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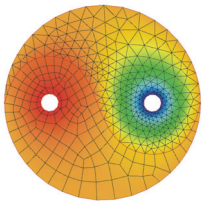

MODELING OF THE NANOSTRUCTURAL DEFECTS BY IMPLEMENTATION OF MOLECULAR STATIC METHOD FOR HETEROGENEOUS HARDWARE ARCHITECTURES

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Abstract

Dynamic development of heterogeneous hardware architectures and the increasing range of their practical applications in recent years influenced not only visualization procedures but also design and implementation of algorithms used in numerical simulations. This paper presents a part of the work on creation of multiscale approach focused on simulations of nanostructural defects in metallic materials. Two aspects are analysed within the paper i.e. qualitative (reliable simulation of interactions between nano particles on the basis of Lenard-Jones and Sutton-Chen potentials) and quantitative (comparison of performance and scalability for different devices). The results obtained for both aspects are presented in the paper and discussed in details.

Key words: nanostructural defects, molecural static, OpenCL

1. INTRODUCTION

Development of heterogeneous hardware architectures (Brodtkorb, 2010) as well as the trend on green computing (Murugesan, 2008) improved computational efficiency of many devices including non-conventional processors and computational devices like Cell Broadband Engine Architecture (CBEA) or General-Purpose Computing on Graphics Processing Units (GPGPUs). Even new projects in this area of science were started e.g. Calxeda (http://www.calxeda.com/), Tilera (http://www.tilera.com/) or Parallela (http://www.kickstarter.com/projects/adapteva/parallella-a-supercomputer-for-everyone), aiming at creation of new kind of integrated computational units. The architectures of these devices are usually based on many low frequency cores, which guarantee high computational as well as energy efficiency. These devices are usually the part of computing nodes equipped with conventional CPUs, thus the hardware architecture is characterized by heterogeneity of internal units. Due to this progress of hardware development as well as availability of many different hardware architectures, the need of unique software implementation technology appeared. This was the first step to create OpenCL approach (http://www.khronos.org/opencl/), supported by a group of the most important hardware providers in the world. It opened the doors to implementation of homogeneous implementation of multiscale numerical simulations on heterogeneous hardware components (Rauch et al., 2011). Modelling of Molecular Static, MS (Mishin et al., 1999; Liu et al., 2004) is also the part of such approach, offering methodology for simulation of nano structures behaviour under various conditions.

The main objective of this paper is to verify efficiency of parallel implementation of MS on different devices, which will give an answer on how to

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choose architecture to the problem or how to adjust implementation of the solution to the specific architecture. The following sections describe the problem, details of algorithms implementation in OpenCL technology and obtained results. The results are twofold i.e. qualitative (verification for A2 nanostructures) and quantitative (performance and scalability).

2. MODELLING OF NANOSTRUCTURAL DEFECTS

2.1. Fundamentals

Numerical simulations of nanostructural defects require calculation of influence between large amount of atoms for relatively small sample of material. Theoretically, all atoms inside analysed structure decide about another atoms locations and influence on each another. In practice, atoms, which are located in significant distance, are omitted in calculations, due to the threshold (cut-off radius) applied on interatomic potentials. Potentials, like Lennard-Jones or Morse, are usually implemented for testing purposes or to simulate behaviour of gases. However, in the case of metallic structures Sutton-Chen potential is much more appropriate to describe multi-atomic common influence. Differences between these potentials are visible in number of formula parameters as well as complexity of calculations, which is directly related to the complexity of neighbourhood.

Structural defects cause increase of the potential values, which have to be minimized by modification of atoms locations. MS aims to obtain the equilibrium configuration of atoms, which is achieved by changing the positions of atoms in each time step, so that the value of the global energy is reduced. The global energy of the system is calculated on the basis of a sum of atoms potentials and information about velocities received indirectly from interatomic driving forces, according to the following equation:

$$\boldsymbol{F}_{ij} = -\frac{\partial\phi(r_{ij})}{\partial r_{ij}}\frac{\boldsymbol{r}_{ij}}{r_{ij}} \qquad \boldsymbol{F}_{ji} = -\boldsymbol{F}_{ij} \quad (1)$$

where F_{ij} is a force of i^{th} particle acting on j^{th} particle, r_{ij} is a distance between these particles and $\phi(r_{ij})$ is a potential function dependent on distance between particles.

2.2. Potentials

As mentioned in previous section various models of interatomic potentials can be used to describe common atomic interactions. However, the main problem is to apply a potential function, which is able to describe physical and chemical properties of materials realistically. These properties depend on atomic structure. The potential energy of N atoms can be described by the formula (Elizondo, 2007; Liu et al., 2006):

$$V(r_1, r_2, \ldots, r_N) = \sum_i \phi_1(\boldsymbol{r}_i) + \frac{1}{2}\sum_{i,j>i}\phi_2(\boldsymbol{r}_i, \boldsymbol{r}_j) + \frac{1}{3}\sum_{i,j>i,k>j}\phi_3(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k) + \cdots \quad (2)$$

where ϕ_i is an i^{th} element potential, $\boldsymbol{r}_i$ is the position vector of an i^{th} atom. The first component of the formula ϕ_1 expresses the external forces of the system, which is ignored in this paper. Atoms interactions described by ϕ_2 and three ϕ_3 are applied. Many models have been presented and discussed in detail by Elizondo (2007) and Liu et al. (2006). In this paper Lennard-Jones and Sutton-Chen potentials are implemented.

2.2.1. Lennard-Jones potential

The diatomic potential model was presented by Lennard-Jones (1924) in the form of:

$$\phi^{\text{L-J}}(r_{ij}) = 4\varepsilon[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}] \quad (3)$$

where, parameter ε is the minimum value of the potential function and σ defines zero potential. Lennard-Jones potential considers only two body interaction, reliable mainly in application to weak interactions between molecules of noble gases (such as argon). It is also used in modelling of solids, because of its simplicity and low computational effort (Elizondo, 2007; Sunyk & Steinmann, 2002). Component $(\frac{\sigma}{r_{ij}})^{12}$ (in equation 3) describes the short-range $(r_{ij} < r_0)$ ionic repulsion to prevent penetration between them. Component $(\frac{\sigma}{r_{ij}})^{6}$ describes van der Waals interaction (attraction between two electric dipoles for $(r_{ij} < r_0)$. Properties of Lennard-Jones potential:

$$r_{ij} = r_0 : \phi^{\text{L-J}} = -\varepsilon = \phi_{min},$$
$$r_{ij} = \sigma : \phi^{\text{L-J}} = 0,$$
$$r_{ij} \to 0 : \phi^{\text{L-J}} \to \infty,$$
$$r_{ij} \to \infty : \phi^{\text{L-J}} \to 0.$$

Force of i^{th} atom influencing j^{th} atom is given by derivative of the potential regarding an interatomic distance r_{ij}:

$$\boldsymbol{f}_{ij} = \frac{24\varepsilon}{\sigma}\left[2\left(\frac{\sigma}{r_{ij}}\right)^{13} - \left(\frac{\sigma}{r_{ij}}\right)^{7}\right]\frac{\boldsymbol{r}_{ij}}{r_{ij}}. \quad (4)$$

2.2.2. *Sutton-Chen potential*

Atomic interactions for solids are more complex than for gases. Therefore, multi-element Sutton-Chen potential is much more reliable to describe behaviour of solids (Sutton & Chen, 1990):

$$\phi^{S-Ch} = \varepsilon\left[\frac{1}{2}\sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^{n} - c\sqrt{\rho_i}\right] \quad (5)$$

where:

$$\rho_i = \sum_j \left(\frac{a}{r_{ij}}\right)^{m} \quad (6)$$

Potential (and the resultant force) for the i^{th} atom is a complex function of the positions of its neighbouring atoms and their neighbours. Unitless parameters, c, n and m in (5) and (6), are specific for each material. Variable ε is scale factor of energy and a is the lattice constant. The force between atoms is calculated from equation (1), which after the transformation can be rewritten as follows:

$$\boldsymbol{f}_{tot} = \sum_{j\neq i} \boldsymbol{f}_{ji}\frac{\boldsymbol{r}_{ji}}{r_{ji}} \quad (7)$$

where f_{ji} is force value between i and j atoms and is given by:

$$f_{ji} = -\varepsilon\left[n\left(\frac{a}{r_{ji}}\right)^{n} - \frac{cm}{2}\left(\frac{1}{\sqrt{\rho_j}} + \frac{1}{\sqrt{\rho_i}}\right)\left(\frac{a}{r_{ji}}\right)^{m}\right]\left(\frac{1}{r_{ji}}\right) \quad (8)$$

3. IMPLEMENTATION DETAILS

The computing methods are implemented by using the OpenCL framework, which is the only framework independent of devices producers. This approach allows to run the same program on different hardware platforms. Proposed program, simulating defects in nanostructures, is composed of the subsequent steps:

1. Generation of non-stable nanostructure,
2. Stabilization of nanostructure,
3. Introduction of nanostructural defects,
4. Stabilization of nanostructure with defects.

The generation of nanostructure is executed on the host side, which means that all computational cost of this procedure is usually handled by CPU. This cost is negligible in the case of large scale computing. Then the data is allocated in the memory of computing devices and kernels are initialized. Kernels are parallel programs, which implements Embedded Atom Method. These are the main solvers of the problem, responsible for stabilization of the moving atoms. Each kernel calculates new positions of *n*/*GWS* atoms, where *n* is total number of atoms in the structure and *GWS* is a Global Work Size, which determines a number of all kernels executed in the device. GWS as well as LWS (Local Work Size) are specific parameters of computing devices. The analysis of GWS and LWS influence on the computational performance of the program is presented in section 4. The algorithm steps are described in details in the following subsections. Stabilization of the nanostructure with and without defects is the same procedure described in section 3.2.

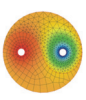
3.1. Structure generation

Generating of nanostructure is based on various primitive cells, e.g. A1, A2, with respect to translational symmetry, which can be done both in 2D and 3D. The distances between each generated pair of atoms do not guarantee immediate stability of the system. The function responsible for generation of the nanostructure takes three arguments as input – one of these parameters is *m*, the number of primitive structures in each of the three dimensions. Therefore, the function returns a rectangular block of atoms in form of one of the nanostructural primitive cells multiplied *m* times in each dimension. Additionally, program implements functionality allowing modification of atoms, thus there exists possibility to add extra or remove existing atom before stabilization.

3.2. Stabilization of the nanostructure

The process of stabilization starts in two cases i.e. with and without defects. The first case is executed after creation of initial nanostructure, while the second one is launched each time the defect is introduced into the structure. The large number of atoms often requires high computational efforts, therefore the procedure solving each move of atoms is implemented in parallel form (described before section 3.1) and the cut-off radius is applied.

The cut-off radius is introduced to avoid situation, when each atom in analysed nanostructure influences the others. In such case of large atomic systems, the



computational cost increases drastically. This influence, according to applied potentials, can be negligible while specific distance between two atoms is obtained. To calculate the force acting on analysed atom the following formula has to be used:

$$F_k = \sum_{i=1, i \neq k}^{n} F(k,i) \qquad (9)$$

where k is an index of analysed atom, i are indexes and n is a number of atoms located in the cut-off radius distance, $F(k, i)$ is a force acting on atom k.

3.3. Introduction of nanostructural defects

Introduction of nanostructural defects causes movement of atoms from their equilibrium positions. Defects in material structures distort the periodicity of structure and influence properties of materials. Three groups of structural defects are implemented in the proposed application i.e. point, linear, planar defects. All the defects can be applied manually by users or randomly to simulate real material structures with specific dislocation density. Point defects include vacancies (figure 1a), self-interstitial atoms (figure 1b), interstitial impurity atoms and substitutional atoms. A disruption of the long-range stacking sequence can produce two other common types of crystal defects: a stacking fault and a twin region. These are planar defects.

4. RESULTS

The calculations were divided into two parts aiming at qualitative and quantitative assessment of the proposed approach implemented by using OpenCL technology.

4.1. Qualitative results

The first group of calculations were performed for regular nanostructures for many different cases

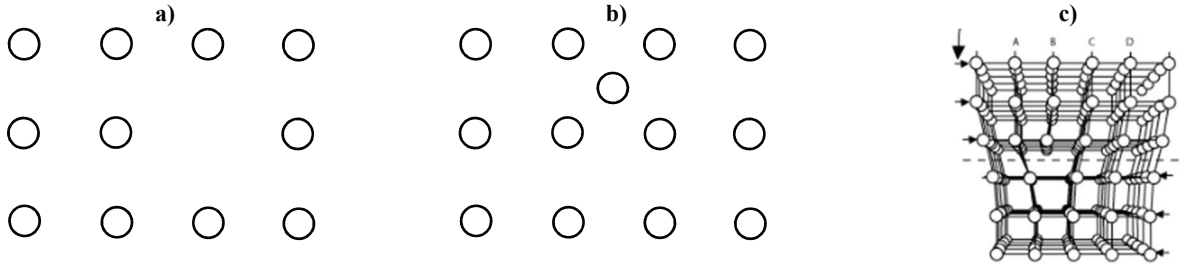


Fig. 1. *Simulated dislocations (a) vacancies, (b) self-interstitial atoms, (c) linear defect.*

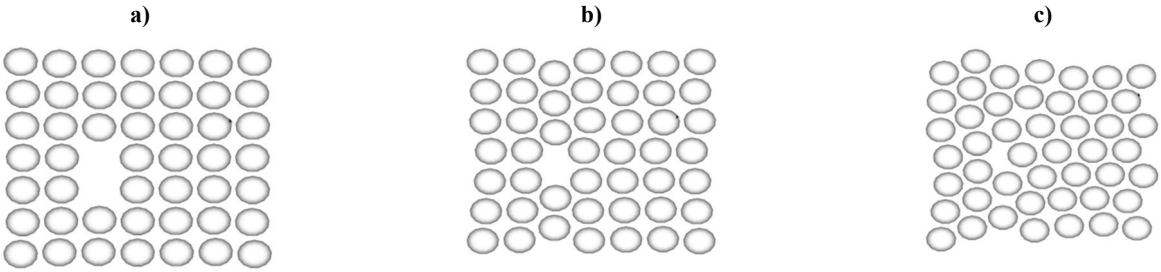


Fig. 2. *Lennard-Jones potential – (a) initial defect, (b) state of the structure in time $t_{0.5}$, (c) stable nanostructure.*

Fig. 3. *Simulation of edge dislocation with Sutton-Chen potential before (a) and after (b) calculations.*

to verify the reliability of proposed approach. The numerical tests were focused on 2D and 3D cases with Lennard-Jones and Sutton-Chen potentials, including all implemented defects. The results of subsequent steps of 2D Lennard-Jones 2-point defect are presented in figure 2. Figure 3 presents initial edge dislocation in 3D structure and final result obtained using Sutton-Chen potential. All the qualitative results were compared to results obtained for the same input (Lennard-Jones and Sutton-Chen potentials) by using Molecular Dynamics Simulator LAMMPS (http://lammps.sandia.gov/). The comparison proved reliability of the solution proposed in the paper.

4.2. Quantitative results

The performance (times and scalability) was analysed for Intel i7 2600 k CPU (theoretical peak = 108 GFLOPs at 4.375 GHz) and GPGPU GTX 570 (theoretical peak = 1405 GFLOPs). Figure 4 presents times obtained for 10 iterations of the method for Lennard-Jones potential on both devices.

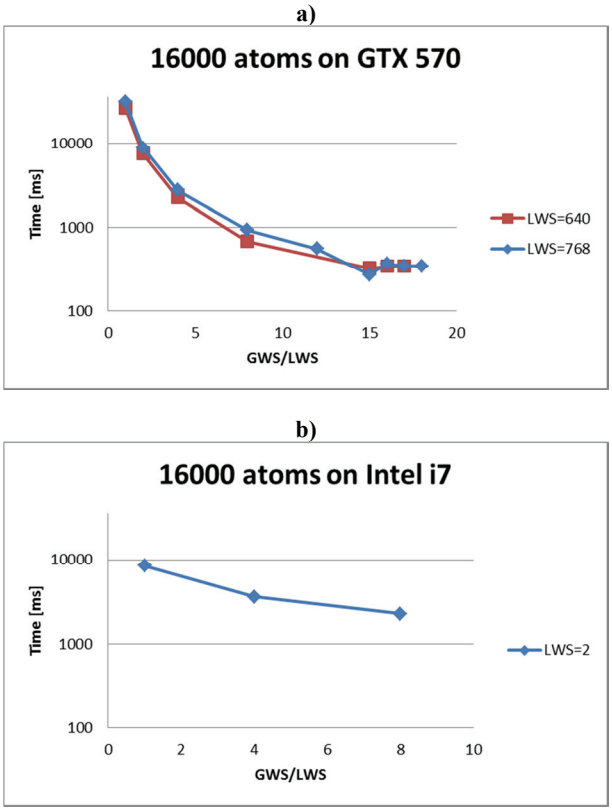


Fig. 4. Times for 10 iterations of the proposed method on GPGPU and CPU (time presented on logarithmic scale).

To obtain results presented in figure 4, LWS parameter had to be determined. It was selected on the basis of series of calculations, where GWS was equal to LWS, which means that only one Streaming Multiprocessor (SM) from GPU was used. Further increase of LWS from 640 to 768 did not offer any additional advantages and the final time obtained for GWS/LWS = 15 for both of these cases was optimal. In the case of CPU similar calculations were performed and LWS was set to 2, which is related to 2 computing threads in one i7 core (the effect of Hyper Threading).

The scalability was calculated for increasing size of the problem as well as for proportionally increasing number of SMs in GTX 570 or cores in i7 (Figure 5). Calculations for GTX 570 started with N = 1000, doubled in subsequent test until 8000. In the last test N = 15000, because of 15 SMs in GPU. In the case of CPU, the calculations stared with N = 2000, doubled each time until 16000 atoms were obtained. The best LWS was selected to perform these calculations for both devices. Calculated scalability is presented in figure 6 a and b for GPU and CPU respectively.

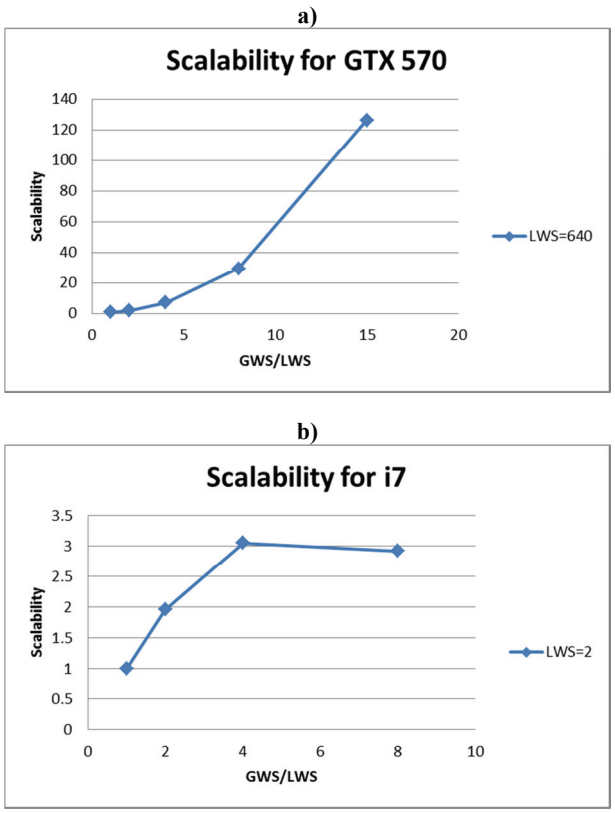


Fig. 5. Scalability of the method for GPGPU and CPU.

Additionally, the values of GFLOPs were calculated for selected devices. The program was changed to avoid random number of operations influenced by cut-off radius. Then, the source code was converted into assembler and floating point operations were counted. The number of these operations divided by computing time resulted in GFLOPs. The best results are as follows:

– 448.255GFLOPs for GWS/LWS = 11520/768, 32000 atoms, 10 iterations on GTX 570,
– 64.468GFLOPs for GWS/LWS = 16/2, 8000 atoms, 10 iterations on i7.

5. CONCLUSIONS

The paper presents parallel implementation of Molecular Static method for simulation of nanostructural defects in metallic materials. Two different interatomic potentials, i.e. Lennard-Jones and Sutton-Chen, and three different defects, i.e. point, linear and planar, were implemented for the purposes of this work. More sophisticated Sutton-Chen potential offered better qualitative results than simple Lennard-Jones potential, which is usually applied to simulate behaviour of gases.

The source code was created in OpenCL technology to compare the same implementation of the method for different computing devices like CPU and GPGPU. Performed calculations proved that used GPGPU finished calculations much faster than CPU for the same size of a selected nanostructure – for 16000 atoms GPGPU time was 329 ms, CPU time was 2280ms, which is 6.93 times slower. However, the peak performance of both devices differs in favour of GPGPU (1405 GFLOPs/108 GFLOPs = 12.96), which suggests that, according to obtained GFLOPs, the usage of this particular CPU, in the case of the selected algorithm, is more efficient than application of GPGPU. Nevertheless, the comparison of these two devices regarding market prices shows that GPGPU offers much shorter times of calculations for similar price level as well as super strong scalability in opposite to i7 CPU.

The proposed approach will be extended with modelling of changing temperatures, which will influence behaviour of atoms. This will allow to simulate real processes like cooling of materials and forming of grains in the metallic structure. Additionally, the influence of memory bandwidth on scalability will be analysed.

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MODELOWANIE DEFEKTÓW STRUKTURALNYCH W SKALI NANO METODAMI DYNAMIKI MOLEKULARNEJ Z WYKORZYSTANIEM HETEROGENICZNYCH ARCHITEKTUR SPRZĘTOWYCH

Streszczenie

Dynamiczny rozwój innowacyjnych architektur sprzętowych powoduje, iż coraz częściej są one stosowane do celów innych niż pierwotnie były zaprojektowane. Artykuł przedstawia krótki przegląd takich architektur heterogenicznych oraz szczegóły dedykowanej dla tych urządzeń implementacji metody statyki molekularnej. Wiarygodność metody została sprawdzona dla symulacji defektów nanostrukturalnych materiałów metalicznych z wykorzystaniem potencjałów Lenarda-Jonesa i Suttona-Chena. Dlatego w pracy przedstawione zostały zarówno jakościowe jak i ilościowe wyniki wykonanych obliczeń. Rezultaty jakościowe obejmują symulacje defektów punktowych, liniowych oraz planarnych, natomiast wyniki ilościowe przedstawiają efekty zrównoleglenia metody. Pracę podsumowuje dyskusja nad otrzymanymi wynikami.

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