Materials Research Proceedings 28 (2023) 1559-1564 https://doi.org/10.21741/9781644902479-168

Evaluation of data transfer methods efficiency in the random cellular automata model of dynamic recrystallisation

PAWLIKOWSKI Kacper[1,a *], SITKO Mateusz[1,b], CZARNECKI Michał[1,c] and MADEJ Łukasz[1,d]

[1]AGH University of Science and Technology in Krakow, Poland

[a]kpawliko@agh.edu.pl, [b]msitko@agh.edu.pl, [c]mczarneck@student.agh.edu.pl, [d]lmadej.agh.edu.pl

Keywords: Random Cellular Automata, Dynamic Recrystallisation, Microstructure

Abstract. Numerical simulations can help predict microstructure morphology evolution under hot forming conditions and support final material properties determination. Cellular Automata (CA) is a commonly used full-field method to model changes in microstructure morphology during different metal-forming processes. However, in the case of microstructure evolution changes during high deformation levels, at higher temperatures, the CA method has some limitations related to computational domain geometry changes. The use of random cellular automata (RCA) allows for a more realistic representation of this phenomenon. However, it involves much more effort during model implementation to optimise the algorithm in terms of execution time, which has to be at an acceptable time. This paper is a part of a larger research aiming at developing the dynamic recrystallisation model (DRX) using the RCA directly incorporated into the finite element (FE) framework. The main goal of the current work is to evaluate the efficiency of data transfer approaches between the two mentioned coupled model components. Particular attention is on shortening the execution time thanks to data streams opened in binary mode.

Introduction

Because of the rapid development of computer technology, current numerical methods can consider not only the macroscopic response of the material but also can track the microstructural changes explicitly. Advanced multiscale models often use different numerical simulation methods to reflect given phenomena at subsequent scales. In general, three major phenomena are responsible for microstructure evolution during the deformation of metallic materials: recrystallisation, phase transformation, and texture development. The former group of phenomena, particularly dynamic recrystallisation (DRX), is critical when evaluating hot metal forming conditions. This phenomenon leads to microstructure restoration during hot working conditions, which eventually influences their final mechanical properties [1].

In principle, DRX consists of two main stages: nucleation and growth of new dislocation-free grains. It is a process driven mainly by a reduction of the dislocation density accumulated in the material during plastic deformation conditions under elevated temperatures. This process occurs directly during deformation at high temperatures, so its direct experimental observations are very demanding. Therefore, various numerical models are used to support and complement experimental analysis [2,3]

The cellular automata (CA) is one of the advanced full-field numerical methods commonly used to represent the microstructure evolution during plastic deformation. This method has been used for DRX simulations for many years, starting from the first simple model that did not consider computational domain deformation developed by Goetz and Seetharaman [4]. They showed that even a straightforward model could approximate the material properties observed during experiments. More and more advanced models appeared over the following years. Xiao et al. [5] introduced the DRX model based on the CA coupled with the topology deformation technique to

account for the influence of grains' topology change during deformation on the kinetics of the DRX. Gawad and Pietrzyk introduced the Cellular Automata Finite Element model (CAFE) [6] with a simplified way to account for the microstructure's evolution in the FE simulation. Complex and more flexible models combining the CA method with FE were also developed [7]. However, all these examples also showed that an accurate description of the deformation of the cellular automata computational domain under plastic forming conditions is a significant limitation of the classic CA approach, which is based on a regular grid of cells (Fig. 1a). Many solutions have been proposed to deal with that issue in recent years. In some works, authors introduced a simple CA space elongation algorithm along a selected axis [8], and as a result, new recrystallised grains were also artificially elongated. Another research developed a technique based on mapping the computational space between two separate coordinate systems [9]. It eliminated many disadvantages of previously reviewed approaches but still considered a series of geometrical assumptions during simulation. An exciting concept of space deformation was introduced in [10]. The authors coupled the CA method with the FE approach and introduced the CA space deformation algorithm directly based on FE mesh geometry. However, because of the regularity of CA space, the remeshing operations were limited in FE software at higher deformation degrees. Therefore, the current paper's authors introduced the concept of coupling the FE deformation model with the random cellular automata (RCA) model of microstructure evolution presented in [11].

In this case, the RCA modifies the definition of a regular CA space and considers it as a cloud of points (Fig. 1).

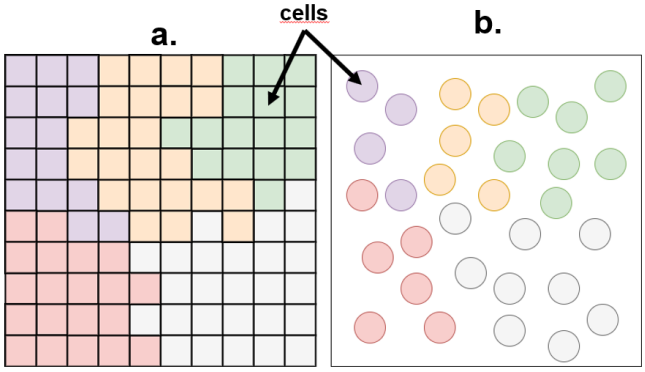

Fig. 1. Comparison of a) CA and b) RCA computational space.

The method retains all general properties of CA without introducing errors during coupling with finite element integration points, which deal with deformation calculations. As a result, the coupled RCAFE model reflects the material's behaviour during deformation more accurately, as it directly considers CA space deformation.

RCAFE DRX Simulation

The material deformation simulations are carried out in the classical J2 plasticity FE framework of Abaqus software. Additionally, each RCA cell from the microstructure evolution model is associated with a single FE integration point (Fig. **2**). Therefore, coordinates of integration points, their displacements and equivalent plastic stresses are transferred from the FE to RCA models in each time step. The described coupling between RCA with the FE model carries the risk that some areas of the material may not be discretized with the correct number of cells, and it can influence the final results. Proper initial FE mesh discretization and remeshing operations should overcome this issue. The RCA model presented in this work can easily incorporate changes introduced by FE remeshing algorithm.

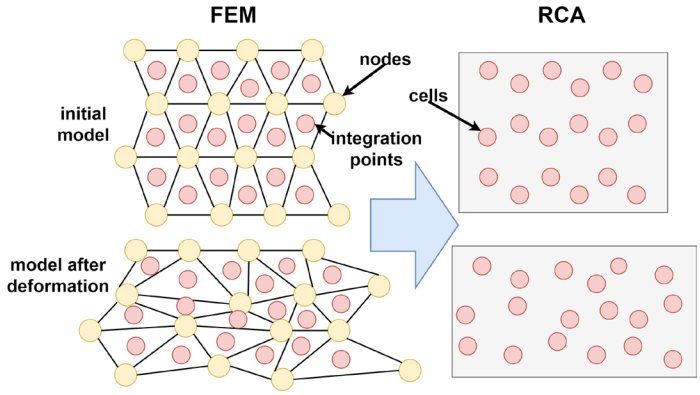

Fig. 2. Transformation of integration points into RCA cells.

In general, the simulation in such a coupled RCAFE model consists of several steps. A the beginning of each iteration, cells in the RCA space are translated based on corresponding integration points coordinates in the FE model. After that, dislocations in each cell are evaluated based on the stress value from Abaqus software:

$$\overline{\rho} = \frac{1}{\rho_0}\left(\frac{\sigma_i}{a_6 G b}\right)^2 \tag{1}$$

where: G is the shear modulus, σ_i is the equivalent stress value calculated by the Abaqus, a_6 is the model constant, b is the magnitude of the Burgers vector, and ρ_0 is the initial dislocation density. When the critical value of dislocation density is reached, new nuclei are incorporated into RCA space with the nucleation rate described by:

$$\dot{N} = c\dot{\varepsilon}\exp\left(-\frac{Q_n}{RT}\right) \tag{2}$$

where: c is constant, $\dot{\varepsilon}$ is the strain rate, Q_n is the activation energy for nucleation, T is the temperature, and R is the universal gas constant.
Finally, in each time step, the cell changes its state from unrecrystallised to recrystallised based on its size and growth velocity value calculated as:

$$V = M_0 \exp\left(-\frac{Q_m}{RT}\right) 2\alpha\tau\left(\rho_{(k,l)} - \rho_{(i,j)}\right) \tag{3}$$

where: M_0 is the initial grain boundary mobility, Q_m is the activation energy for grain boundary motion, α is a coefficient from the range (0,1), $\rho_{(k,l)}$ - dislocation density in the analysed and neighbouring cell, and τ is the energy required for dislocation movement.

The flow of the simulation in such a basic version of the DRX model is presented in Fig. 3.

Materials Research Proceedings 28 (2023) 1559-1564 https://doi.org/10.21741/9781644902479-168

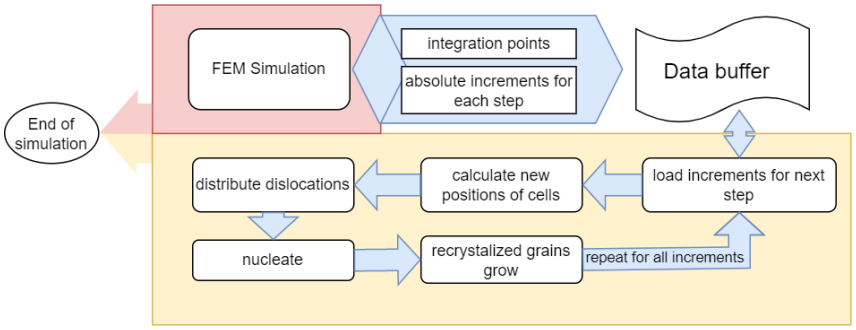

Fig. 3. Flow of implemented DRX simulation process.

Initial research on this topic clearly pointed out that the major disadvantage of the coupled RCAFE solution is the excessive computational time. The improvements in the RCA code itself, related to designing specific neighbourhood types and neighbourhood search algorithms, have already been carried out in [15]. Therefore, the current research is directly focused on further optimising the algorithmic solution to increase the model efficiency, particularly developing effective data transfer mechanisms between the RCA and FE methods.

Results

A two-dimensional digital material representation (DMR) model consisting of six grains discretised by 50 000 elements was selected as a case study for the current research (Fig. 4). The DMR model was deformed by 30% at 1100°C within the FE framework. In each FE element time step, the data from FE integration points were directly transferred to the corresponding RCA points, where the progress of dynamic recrystallisation was simulated within the in-house code.

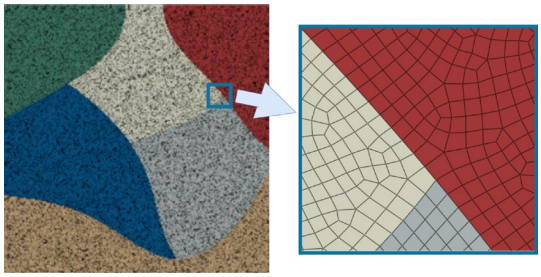

Fig. 4. Illustration of the DMR model used for the FE simulations.

Obtained microstructure evolution results in the RCA computational domain are presented in Fig. 5; blue cells represent unrecrystallised grains, and cells in the red-scale colours represent new, recrystallised ones. It is seen that nucleation starts from grain boundary regions, where higher dislocation densities are expected. The nuclei can also appear inside grains, but only after reaching significant deformation levels, which replicates well-known experimental observations. It should be clearly pointed out that despite the very small model used as a case study, the calculation time was quite long, reaching approx. 28 s. This time in the case of models with a larger number of grains and significantly refined FE mesh in 3D space, will lead to unacceptable simulation times. While the RCA simulation itself can be accelerated with the use of parallelisation techniques, the bottleneck of the coupled RCAFE solutions is transferring a large amount of data between the two models. In the evaluated case, the data transfer took about 30% of the entire simulation time.

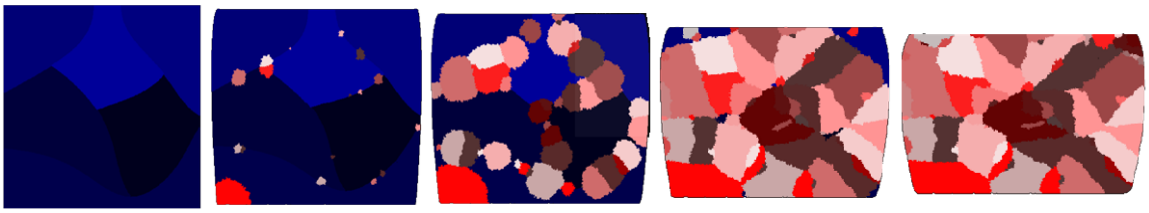

Fig. 5. The results of subsequent simulation steps for a model consisting of 50 000 elements.

As mentioned, the described technique should ultimately simulate much larger DMR models in 3D space. Therefore, as the first step, we decided to look at the possibility of reducing the time of data transfer. Two different methods of handling data transition from FE to RCA were implemented and compared. Both approaches differ in the format of the files stored in the buffer linking the two models. In the basic approach, data files from Abaqus with subsequent changes in stress values and positions of FE integration points were saved in a standard text form. In the second approach, files were saved and loaded in binary mode. The concept of communication between FE and RCA models is presented in Fig. 6.

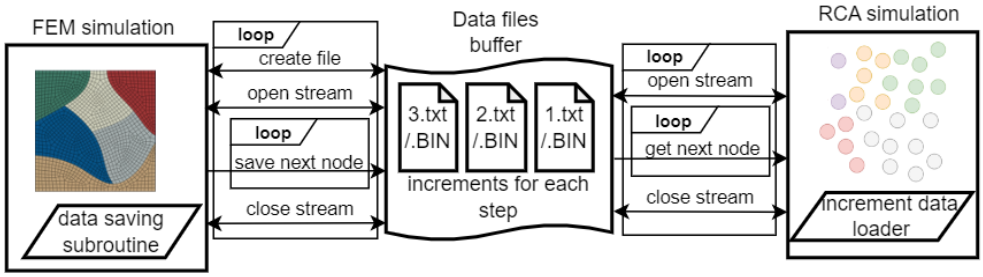

Fig. 6. Diagram of communication between FE and RCA models.

A series of simulations with increasing FE discretization levels was carried out to evaluate the differences between the two solutions. The summary of realised measurements shown in Fig. 7 proves that thanks to the application of binary files, it is possible to save up to 10% of the time for the largest model. Nevertheless, the time effort associated with the data transfer is still quite excessive in comparison to the pure simulation time.

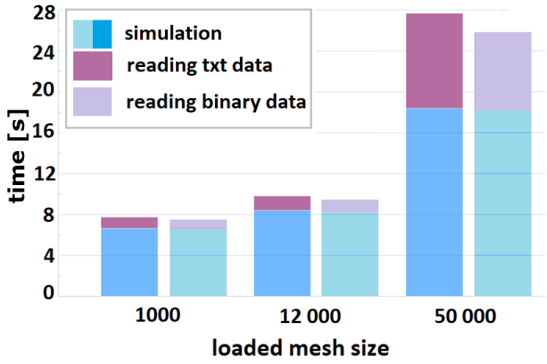

Fig. 7. Comparison of simulation and data transfer times for the text and binary files, respectively.

Summary

The use of the RCA concept allowed for the implementation of the DRX microstructure evolution model that, thanks to the flexibility of this solution, can be directly coupled with material

deformation data obtained from FE simulations. As a result, it is possible to take into account the influence of cellular automata space deformation on the progress of dynamic recrystallisation. At this research stage, the developed RCA DRX model considers only basic components like dislocation distribution, nucleation and dislocation density-driven grain growth and will be further developed. It was proven that in the coupled RCAFE simulation, the data transfer procedure between the commercial and in-house codes generates a major overhead in total simulation time. It was shown that the use of binary files could already speed up the analysis in comparison to the standard text files; however, further improvements in this aspect are also required. The further concept assumes direct information exchange inside subroutine code to eliminate the need for the files.

Acknowledgement
The financial assistance of the National Science Centre project No. 2019/35/B/ST8/00046 is acknowledged. This research was supported in part by PLGrid Infrastructure.

References
[1] K. Huang, R.E. Logé, A Review of Dynamic Recrystallization Phenomena in Metallic Materials, Mater. Des. 111 (2016) 548-574. https://doi.org/10.1016/j.matdes.2016.09.012
[2] M. Bernacki, R.E. Logé, T. Coupez, Level Set Framework for the Finite-Element Modelling of Recrystallization and Grain Growth in Polycrystalline Materials, Scripta Mater. 64 (2011) 525-528. https://doi.org/10.1016/j.scriptamat.2010.11.032
[3] T. Takaki, A. Yamanaka, Y. Tomita, Phase-Field Modeling for Dynamic Recrystallization, Adv. Struct. Mater. 64 (2015) 441-459. https://doi.org/10.1007/978-3-319-19440-0_20
[4] R.L. Goetz, V. Seetharaman, Modeling Dynamic Recrystallization Using Cellular Automata, Scripta Mater. 38 (1998) 405- 413. https://doi.org/10.1016/S1359-6462(97)00500-9
[5] N. Xiao, C. Zheng, D. Li, Y. Li, A Simulation of Dynamic Recrystallization by Coupling a Cellular Automaton Method with a Topology Deformation Technique, Comput. Mater. Sci. 41 (2008) 366-374. https://doi.org/10.1016/j.commatsci.2007.04.021
[6] J. Gawąd, M. Pietrzyk, Application of Cafe Multiscale Model to Description of Microstructure Development during Dynamic Recrystallization, 2007.
[7] Ł. Madej, M. Sitko, K. Radwanski, R. Kuziak, Validation and Predictions of Coupled Finite Element and Cellular Model: Influence of the Degree of Deformation on Static Kinetics Case Study, Mater. Chem. Phys. 179 (2016) 282-294. https://doi.org/10.1016/j.matchemphys.2016.05.040
[8] H. Hallberg, M. Wallin, M. Ristinmaa, Simulation of Discontinuous Dynamic Recrystallization in Pure Cu Using a Probabilistic Cellular Automaton, Comput. Mater. Sci. 49 (2010) 25-34. https://doi.org/10.1016/j.commatsci.2010.04.012
[9] N. Yazdipour, C.H.J. Davies, P.D. Hodgson, Microstructural Modeling of Dynamic Recrystallization Using Irregular Cellular Automata, Comput. Mater. Sci. 44 (2008) 566-576. https://doi.org/10.1016/j.commatsci.2008.04.027
[10] H. Li, X. Sun, H. Yang, A Three-Dimensional Cellular Automata-Crystal Plasticity Finite Element Model for Predicting the Multiscale Interaction among Heterogeneous Deformation, DRX Microstructural Evolution and Mechanical Responses in Titanium Alloys, Int. J. Plast. 87 (2016) 154-180. https://doi.org/10.1016/j.ijplas.2016.09.008
[11] L. Madej, M. Sitko, A. Legwand, K. Perzynski, K. Michalik, Development and Evaluation of Data Transfer Protocols in the Fully Coupled Random Cellular Automata Finite Element Model of Dynamic Recrystallization, J. Comput. Sci. 26 (2018) 66-77. https://doi.org/10.1016/j.jocs.2018.03.007