

Numerical modelling based on the digital material representation idea, which explicitly introduces microstructure elements into the simulation (grains, grain boundaries, inclusions, particles, phase boundaries, etc.), is being rapidly developed in the leading scientific centres. Simulation-based on this approach allows the analysis of material behaviour to an extent that was not possible with the use of the conventional modelling approaches where microstructure is treated as a homogeneous material.

The digital material representation concept combined with the discrete modelling techniques, e.g. cellular automata (CA), provides an opportunity to perform microstructure evolution simulations during various metal-forming and heat treatment operations, directly replicating and further extending experimental monitoring capabilities.

That kind of simulation is a powerful computational tool because it allows control of many aspects of material microstructure evolution during various metal-forming processes. **A lot of publications dedicated to simulation based on this approach can be found in the scientific literature. However, the major problem of these models still lies in the high computational cost, which is a limiting factor in practical application in designing new metal-forming technologies. Due to that, the application of the approach at an industrial scale is practically impossible.**

There are two approaches that can minimize the CA model's computational complexity and simulation time. The first is based on the frontal cellular automata approach, which assumes that computations are realized only in selected areas of the investigated microstructure, e.g., grain boundaries. The second approach takes advantage of modern computer centres, also known as supercomputers. They are equipped with hundreds and sometimes even thousands of computational units, providing enormous computational power.

The first approach reduces the computation time; however, this reduction is associated with a significant reduction in the computational domain complexity, which also causes a decrease in the accuracy of calculations. Therefore, this project decided to use the second approach based on the idea of parallel and distributed computing within high-performance computing centres. Performing parallel calculations on massive computing units will significantly reduce simulation time to an acceptable amount. Such an approach is possible due to the rapid development of technology observed in recent years, which favours the emergence of an increasing number of computing centres supporting simulations on supercomputers. However, mapping microstructure evolution models onto this type of architecture is constrained by problems related to the even distribution of simulation tasks among the various computing units. With the increase of resources used, the issue of uneven load work during simulations builds up, which causes a drastic reduction in the scalability of developed solutions.

Within the project, a distributed version of the model of microstructure development based on the cellular automata method is planned to be developed and implemented, which will be able to adapt to specific simulation division conditions automatically. Such adaptation will be possible thanks to graph theory, which will directly allow tracking interactions between individual computational units and provide conditions for carrying out the so-called load balancing procedure. Static and dynamic load balancing adaptation will avoid situations in which computing units are overloaded or unused, resulting in faster parallel computing. The combination of these two methods will allow to manage computing resources effectively and maximize the potential of parallel processing. Efficient models will support the development of technologies for manufacturing various components from modern metal alloys with controlled properties in the future. A model of the static recrystallization phenomenon will be used as an example of the practical application of the cellular automaton method.

A basic cellular automaton algorithm dedicated to parallel simulation of static recrystallization has been implemented and initially verified with literature data at the preliminary research stage. This project will use the collected experience to adapt the existing algorithms and develop a self-adaptive solution for load balancing in a distributed environment using graph theory. The work will be based on the object-oriented C++ language in the Visual Studio environment. The creation of highly computationally efficient algorithms will require the use of additional libraries containing tools to perform communication in parallel execution of applications both for units consisting of multiple processors (multi-threaded application using the OpenMP library) and for platforms consisting of multiple computers (multi-threaded application using Message Passing Interface MPI).