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Evaluation of code parallelization solutions in the static recrystallization cellular automata model

Mateusz Sitko*, Lukasz Madej

AGH University of Science and Technology, Mickieiwicza 30 av., Krakow 30-059, Poland

Abstract

A parallel implementation of the cellular automata static recrystallization model is the subject of the present paper. First, a description of theoretical assumptions of the static recrystallization model including nucleation and grain growth stages is summarized. After that crucial modifications that have been introduced to the model to handle parallel execution are presented. Particular attention is put on evaluation of the influence of recrystallized fraction on parallelization efficiency and computational time. The classical parallelization indicators in a form of computational speedup and computation time are presented in that part. Finally, microstructure morphology results for different simulation settings are presented and discussed.

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Keywords: Cellular automata, Static recrystallization, Parallelization, MPI standard, Computation efficiency

1. Introduction

Through a suitable combination of thermo-mechanical treatment operations like heating, hot rolling, cooling, cold rolling, etc. series of sophisticated properties of final metallic products can be achieved. There are several major phenomena, that allow to control microstructure evolution during and after deformation e.g. recovery, recrystallization, precipitation, phase transformation etc. [1]. The numerical modelling of microstructure evolution is recently a very important part of development of different innovative metal forming operations as well as new functional materials as it broadens experimental research capabilities and limits costs. Modern material models are often based on full field

* Corresponding author. Tel.: +48 12 617 50 08;
E-mail address: msitko@agh.edu.pl

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techniques like the cellular automata [2, 3], the Monte Carlo [4, 5], the phase field [6, 7], the level-set [8, 9] approaches. These methods take into account not only general behavior of the material but also microstructure morphology changes under heat treatment conditions [10]. Unfortunately, a computational time of this class of models, especially in the 3D, is still an enormous obstacle and currently it is impossible to apply these models at the industrial scale. One of the solutions to eliminate this problem, investigated within the work, is application of capabilities provided by modern computer architectures and parallelization scenarios. The static recrystallization cellular automata model [2, 11] was selected as a case study for the present investigation.

2. Static recrystallization model

In the static recrystallization model three major stages are considered: the microstructure generation, the nucleation and the grain growth, respectively. The present paper is primarily focused on parallelization aspects of the model, thus the initial microstructure was simplified and generated based on the unconstrained grain growth algorithm [12] with non-uniform energy distribution. The other two stages of nucleation and grain growth are based on the earlier authors work described in [13] and only major assumptions summarized below.

The nucleation is based on physical rules and takes into account the influence of a temperature and an energy accumulated during a deformation. The number of nuclei that can appear in the material volume per unit of time is controlled by the equation:

$$N = M_N \exp\left(-\frac{Q_{nuc}}{RT}\right), \tag{1}$$

where Q_{nuc} is the activation energy for nucleation, R is the universal gas constant, T is the temperature and M_N is the coefficient computed using the formula:

$$M_N = C_0\left(H_i - H_C\right), \tag{2}$$

where C_0 is the scaling parameter, H_i is the amount of energy in the particular cell obtain from deformation in Abaqus software [11] or artificially distributed in material and H_C is the critical amount of energy, which is necessary to trigger nucleation. H_C is calculated from the formula:

$$H_C = \frac{\varepsilon_c}{a\varepsilon_c + b}\gamma_{lagb}, \tag{3}$$

where ε_c is the critical plastic strain, a and b – parameters, which are fitted during the experimental analysis and γ_{lagb} is the low angle grain boundary energy.

The probability of nucleation in the unit of time is computed as:

$$P_n = NS_N t_{step}, \tag{4}$$

where S_N is the the volume in which the nucleus can appear and t_{step} is the length of time step in each cellular automata iteration.

Recovery phenomenon is consider at the beginning of each cellular automata iteration. During this stage the amount of accumulated energy is reduced in the particular cell by the following formula proposed in [14]:

$$H_i = \left[{H_{i0}}^{1/2} - C_1 \mu^{-1/2} kT \ln\left(1 + \frac{t}{\tau_0}\right)\right]^2, \tag{5}$$

where H_{i0} is the initial stored energy value, C_1 is a fitting parameter, k is the Boltzmann constant, τ_0 is the time constant

which is set as 1s, t - time.

The kinetics of the growing nuclei is described by the standard velocity equation:

$$v_E = MP, \tag{6}$$

where M is the grain boundary mobility and P is the net pressure on the grain boundary.

The value of M is computed according to the formula:

$$M = M_\theta \frac{D_0 b_B^{\,2}}{kT} \exp\left(-\frac{Q_b}{RT}\right), \tag{7}$$

where D_0 is the diffusion constant, b_B is the magnitude of Burgers vector, Q_b is the activation energy for grain boundary motion and M_θ is the influence of crystallographic orientation difference between two grains, computed as:

$$M_\theta = 1 - \exp\left(-\left(\frac{\theta_1 - \theta_2}{\theta_{cr}}\right)^n\right), \tag{8}$$

where n is the constant (equal 3) and θ_{cr} is the critical misorientation angle set as 15°.

The value P, on the other hand, is calculated with a consideration of the accumulated energy due to deformation, the pinning force from possible precipitates proposed in [15] and the grain boundary curvature effect within the microstructure:

$$P = H + \left(-\frac{3}{2}\gamma_{lagb}\frac{f}{r}\right) + \kappa\,\gamma_{hagb}, \tag{9}$$

where f is the volume fraction of spherical particles, r is the particle radius, γ_{hagb} is the high angle grain boundary energy and κ is the grain boundary curvature calculated as:

$$\kappa = \frac{A}{c_s}\frac{Kink - c}{N'}, \tag{10}$$

where A is the fitting parameter, c_s is the cellular automata cell size, *Kink* is the number of cells, which create flat grain boundary (with classical CA the values of 15 and 75 for 2D and 3D models, respectively), c is the number of cells within the neighborhood with the same state as investigated cell and N' is the number of all cells belonging to the long range Moore's neighborhood (the values of 25 and 125 for 2D and 3D models, respectively).

With presented calculations the recrystallized volume fraction in the CA cell is evaluated by:

$$RX_{i,j,t}^{\,fraction} = RX_{i,j,t-1}^{\,fraction} + \sum_{k=1}^{rx}\left(\frac{v_E t_{step}}{c_s}\right), \tag{11}$$

where $RX_{i,j,t-1}^{\,fraction}$ is the level of coverage in the *t-1*-th time step, *rx* is the number of recrystallized neighbors (stored energy driving force) and v_k is the velocity of the recrystallization front.

Thus, based on the above equations transition rule describing changes in the CA cell state from the *unrecrystallized* to *recrystallized* is defined as:

$$Y_{i,j,t+1} = \begin{cases} SRX \Leftrightarrow RX_{i,j,t}^{fraction} > 1.0 \\ Y_{i,j,t} \end{cases}, \tag{12}$$

where $Y_{i,j,t}$ is the state of the neighboring CA cell (i,j) in a particular time step t.

Described cellular automata static recrystallization model was already validated in earlier authors research works [13] and proved its predictive capabilities. However, as mentioned, to increase its computational efficiency in the present work the code was modified to allow the parallel execution on multi core processor computing machines.

3. Parallelization of cellular automata code

The first crucial step in a parallel implementation of the cellular automata algorithm is development and implementation of proper division of the cellular automata space between subsequent processor units (CPUs). The Message Passing Interface (MPI) standard [16, 17] was selected as a framework for parallelization of the cellular automata static recrystallization code. The developed concept of the cellular automata space division scheme is based on an equal rectangular computational domains, which are distributed between set of computing CPUs.

At the beginning of each simulation the *master* process, which is an instance of the cellular automata static recrystallization program, with id = *p0* performs loading operation of the initial microstructure morphology with: the grain id, the orientation and the energy value as well as the set of simulation parameters (Fig. 1(a)). After that, based on a number of processes on which simulation is carried out the cellular automata computational domain is divided to smaller subdomains. Each subdomain contains again a set of appropriate microstructure data, which are handled by set of *slave* processes with ids = *p1 – pn*, as seen in the Fig. 1(b).

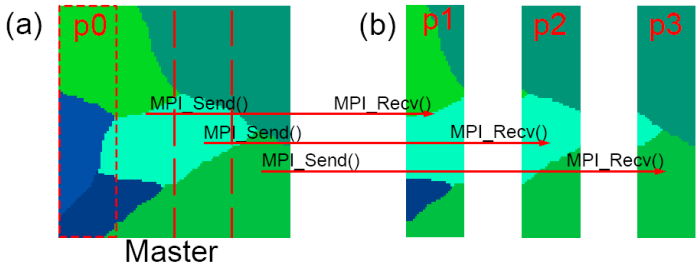

Fig. 1. Concept of cellular automata domain decomposition between subsequent processes (a) Master process: *p0,* (b) other processes: *p1 – p3*.

After each process finishes execution of a single cellular automata static recrystallization program iteration, the information about boundary cells at each subdomain edge is exchanged between neighboring subdomains to maintain cellular automata space continuity (*MPI_Send()/MPI_Recv()* pair is created) as schematically presented in the Fig. 2. Moreover information on partial kinetics and average grain sizes are send to the *master* process, with the use of *MPI_Reduce()* function. Obtained data at each time step are finally agglomerated by the *master* process (*p0*) and the complete microstructure is restored. Such communication involving the cellular automata space division, static recrystallization calculations and finally the cellular automata space agglomeration is performed in each time step until the stop criterion is reached.

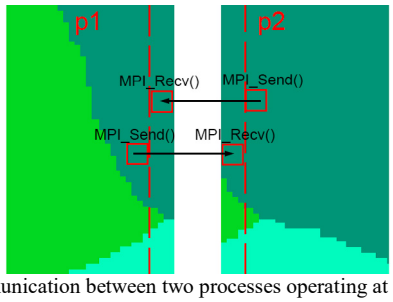

Fig. 2. Concept of communication between two processes operating at neighboring subdomains.

To investigate the effectiveness of implemented parallel solution, calculations on the 2D cellular automata space with 1000 × 1000 cells containing information on microstructure morphology and accumulated deformation energy have been performed. The initial model parameters for the cellular automata static recrystallization model were taken from [2]. Simulations were realized on the one workstation with two Intel Xeon E5-2420v2 @2.20GHz processors with different number of available processes varying between 1 and 10.

During computations three different scenarios were selected with simulation parameters set to obtain at the end of calculations approx.: 20%, 50% and 100% recrystallized fraction (RXF) within the same amount of iterations in each case study. A comparison of the computational time for all cases is presented in the Fig. 3(a).

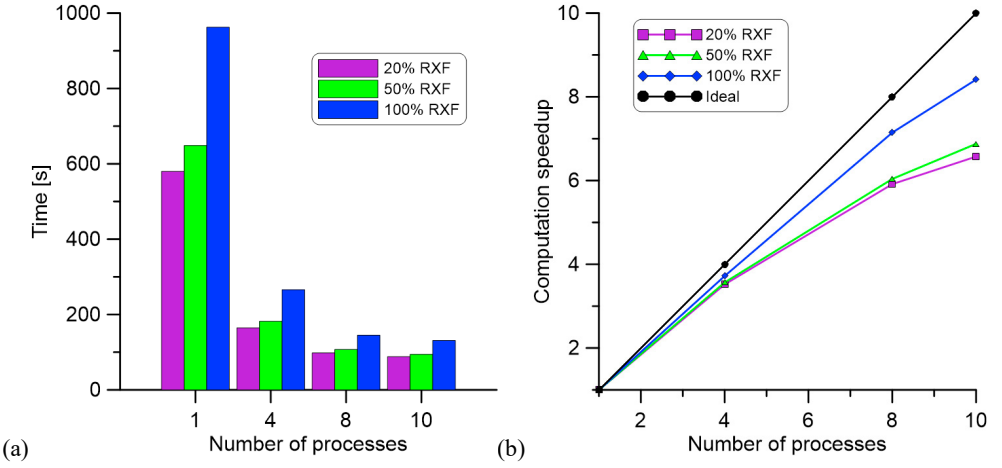

Fig. 3. Comparison of computational (a) time and (b) speedup, for a set of simulations with different final recrystallized volume fractions.

As can be noticed in the Fig. 3(a) simulation time for the scenario with 100% recrystallization fraction as a function of different number of processes always take more time than other two case studies. This situation is related with increasing number of recrystallized cells that are subjected to calculations due to growth of new grains. However, in each scenario the computational time with a parallel execution is significantly reduced. To evaluate parallelization effectiveness a computational speedup for each scenario was calculated and presented in the Fig. 3(b). As can be seen, the more calculations the cellular automata program performs during simulation the more effective the parallelization is. Additionally, to confirm that the developed modifications to the parallel version of the cellular automata algorithm do not introduce any unphysical artefacts, recrystallization kinetics have been investigated. Model with the same initial setup was executed on different amount of processes and obtained recrystallization kinetics were compared and proved the model robustness as seen in the Fig. 4. Corresponding selected microstructure morphologies are presented in Fig. 5.

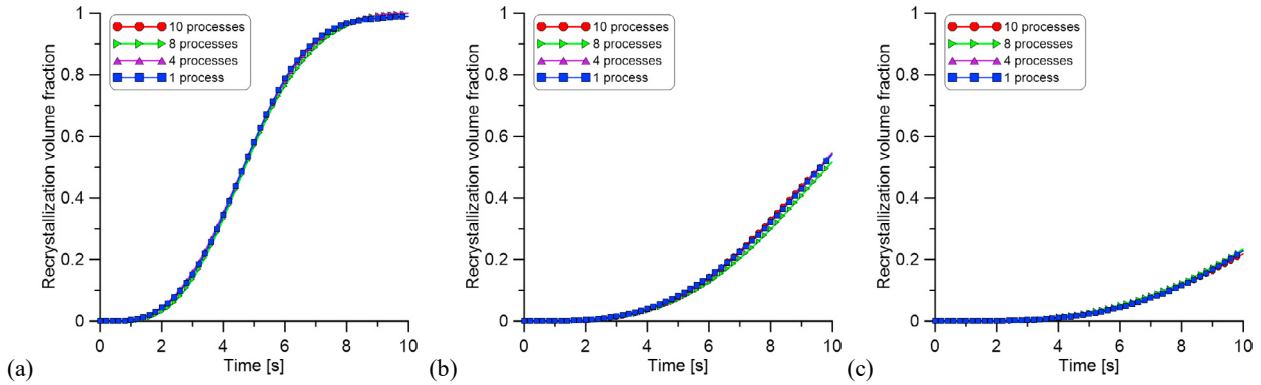

Fig. 4. Comparison of recrystallization volume fraction for different execution variants for simulations with (a) 100%, (b) 50% and (c) 20% RXF.

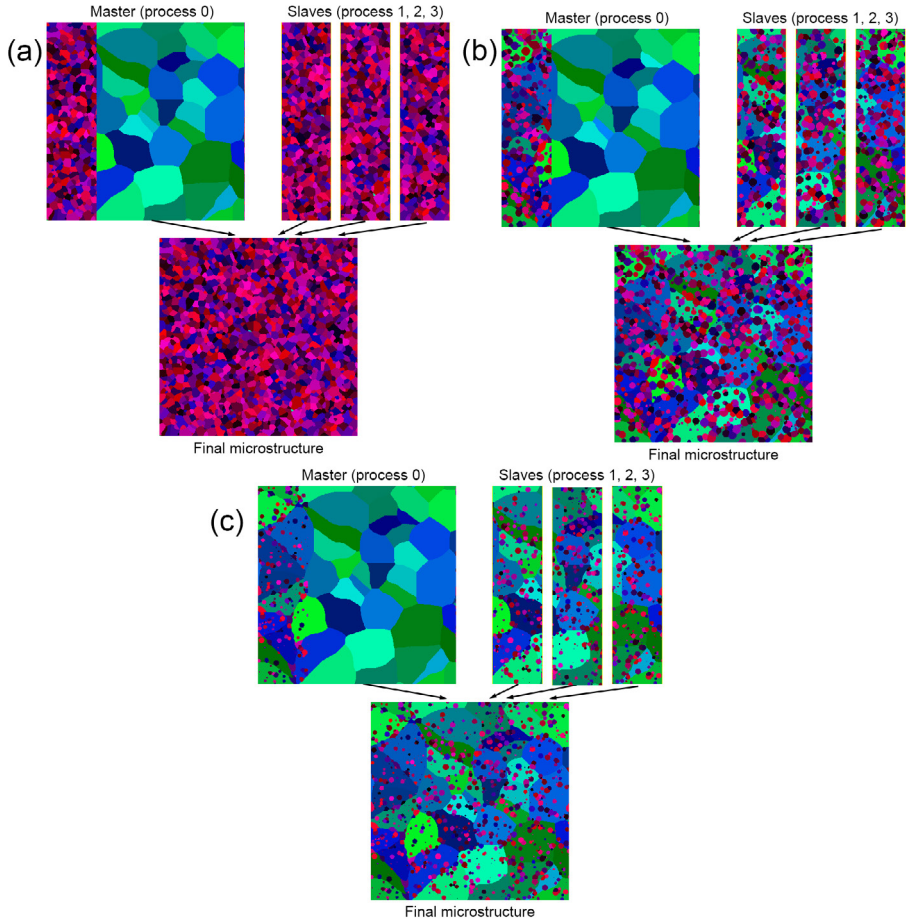

Fig. 5. Selected material morphologies for different execution variant on 4 processes for simulations with (a) 100%, (b) 50% and (c) 20% RXF.

The small differences in kinetics visible in the Fig. 4 are related to stochastic elements of the cellular automata model, e.g. slightly different positions of new nuclei occurring during static recrystallization. As presented, the parallelization seems to be an effective and robust approach to decrease computing times of the cellular automata calculations. Further studies in the area will be conducted, especially with the focus on development of other communication mechanisms between subdomains.

4. Conclusions

Based on presented results it can be concluded that:

- The Message Passing Interface standard can be effectively used to parallelize cellular automata microstructure evolution models.
- Introduced modifications to the cellular automata static recrystallization code related with division and agglomeration of computational domain did not introduce any unphysical artefacts to the model predictions.
- The parallelization is more effective with increasing number of cellular automata cells that are processed during the entire simulation.
- More elaborated communication scheme should be used to further decrease the computational time. This will be the subject of further study.

Acknowledgements

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