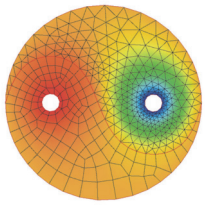
Publishing House
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 16, 2016, No. 3



OPTIMIZATION OF CARBON BASED FLAT STRUCTURES TOPOLOGIES BY USING PARALLEL COMPUTING

WACŁAW KUŚ[1*], ADAM MROZEK[2]

[1] *Silesian University of Technology, Poland*
[2] *AGH University of Science and Technology, Poland*
**Corresponding author:* waclaw.kus@polsl.pl

Abstract

The optimization algorithms based on global techniques like evolutionary algorithms tend to be time consuming due to a very high number of objective function evaluations. The computational effort can be reduced when the parallel approach is used. The paper is devoted to parallel versions of optimization algorithm developed for a multicore computer, manycore coprocessor and a supercomputer. The idea of dividing tasks between available cores is described. The optimization of carbon based flat structures problem is used as a test problem in the paper. The paper is focused mainly on the efficiency and scalability of the proposed algorithms.

Key words: optimization, parallel, memetic algorithm, graphene, flat structures

1. INTRODUCTION

The parallel algorithms for the optimization of structures like evolutionary algorithms have been well known for years (Burczyński et al., 2004; Kuś & Burczyński, 2008). The main idea of modification of algorithms is focused on fitness function evaluation in a parallel way. Some of the optimization problems were solved by parallelizing the optimization algorithm and the direct solving algorithm in a hierarchical way. The memetic algorithms used in the paper are based on a hybrid of evolutionary algorithm and gradient based local optimization technique. The algorithm is tested with the use of the topology carbon based flat materials optimization problem in the following sections. Carbon is well known for the creation of allotropes like graphene. Graphene is a flat structure with very high stiffness. The optimization problem presented in the paper is connected with searching for a new stable atomic, flat, carbon based structures. The new structures should be stable and the mechanical stability of them can be checked on the basis of the energy of the structure. The problems are solved using parallel memetic algorithm. The paper is organized as follows: first, the optimization problem is formulated. Then, the optimization memetic algorithm is described. The numerical tests of the algorithm with the use of different computational resources are shown in section 4.

2. THE OPTIMIZATION PROBLEM FORMULATION FOR CARBON BASED FLAT STRUCTURES

Graphene and similar two dimensional materials are the subjects of particular interest of researchers in recent years (Cranford & Buehler, 2011; Enyashin & Ivanovskii 2011; Narita et al., 2000; Peng et al., 2012; Scarpa et al., 2009) because of unique electronic, thermal and mechanical properties of such structures. The mechanical properties of flat structures are addressed in the paper. Two dimensional carbon based materials can be considered as period-

 ISSN 1641-8581

ic, flat atomic networks, made of stable configurations of carbon atoms in certain hybridization states. Depending on the arrangement of the considered structure, a rectangular or triclinic unit cell of a given size and atomic density can be identified for each type of the flat periodic network. An overview of such structures (like graphyne and supergraphene), along with detailed description and investigation of their structural and electronic properties using thight-binding method, can be found in the work by Enyashin and Ivanovskii (2011).

The stable configurations of atoms correspond to the minima on the Potential Energy Surface (PES), such a task can be considered as an optimization problem. However, searching for the global minimum on the PES is a non-trivial, NP-hard problem, because the number of local minima increases almost exponentially with the number of atoms in the considered structure.

The search for a new stable configuration of carbon atoms in flat structures were described by the authors in the paper Mrozek et al. (2015b). The potential energy, as well as neighborhood-dependent behavior of the carbon atoms is determined using Adaptive Intermolecular Reactive Bond Order (AIREBO) potential (Stuart et al., 2000), an extended REBO model proposed by Brenner et al. (2002) with additional terms.

The design vector contains coordinates of the atoms, due to two dimensional structure, two coordinates per atom are stored. The constraints on the atom positions are imposed. The atoms should be inside the unit cell under consideration. The goal of the optimization is to obtain stable atomic structure. The stable means the structure will not change after constructing such material, and the mechanical stability is defined by energy of the structure. The minimal energy guarantee the mechanical stable structure. The energy depends on energies of bonds between atoms. The objective function F depends on the energy computed for the structure defined by design vector:

$$F = \sum_{i} \sum_{j \neq i} \left(E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{kijl}^{TORSION} \right) \quad (1)$$

where i, j, k, l are atoms numbers, E^{REBO} is potential model defined by REBO model, $E^{TORSION}$ is torsion and E^{LJ} are long range terms. The application of the AIREBO potential to the examination of mechanical properties of two dimensional graphene-like materials that has already been performed by Mrozek and Burczyński (2013) yields good agreement with results obtained by other researchers.

3. MEMETIC OPTIMIZATION METHOD

The proposed memetic optimization algorithm method combines two optimization techniques, the global optimization Evolutionary Algorithm (EA) and local Conjugated Gradient (CG). The EA (Michalewicz, 1996) is based on the well known mechanisms from biological evolution of species. The local optimization algorithm allows to decrease the drawback of the global algorithm - the slow convergence near the optimum. The drawbacks of local search, like a very high probability of finding local optimum, is only balanced by the global optimum part of the algorithm. The design vector is described by chromosomal genes in the algorithm. The presented approach uses the floating point representation of genes, making the process of coding coordinates into genes straightforward (Kuś & Burczyński, 2008). One-chromosome individuals are used.

Each individual (chromosome) represents a certain, constant number of atoms with randomly generated coordinates placed in the area of the unit cell with periodic boundaries. Dimensions and type (rectangular or triclinic) of the unit cell, as well as a number of atoms, are part of the set of parameters of the simulation. Such approach allows for the regulation of atomic density of the created structure. The local search algorithm is applied for each atomic structure. The minimization algorithm from LAMMPS library (Lammps, 2016) is used for each chromosome in the population. The fitness function is equal to the total potential energy given by equation 1.

The local optimization is the most time consuming part of the algorithm. To overcome this problem, the authors decided to parallelize the proposed algorithm and make it suitable for running on multicore computers and coprocessors. The population is scattered into a certain number of parts using the MPI library or OpenMP. In the next step, each part is further processed in a parallel way using a dedicated instance of LAMMPS library running on a separate core or processor of the computer. The maximum number of parallel cores is equal to the number of chromosomes in the population. The computation can be parallelized in the future with the use of parallel local optimizer from LAMMPS library. The parallel computation inside one LAMMPS instance

will be important when structures with hundreds or thousands of atoms will be considered.

The EA performs selection and invokes evolutionary operators like mutation and crossover in the next step. The selection chooses chromosomes for a new parent subpopulation taking into account the values of the fitness function. Evolutionary operators change chromosomal genes and create new chromosomes for the offspring population. The uniform and Gaussian mutations, the simple crossover and ranking selection were implemented in the presented algorithm (Kuś & Burczyński, 2008). The stop condition is formulated as the maximum number of iterations. The flowchart of the optimization algorithm is presented in figure 1.

4. TESTS OF THE PARALLEL OPTIMIZATION ALGORITHM

The tests of the optimization algorithm were performed for the problem described in Mrozek et. al., (2015a). The search for the new stable configurations of 14 carbon atoms placed in the 7Å×6Å rectangular unit was performed by the optimization algorithm. 512 chromosomes in the population were used, the total number of genes was 28. The Gaussian mutation with probability parameter equal to 70%, uniform mutation with probability parameter 20%, the simple crossover with probability parameter 10% and range selection were applied.

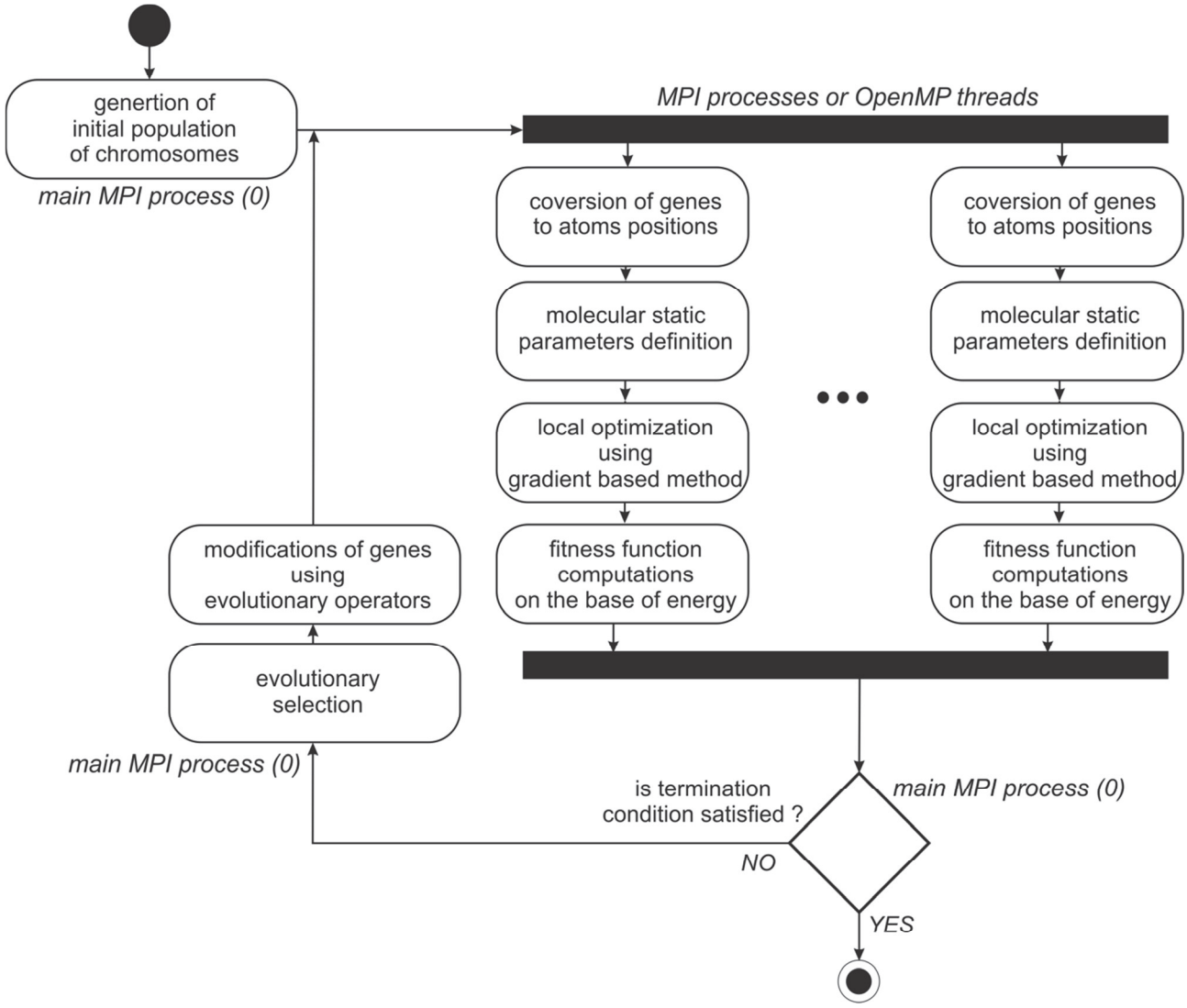


Fig. 1. *The parallel memetic optimization algorithm*

The exemplary progress of optimization is shown in figure 2. The arrangement of the atoms, a flat polycyclic network made of dodecagons is shown in figure 3a. A more detailed view of the unit cell, along with atoms potential energies and bond lengths, is shown in figure 3b.

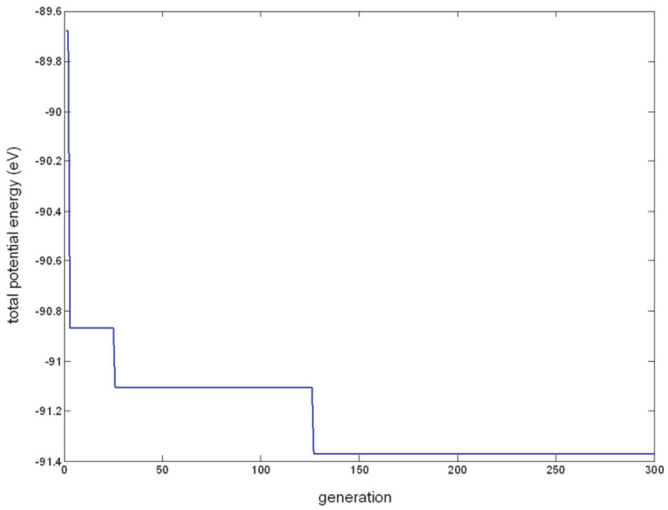


Fig. 2. *Progress of minimization of total potential energy (Mrozek et al., 2015a)*

The speedups were measured and presented in figure 4. The maximum speedup was near 10 for 16 cores.

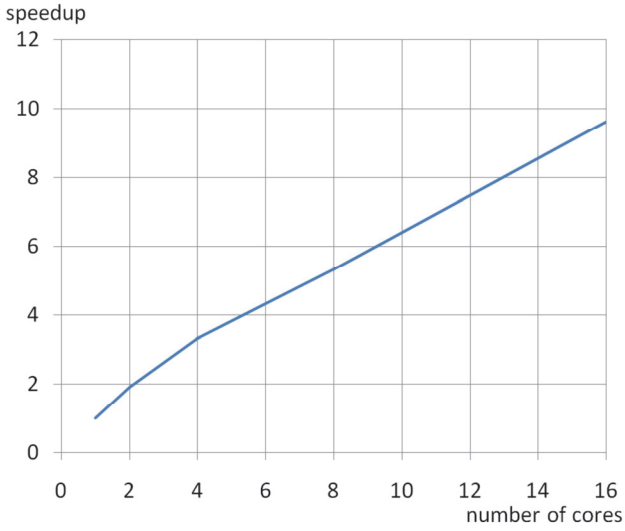


Fig. 4. *The scalability of optimization algorithm on multicore architecture*

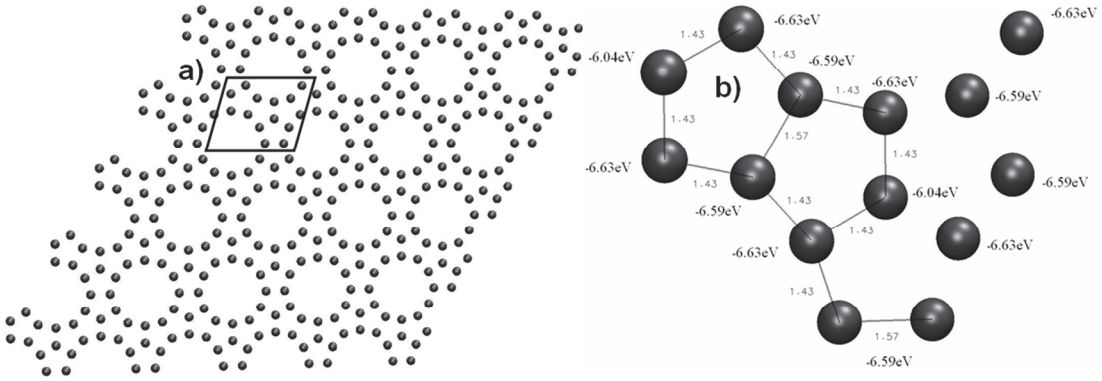


Fig. 3. *New carbon network found by optimization algorithm: a) structure, b) unit cell (Mrozek et al., 2015a)*

The tests were performed on three types of computational resources. First, a common multicore architecture with two processors was used. Next, the algorithm was executed on supercomputer IBM BlueGene/Q. Finally, the tests were performed on a manycore coprocessor. The starting seed for random generators was the same, so the same results can be obtained independent of the computing platform. The speedups of computation were measured for the resources under consideration.

A computer with two Xeon E5-2695 processors containing 12 cores each was used to test the algorithm in multicore environment. The MPI library provided communication during program execution. The tests were performed for 1, 2, 4, 8, 16 cores.

The second computing platform was IBM BlueGene/Q supercomputer located at ICM Warsaw. The supercomputer is build from 16-core one chip IBM PowerPC A2 1.6 GHz nodes connected by using 5D torus 40Gb low latency network. Each of the nodes has 16GB RAM, if all cores are used then 1GB per core is available. The tests were performed for 1, 8, 16, 32, 64, 128, 256 and 512 cores. The lowest possible numbers of nodes were chosen (1 node for 1, 8, 16, 2 nodes for 32, 4 nodes for 64, 8 nodes for 128, 16 nodes for 256 and 32 nodes for 512 cores). The MPI library was used in parallelization of optimization algorithm. The speedup of the computations were computed and presented in figure 5. The max-

imum speedup was approximately 167 for 512 cores (Mrozek et al., 2015a).

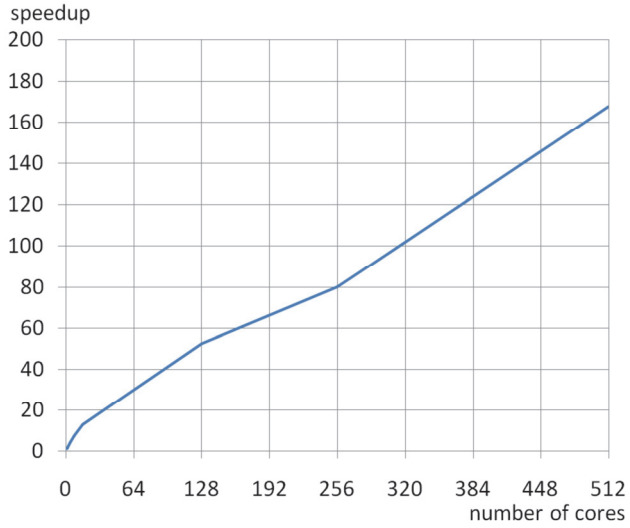


Fig. 5. *The scalability of optimization algorithm on IBM BlueGene/Q.*

The third architecture Intel MIC is a coprocessor which contains a chip with many cores (61 in the case of Intel Phi 7120P – code name Knights Corner) connected using a bidirectional ring bus. Each of the cores has 4 threads. The cores are equipped with cache-coherent L2 cache and the coprocessor is equipped with a few (8 in Intel Phi 7120P) memory controllers. The Intel Phi 7120P coprocessor has up to 16GB of GDDR5 memory with the total throughput of 352 GB/sec. The communication between host and coprocessor is based on PCIe bus. The low speed of the PCIe bus should be taken into account during the development of algorithms, the lowest possible communication between host and coprocessor is an important factor. One of the cores is used to manage the system operations on the coprocessor. The user can use 60 cores with 4 threads which gives up to 240 threads per coprocessor card. The programs on the coprocessor were executed in the coprocessor native mode - the program is compiled for the coprocessor only and cannot be executed on host processor. However, special coprocessor instructions, like AVX512, can be used to improve the performance of the program. The OpenMP was chosen as a parallel library for programs presented in the paper. The minimization with the use of memetic algorithm was performed in a parallel way. The optimization was executed on coprocessor Intel Phi 7120P. The scatter type of distribution of threads was used. The obtained speedup (Kuś et al., 2016) for a different number of threads is shown in figure 6.

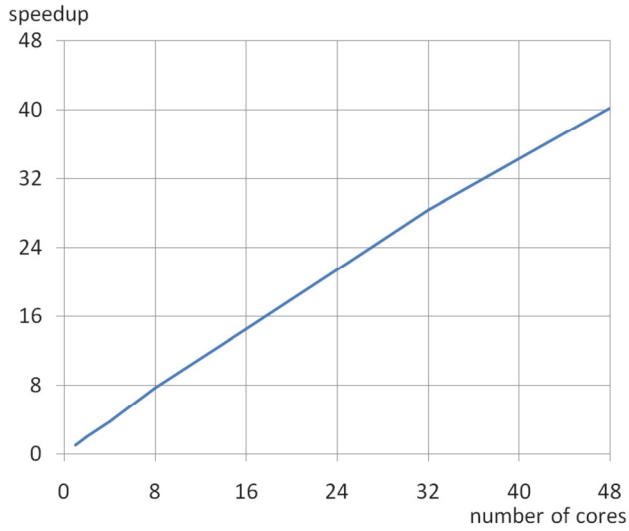


Fig. 6. *The scalability of optimization algorithm on Intel PHI coprocessor.*

The scalability of optimization algorithm in presented results is good. The main problem in presented optimization problem is connected with time needed for one objective function evaluations which can vary up to four times between chromosomes. The static distribution of chromosomes between MPI processes were used and it can be observed in results obtained for two platforms. The OpenMP dynamically distributed resources and the scalability was much better on Intel PHI coprocessor. The future modifications of the MPI versions of the code will take into account dynamic distribution of chromosomes and prediction of computing time of chromosome on the base of history of chromosomes parents computing time.

5. CONCLUSIONS

The parallel approach during memetic optimization allows for a significant reduction of wall time of computations. The speedups obtained for all computing platforms: multi, manycore and supercomputer show the utility of the presented approach. The efficiency of the algorithms for a high number of cores is not very good and future improvements of the codes should be implemented. However, from the point of view of the optimization problems, the memetic algorithm can significantly reduce computation time on the presented platforms. The optimization problem is complicated and sometimes the choice of initial parameters (like the size of the unit cell, number of the atoms) are crucial. The optimization process can be shortened significantly with the use of parallel approach presented in the paper.

ACKNOWLEDGEMENT

Calculations were performed in part at the Interdisciplinary Centre for Mathematical and Computational Modelling at the University of Warsaw under grant G56-1. The authors are grateful to Czestochowa University of Technology for granting access to Intel CPU and Xeon Phi platforms provided within MICLAB project No. POIG.02.03.00.24-093/13

REFERENCES

Brenner, D.W., Shenderova, O.A., Harrison, J.A., Stuart, S.J., Ni B., Sinnott, S.B., 2002, A second generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons, *Journal of Physics: Condensed Matter*, 14, 783-802.

Burczyński, T., Kuś, W., Długosz, A., Orantek, P., 2004, Optimization and defect identification using distributed evolutionary algorithms, *Engineering Applications of Artificial Intelligence,* 17(4), 337-344.

Cranford, S.W., Buehler, M.J., 2011, Mechanical properties of graphyne, *Carbon*, 49, 4111-4121.

Enyashin, A.N., Ivanovskii, A.L.,2011, Graphene Allotropes, *Physica Status Solidi*, 248, 8, 1879-1883.

Kuś, W., Mrozek, A., Burczyński, T., 2016, Memetic Optimization of Graphene-Like Materials on Intel PHI Coprocessor, *Artificial Intelligence and Soft Computing*, *Lecture Notes in Computer Science*, 9692, 401-410.

Kuś, W., Burczyński, T., 2008, Parallel bioinspired algorithms in optimization of structures, Parallel processing and applied mathematics, PPAM 2007, 7th International conference, *Lecture Notes in Computer Science*, 4967, 1285-1292, Springer.

Lammps homepage: Available online at: http://lammps.sandia.gov accessed: 02.09.2016

Michalewicz, Z., 1996, *Genetic algorithms + data structures = evolutionary algorithms,* Springer-Verlag, Berlin.

Mrozek, A. Kuś, W., Burczyński, T., 2015a, Hybrid Parallel Evolutionary Algorithm in Optimization of 2d Grapehene-Like Materials, *Computer Methods in Materials Science*, 15, 103-110.

Mrozek, A. Kuś, W., Burczyński, T., 2015b, Nano level optimization of graphene allotropes by means of a hybrid parallel evolutionary algorithms, *Computational Materials Science*, 106, 161-169.

Mrozek, A., Burczyński, T., 2013, Examination of mechanical properties of graphene allotropes by means of computer simulation, *Computer Assisted Methods in Engineering and Science*, 20, 4, 309-323.

Narita, N., Nagai, S., Suzuki, S., Nakao, K., 2000, Electronic structure of three-dimensional graphyne, *Physical Review B*, 62, 16, 11146-11151.

Peng, Q., Ji, W., De, S., 2012, Mechanical properties of graphyne monolayers: a first-principles study, *Physical Chemistry Chemical Physics*, 14, 38, 13385-13391.

Scarpa, F., Adhikari, S., Phani, A.S., 2009, Effective elastic mechanical properties of single layer graphene sheets, *Nanotechnology*, 20.

Stuart, S.J., Tutein, A.B., Harrison, J.A., 2000, A reactive potential for hydrocarbons with intermolecular interactions, *The Journal of Chemical Physics*, 112, 14, 6472-6486.

OPTYMALIZACJA TOPOLOGII PŁASKICH STRUKTUR ATOMOWYCH WĘGLA Z UŻYCIEM PRZETWARZANIA RÓWNOLEGŁEGO

Streszczenie

W artykule przedstawiono metodę oraz algorytm równoległej optymalizacji mimetycznej w zastosowaniu do optymalizacji płaskich struktur atomowych opartych na węglu. W artykule wykorzystano trzy rodzaje zasobów obliczeniowych, typowy komputer wieloprocesowy z wieloma rdzeniami, superkomputer IBM BlueGene/Q oraz koprocesor Intel PHI. Obliczenia przeprowadzono dla problemu optymalizacji rozkładu atomów węgla przy użyciu funkcji celu związanej z energią struktury. W pracy porównano skalowalność przedstawionego algorytmu optymalizacji dla różnych platform sprzętowych.

Received: November 10, 2016
Received in a revised form: November 21, 2016
Accepted: December 16, 2016