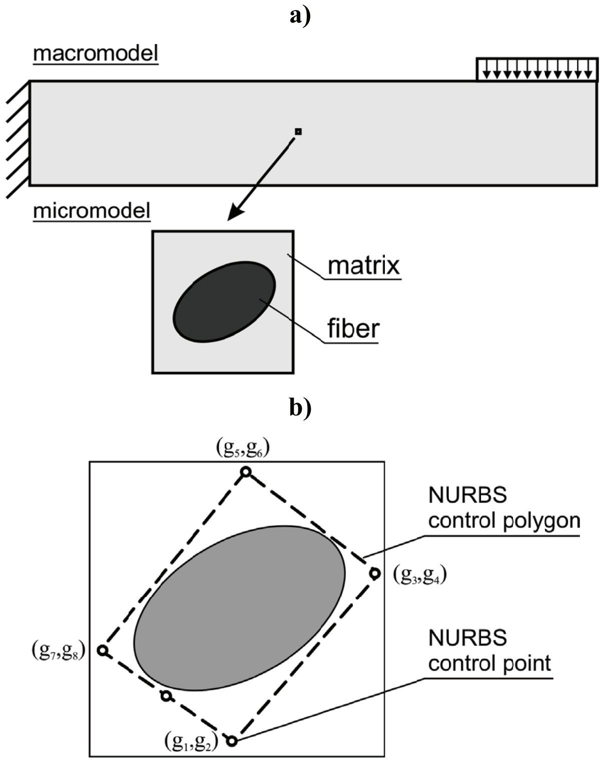

Fig. 4. a) The analysed 2D beam, macro and micro model, b) the fiber shape definition using.

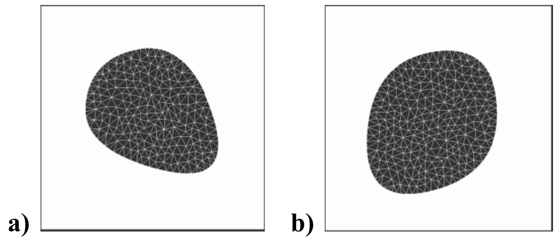

Fig. 5. The best result of optimization a) after the first generation, b) after optimization.

5.2. Optimization with the use of parallel evolutionary algorithm and the parallel homogenization

The previous numerical example is considered. The optimization algorithm operates on the same starting population during tests. The parameters of the evolutionary algorithm as the number of chromosomes, the number of subpopulations and operators are the same in each test. The goal of the numerical tests is to obtain speedups of computation when parallel algorithm are used. The parallel evolutionary algorithm and parallel analysis of 2D homogenization is considered. The analysis of the microstructure model is parallelized in homogenization method. The tests are performed using two quad core processors SMP computer (8 cores in a box, common hard disk). The homogenization are used in serial or parallel mode in tests. The parallel mode used 3 cores. The parallel evolutionary algorithm used 2, 4, 8 parallel fitness

***Table 1.** Optimizations times and speedups.*

Test number	Number of cores used in parallel homogenization	Number of parallel fitness function evaluations	Number of threads	Total number of used cores	Number of boxes	Time s	Speedup
1	1	1	1	1	1	1905.3	1
2	3	1	3	3	1	1215.4	1.57
3	1	2	2	2	1	1230.0	1.55
4	3	2	6	6	1	826.4	2.31
5	1	4	4	4	1	867.8	2.20
6	1	8	8	8	1	707.9	2.69
7	3	8	24	16	2	622.3	3.06

function evaluations. The tests run for 50 generations of the evolutionary algorithm. The total number of chromosomes was 10. The time need to perform optimization and speedups are shown in table 1.

The results depend on computer hardware, the common hard disk and common memories slow down parallel computations. It can be seen that the parallel evolutionary algorithm gives better speedups in tests 3, 5, 6. The use of the parallel homogenization algorithm is very important when the number of available cores is greater than number of chromosomes, the parallel evolutionary cannot scale up and the fitness function should be parallelized. The results depend hardly on the multiscale problem and presented data should be verified for other models before performing optimizations.

6. CONCLUSIONS

The evolutionary approach to optimization problems in the multi-scale modelling was presented. The aim of optimization problem was to find optimal parameters of the microstructure which ensures the best performance of the macrostructure for an assumed optimization criterion. It is seen that coupling FEM, the computational homogenization and the evolutionary computing enables to solve optimization and identification problems in multiscale modeling. The experimental analysis of parallelization of the evolutionary algorithm and homogenization was performed. The results show advantages of using the parallel evolutionary algorithm combined with the parallel homogenization when number of available processing elements is bigger than number of chromosomes.

ACKNOWLEDGEMENT

The research is financed from the Polish science budget resources in the years 2008-2010 as the research project.

REFERENCES

1. Burczyński, T., Osyczka, A. (eds), Evolutionary Methods in Mechanics, Kluwer Publishers Dordrecht, 2004.
2. Burczyński, T., Kuś, W., Optimization of structures using distributed and parallel evolutionary algorithms, Lecture Notes on Computational Sciences, 3019, 2004, 572–579.
3. Burczyński, T., Kuś, W., Microstructure Optimization and Identification in Multi-scale Modelling, ECCOMAS Multidisciplinary Jubilee Symposium, Computational Methods in Applied Sciences, Springer, Berlin, 2009 (in print).
4. Kaczmarczyk, Ł., Numerical analysis of selected problems of heterogeneous solids, Ph.D Thesis TU Cracow, Poland, 2006.
5. Kuś, W., Grid-enabled evolutionary algorithm application in the mechanical optimization problems, Engineering Applications of Artificial Intelligence, 20, 2007, 629–636.
6. Kouznetsova, V. G., Computational homogenization for the multi-scale analysis of multi-phase materials, Ph.D. Thesis TU Eindhoven, 2002.
7. Madej, Ł., Mrozek, A., Kuś, W., Burczyński, T., Pietrzyk, M., Concurrent and upscaling methods in multi scale modeling - case studies, Computer Methods in Materials Science, 8 (1), 2008, 1-15.
8. Liu, W. K., Karpov, E. G., Park, H. S., Nano Mechanics and Materials, Theory, Multiscale Methods and Applications, Willey, 2006.
9. Michalewicz, Z., Genetic Algorithms + Data Structures = Evolutionary Programs, Springer Verlag, Berlin, 1992.
10. MSC.Nastran User Guide, 2006.
11. Zhodi, T. I., Wriggers, P., Introduction to Computational Micromechanics, Springer, Berlin, 2005.
12. Zienkiewicz, O. C., Taylor, R. L., The Finite Element Method, Butterworth-Heinemann Oxford, 2000.

RÓWNOLEGŁA OPTYMALIZACJA EWOLUCYJNA W ZAGADNIENIACH WIELOSKALOWYCH

Streszczenie

Artykuł poświęcony jest optymalizacji w problemach wieloskalowych. Rozważany jest kompozyt modelowany jako ciało makroskopowe z mikroskopową strukturą lokalnie periodyczną Analiza wielkoskalowa przeprowadzona jest z użyciem metody homogenizacji komputerowej. Zastosowanie w obliczeniach równoległego algorytmu ewolucyjnego pozwoliło na skrócenie czasu obliczeń. Wyznaczanie wartości funkcji przystosowania również przeprowadzono stosując obliczenia równoległe. Artykuł zawiera opis równoległego algorytmu ewolucyjnego, metody homogenizacji, sformułowanie problemu optymalizacji oraz przykład numeryczny.

Submitted: October 30, 2008
Submitted in a revised form: December 5, 2008
Accepted: December 6, 2008