AGH

UNIVERSITY OF SCIENCE AND TECHNOLOGY CRACOW

Metals Engineering and Industrial Computer Science

Multiscale Modelling 2nd Report:

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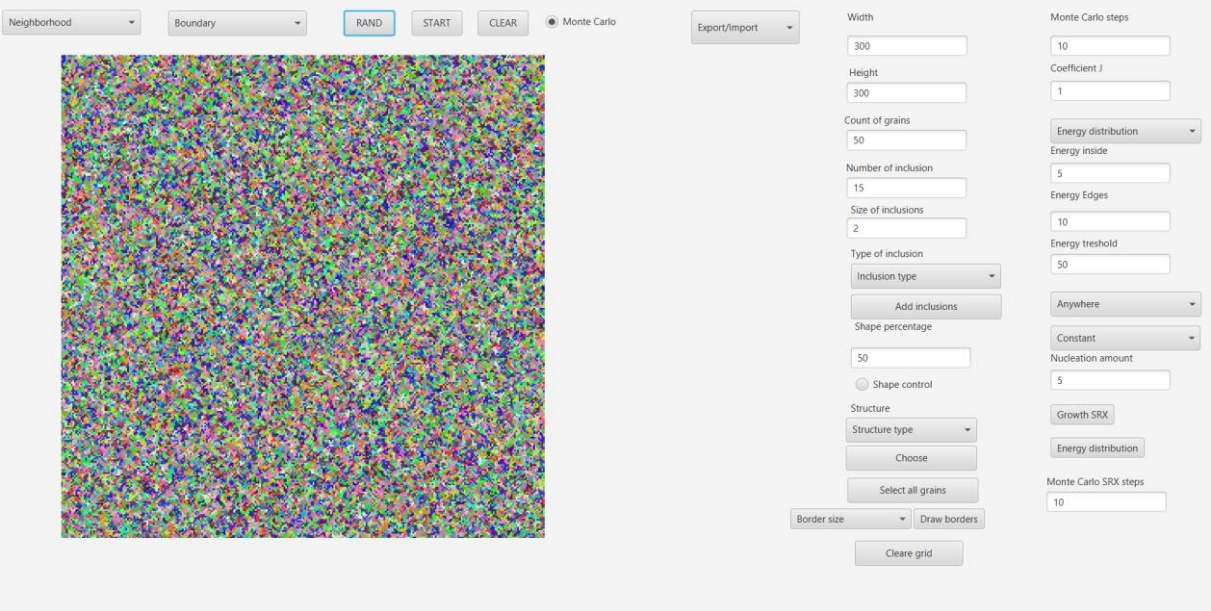
Group:	**1**
Repository:	**https://github.com/MarcelinaBalamut/MulticaleModeling**
Course:	**Multiscale Modeling**

1. User interface

To fulfillment the simulation of grain growth using the Monte Carlo method, the user interface that was created for the first project was extended. Additional buttons, comboboxes and necessary text fields have been added. The main application window is shown in Pic.1.



Pic.1. Main application window

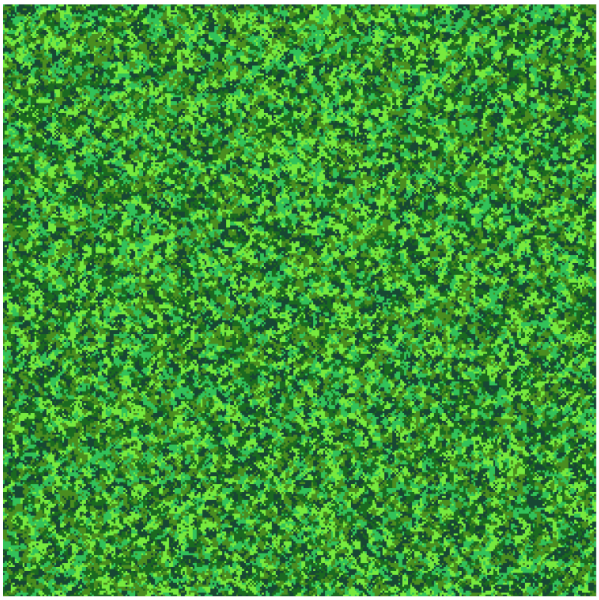
2. Functionalities

2.1. Monte Carlo grain growth

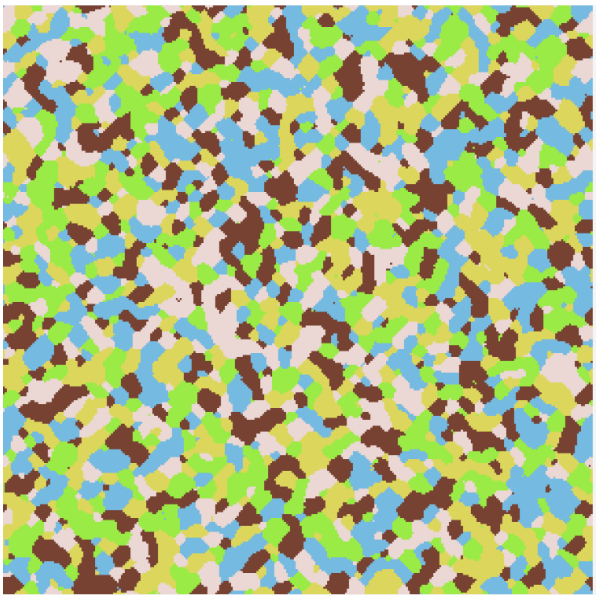
The first action the user should take is to set the mesh size to be generated. It is also necessary to check the "Monte Carlo" option, which means that from now the application will be based on the Monte Carlo method. Next, the user have to select the number of grains to draw. To simulate grains random using the Monte Carlo method, it is required to set the coefficient J (less or equal than 1) and the number of iteration steps. After clicking on the Random button, we get the number of grains randomly distributed over the entire surface of the grid. It was necessary to apply a random with returning. The next step of the algorithm was the calculation of energy for a given cell, taking into account its neighbors. The most important aspect is the calculation of the Kronecker delta. This formula consists in calculating the number of states of neighbors, different from the state of a given cell. The cell state is randomly drawn from the range of neighbor states and then, count number of neighbor cell states different from the

random state. The last part of the algorithm is to compare two deltas and select the larger one. Its value becomes the state of the cell. The whole algorithm is repeated the number of steps entered by the user. The grid looks different depending on the number of steps.

In the Pic.2, the grid is shown after the drawing of 5 grains at 3 number of steps, while in Pic.3, for 5 grains and 50 steps and coefficient J is equal to 0.8.



Pic.2 Grid with randomly distributed grains for 3 steps.



Pic.3 Grid with randomly distributed 5 grains for 50 steps.

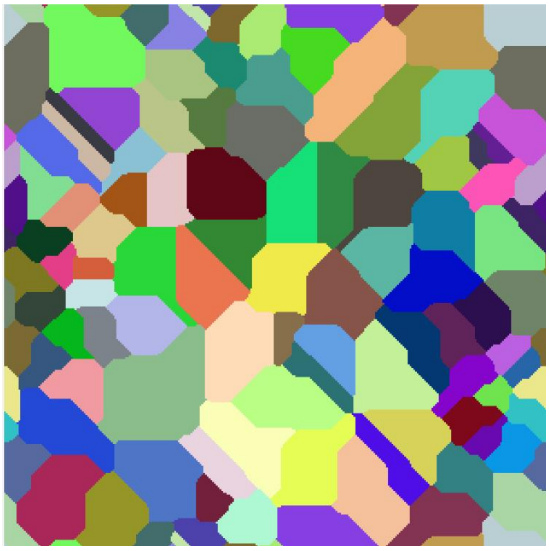
2.2. Dual phase microstructure

The next functionality which provides application is dual phase microstructure with different variants. Is possibility to generate dual phase microstructure for: (CA) -> (CA or MC) and (MC) -> (CA or MC), which are described in the following sections.

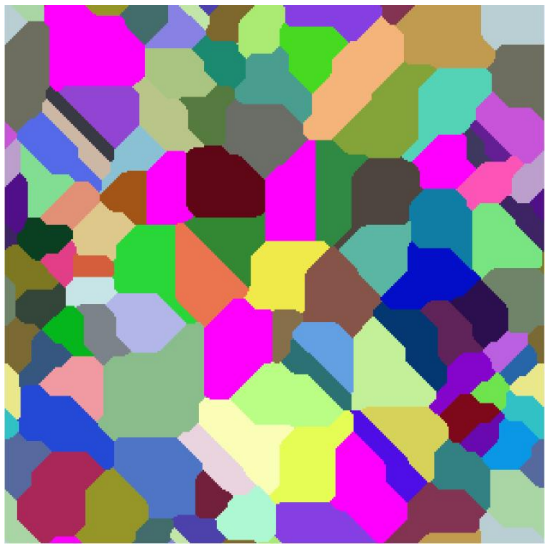
- Cellular Automata -> Monte Carlo

  The first step is to generate the grid with simple grains growth described in report 1, what is shown on Pic. 4. For such a generated grid, a dual-phase structure can be generated. Choose dual-phase as the structure type and choose grain as is shown on Pic.2, with the mouse click and click on “Choose” button. All grains except the selected ones will be cleaned as in the Pic.6. Next, select the "Monte Carlo" option and set the number of steps and coefficient J. Is important to choose number of grains, also. The, user have to click on “Rand” button. After that, the Monte Carlo simulation will be

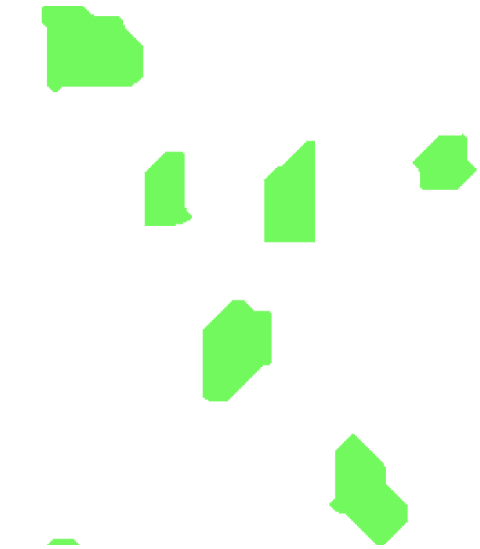
applied to the grid containing the selected grain using CA method. The result is the Pic.7.



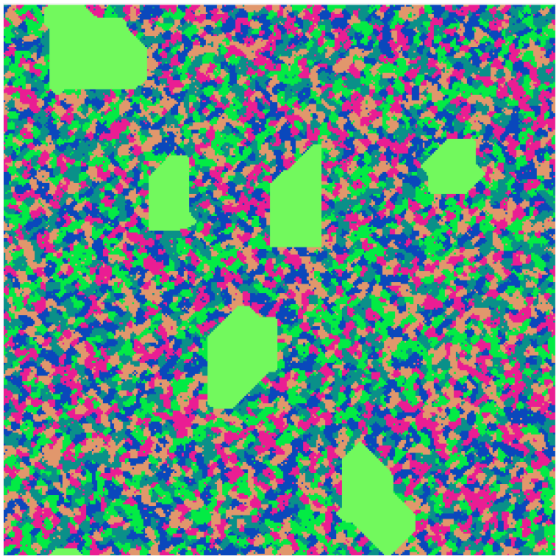
Pic.4 Generated grid by CA method for 100 grains.



Pic.5 Grid with selected grains marked on the magnet color.



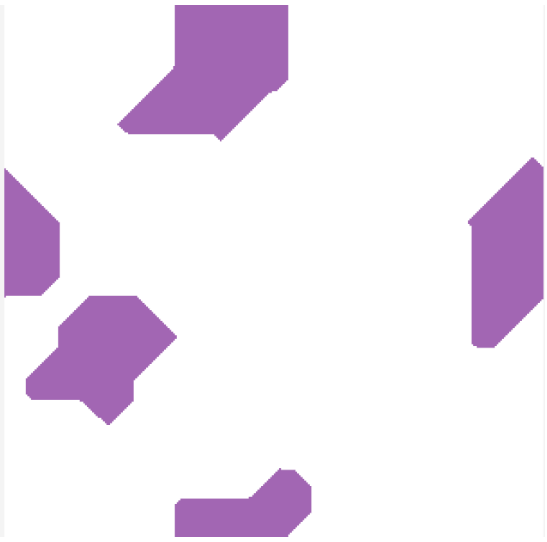
Pic. 6 Condition after cleaning unselected grains for the dual-phase structure.



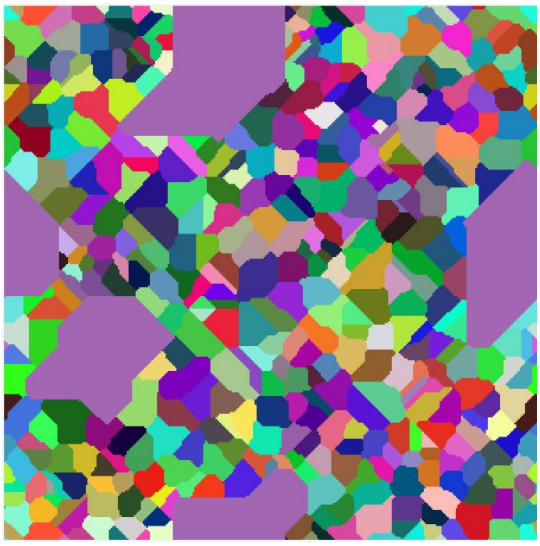
Pic.7 Grid for CA-> MC for 5 grains, coefficientJ equal to1, and 10 steps.

- Cellular Automata -> Cellular Automata

  This type has been described in more detail in Report 1. In this case, generate a grid and perform CA simulation. Then, as before, select the grains by clicking the mouse, clean the mesh from the remaining grains. The condition of the grid for this stage is shown at Pic.8. The next step is random grains again and perform simulation as before. Both the grains created during the new simulation and the remaining ones resulting from the creation of dual phase structures are placed on the grid and shown in the Pic.9.



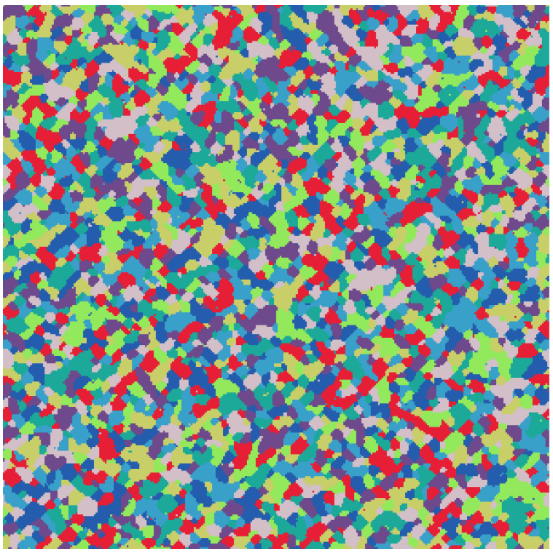
Pic.8 Selected grains after CA stimulation to dual-phase for 20 grains.



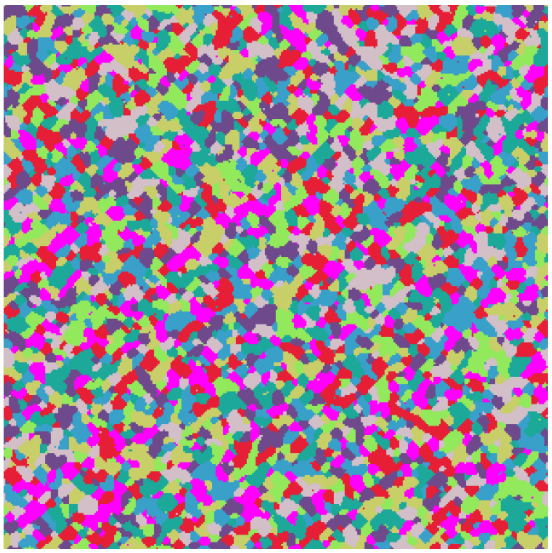
Pic.9. Grid for CA(20 grains)->CA(300 grains).

- Monte Carlo -> Cellular Automata

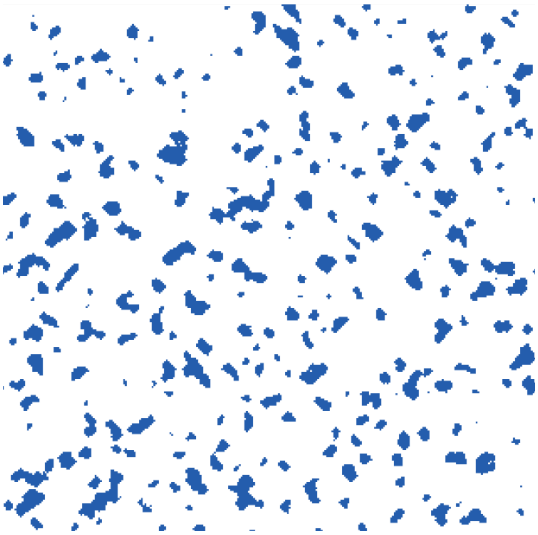
  The first step is to perform the Monte Carlo simulation. To do this, set the number of grains, value of coefficient J and number of steps, and click on the "Random" button. This image is shown in Pic.10. The next step is choosing the dual-phase option, choosing the grains shown in Pic.11 and pressing the "Choose" button. Selected grains with a cleaned up area are shown in Pic.12 Next, the user should deselect the "Monte Carlo" option, select the number of grains and perform a CA simulation, which is shown in Pic.13.



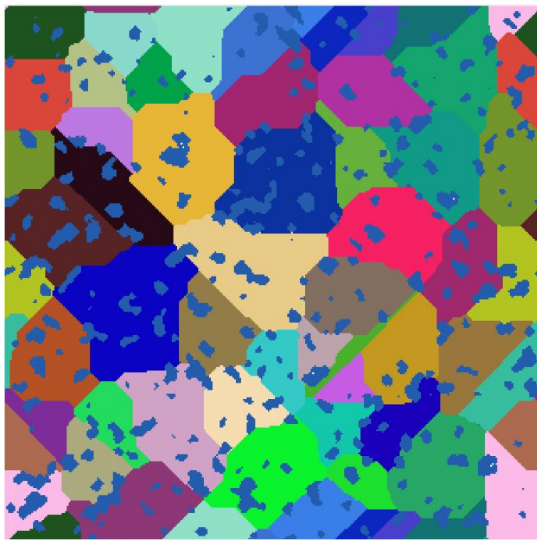
Pic.10. Gris after perform Monte Carlo method for 50 steps.



Pic.11 Selected grains for dual-phase structure.



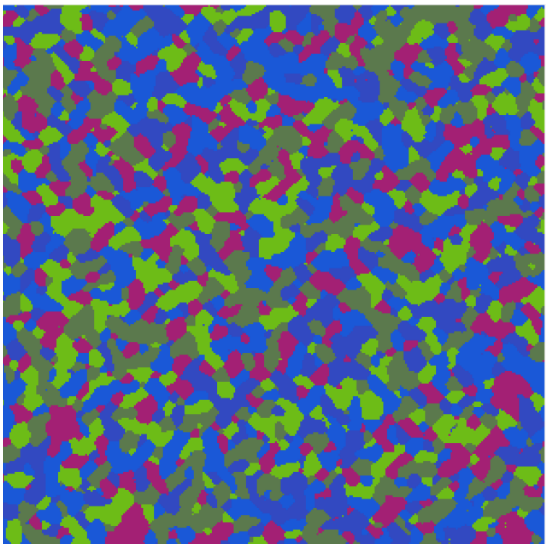
Pic.12 Cleared grid area for selected grains.



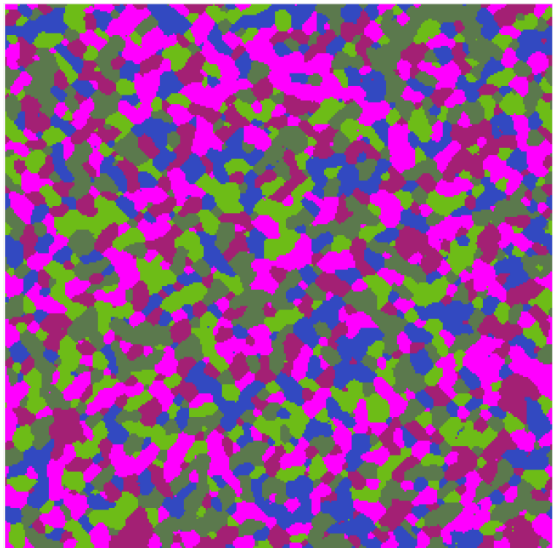
Pic.13 Grid after performed CA simulation for MC->CA.

- Monte Carlo -> Monte Carlo

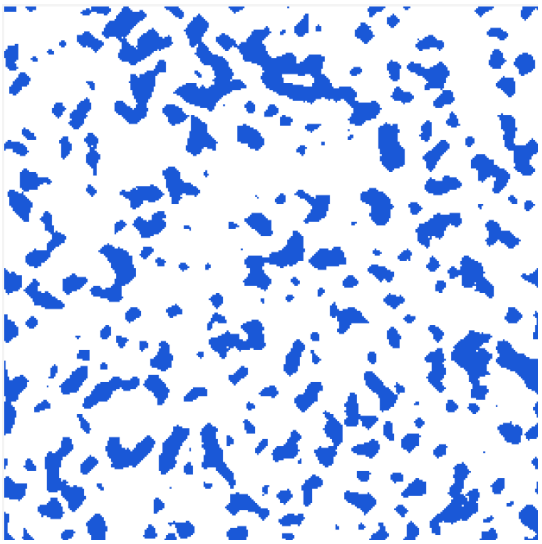
  The first step is to select the Monte Carlo option, select the coefficient J, the number of grains and the number of steps, what is shown in Pic.14. Then select dual-phase and select the number of grains shown in Pic.15 and press "Choose". Cleared gris is shown in Pic.16. Next, set the Monte Carlo method parameters again and click on the Rand button again. Result is shown on Pic.17.



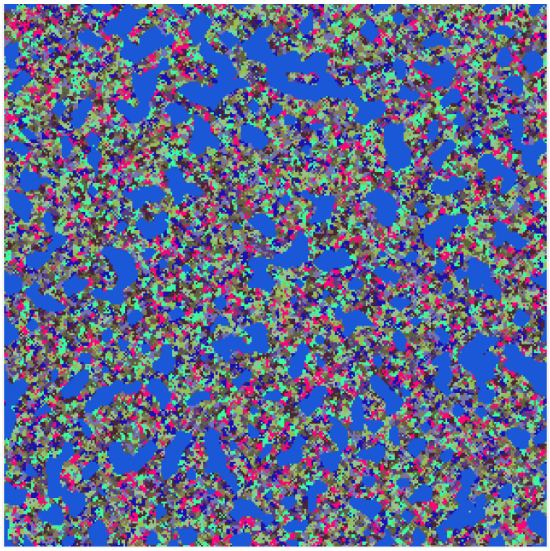
Pic.14 Grid generated by Monte Carlo method for 50 steps, 5 grains and coefficient 1.



Pic.15 Selected grains for dual-phase.



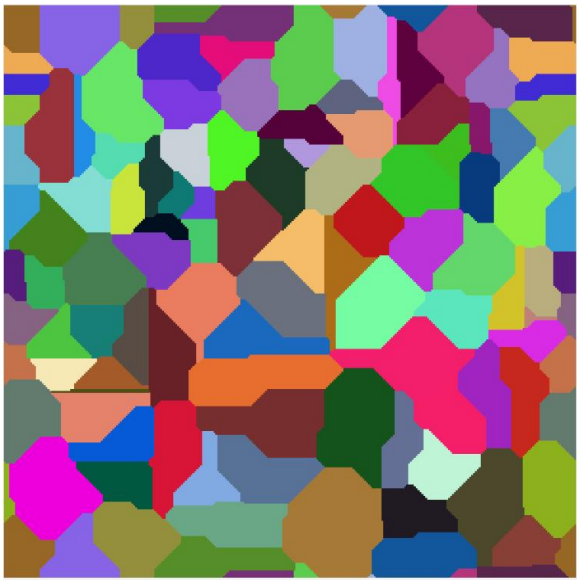
Pic.16 Cleared area for selected grains.



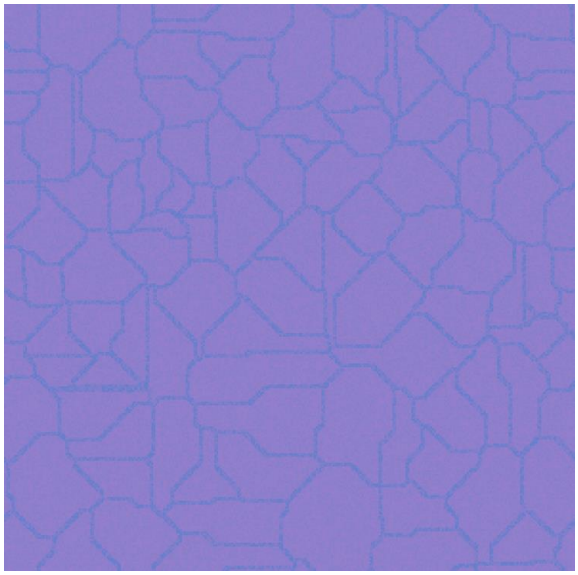
Pic.17 Grid after reapplication MC method for 10 steps, 10 grains and coefficient J 1.

2.3. SRX Monte Carlo

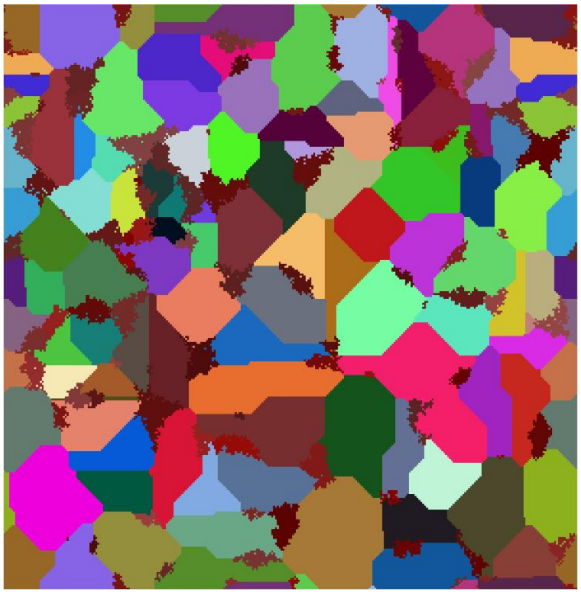
Another functionality allows the user to perform nucleation and to grow grains that have been recrystallized. The first step to perform this functionality is to generate a grid using the Monte Carlo method or Cellular Automata. Subsequently, the user have to select the type of energy distribution. There are two ways: homogenous and heterogeneous. Distribution using homogenous method is based on the even distribution of energy between the cells. Heterogeneous allows an imbalanced distribution of energy. At the grain boundaries, this energy is different from the energy within the grains. The next step that the user have to take is to set the value of the coefficient J, energy on both inside the grains and on their borders (in the case of heterogeneous), and the threshold value. In the homogeneous method, the energy value inside the grains is equal to the energy at their boundaries. The next step is to press the button "Distribute energy ". As a result, the image of energy distribution appears on the screen. The next step is the nucleation and growth of the grains of the recrystallized grains. To do this, select nucleation location and nucleation type. Location from nucleation can be anywhere and on borders. For the boundaries option, only cells at the grain boundaries are taken into account, whereas in the second case all cells are taken into account. For the type of nucleation, the user can choose nucleation at the beginning, constant nucleation, or increasing, where the number of grains increases. Additional information that the user must enter is the number of steps and the number of grains. The last step is to press the Growth SRX button, which starts the growth.



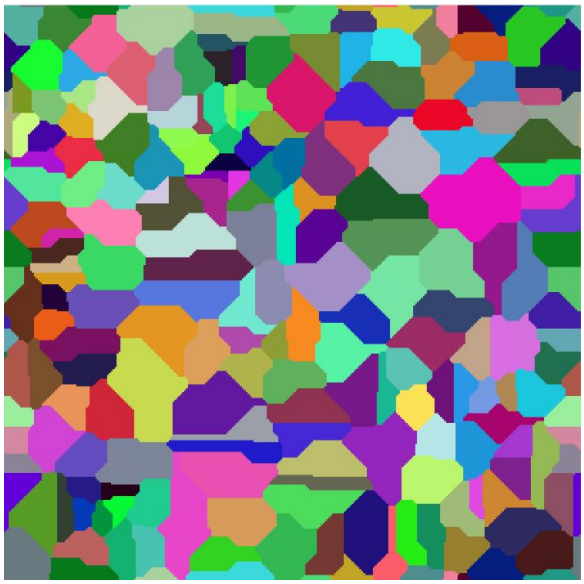
Pic.18 Grid generated using CA method for 100 grains.



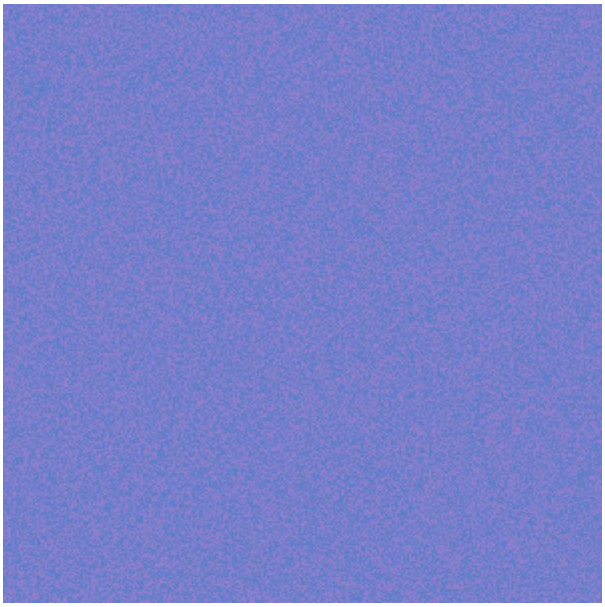
Pic.19 Distributed energy using heterogeneous method for energy inside 2, energy on boundaries 10 and threshold 50.



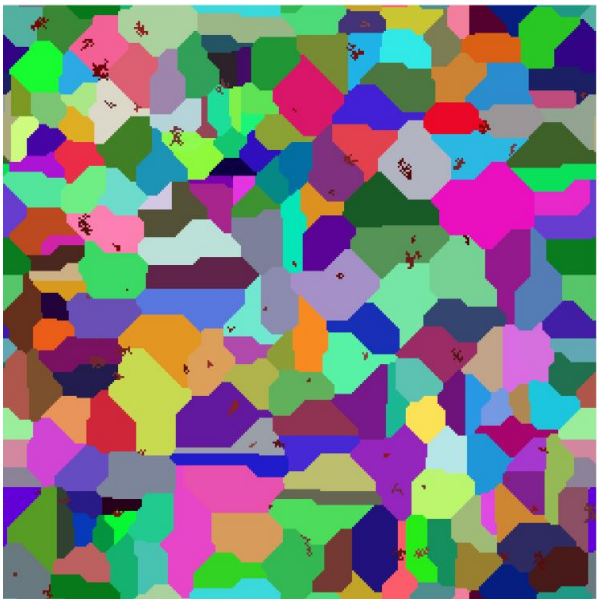
Pic.20 Nucleation located on boundaries, constant nucleation type for 10 nucleation and 10 steps.



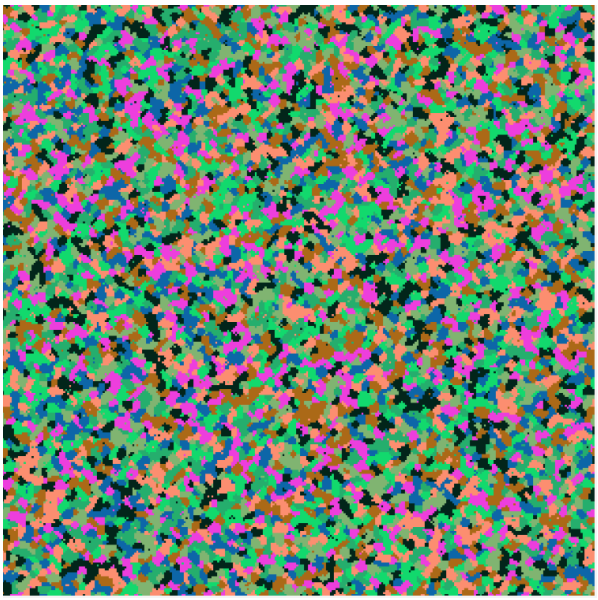
Pic.21 Grid generated using CA method for 200 grains.



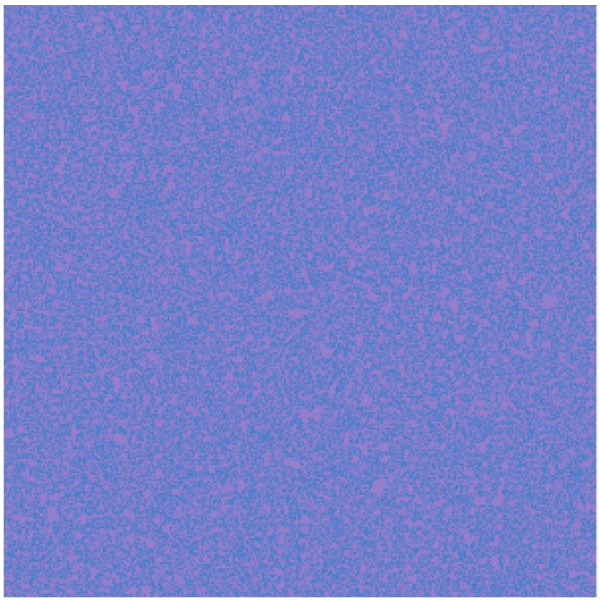
Pic.22 Distributed energy using homogenous method for energy inside 10, energy on boundaries 20 and threshold 85.



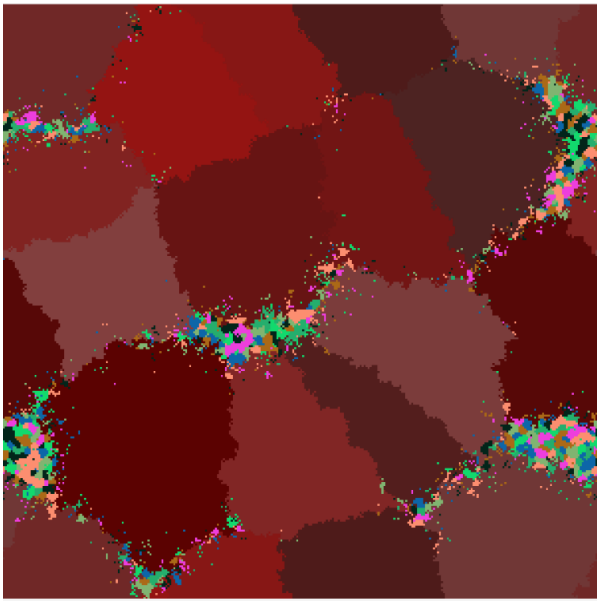
Pic.23 Nucleation located anywhere, increasing nucleation type for 20 nucleation and 2 steps.



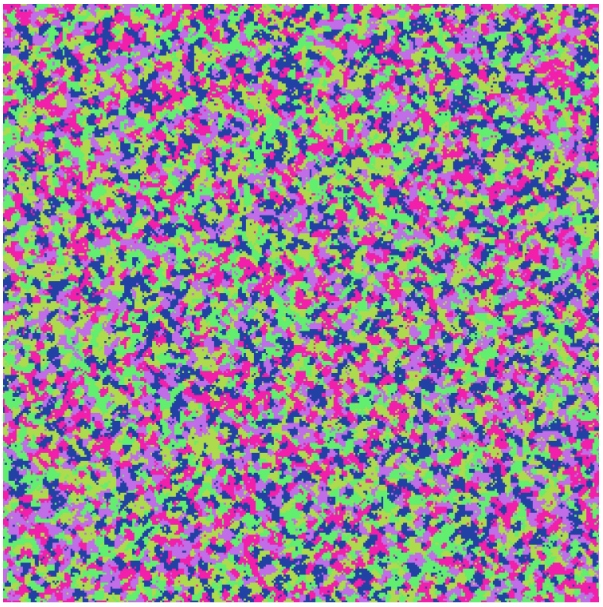
Pic.24 Grid generated using MC method for 8 grains, 20 steps and coefficient 1.



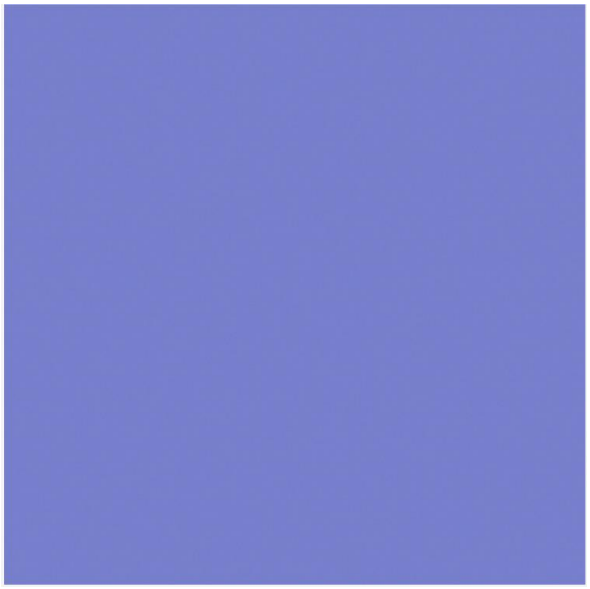
Pic.25 Pic.19 Distributed energy using heterogeneous method for energy inside 2, energy on boundaries 12 and threshold 90.



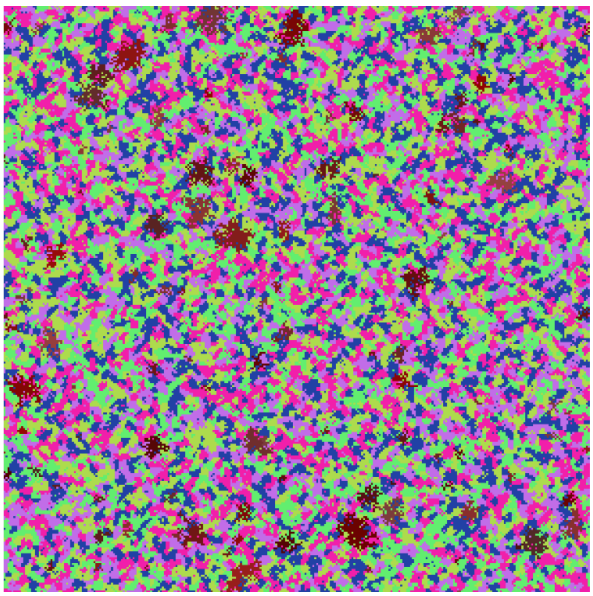
Pic.26 Nucleation located on boundaries, at the beginning nucleation type for 20 nucleation and 2 step.



Pic.27 Grid generated using MC method for 5grains, 7 steps and coefficient 1.



Pic.28 Distributed energy using homogenous method for energy inside 10, energy on boundaries 15 and threshold 8.

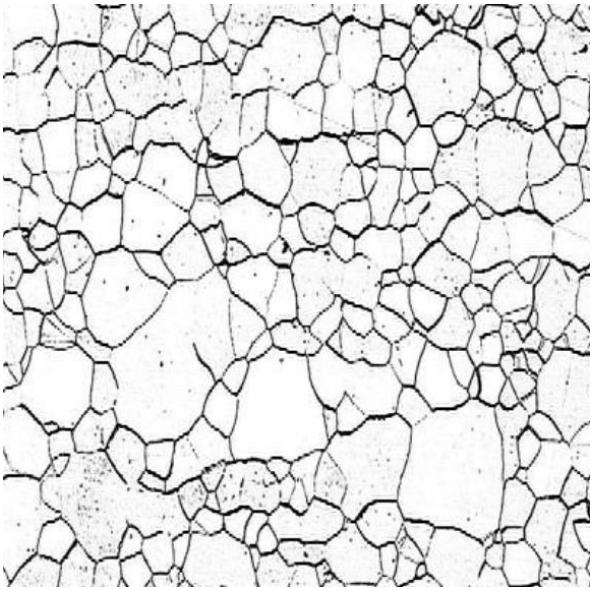


Pic.29 Nucleation located anywhere, increasing nucleation type for 8 nucleation and 4 steps.

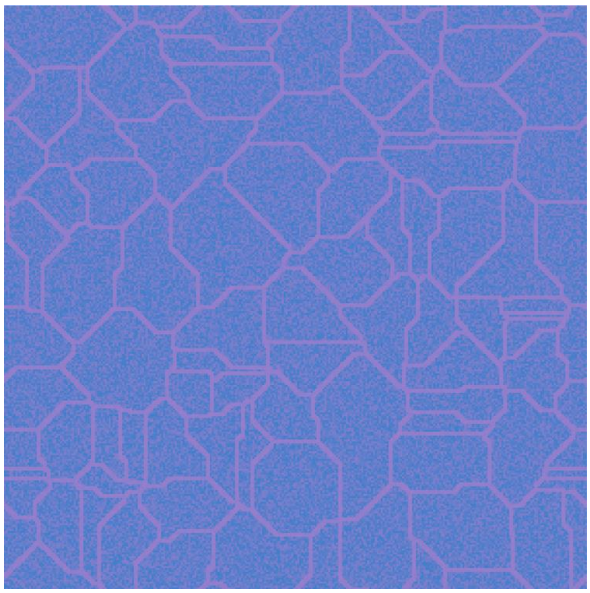
Pic.18 and Pic.19 show grids created using CA method and in Pic.24 and Pic.27 grid created Monte Carlo method what is needed to perform next simulations steps. On Pic.19 and Pic.25 is shown energy distribution method called heterogeneous. User can see a lot of differences between the colors on the border and inside the grains, which indicates different energy sizes. However, on Pic.22 and Pic.28 the homogenous method is presented. The distribution of nucleons at borders is presented on Pic.20 and Pic.26. Here user can see that the red spots are visible only at the grain boundaries. On Pic.23 and Pic.29 nucleons are arranged throughout the grid, regardless of whether grains ate place on the border or inside the grains.

3. Summary

Nowadays, grain growth simulation used in many areas is a very important aspect. Thanks to such simulation, very similar mapping of the real material structure is possible. Appropriate techniques and methods should be selected to generate a similar microstructure. Below are comparisons of real microstructures with microstructures generated by applications.



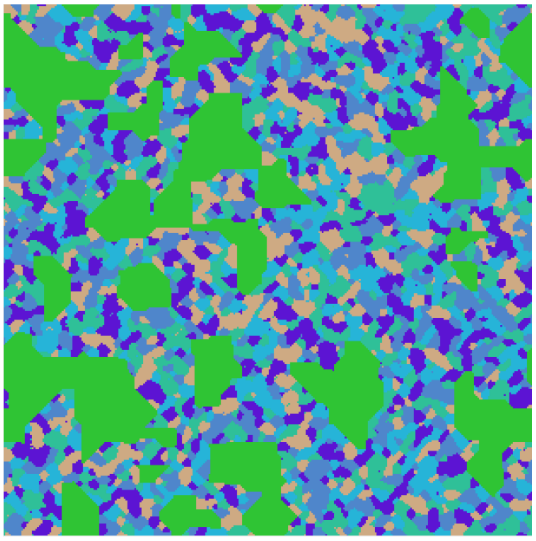
Pic.29 Microstructure and grain sizes of the ULC steel specimens after the annealing cycle.



Pic.30 Microstructure generated using CA method and heterogeneous energy distribution.

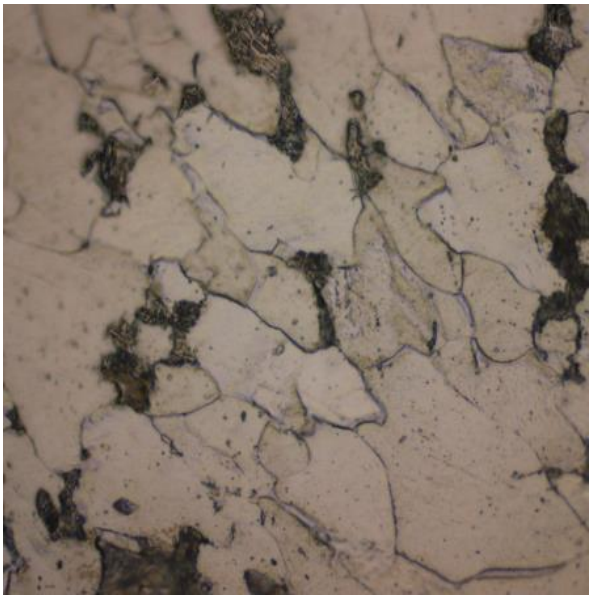
Pic. 29 shows the microstructure of UCL steel. The picture shows the exact size and grain boundaries. Pic.30 presents the mapping generated by the application using the Cellular Automata method, followed by the heterogeneous energy distribution method at 60 threshold, energy inside 3 grains, and energy at equal 15. As can be seen in the above drawings, both microstructures are very similar to each other.

Pic.31 Microstructure for MY 3200.

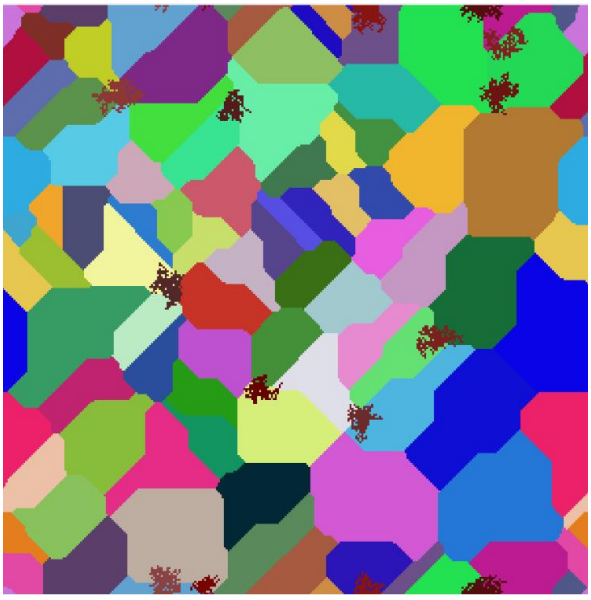


Pic.32 Microstructure generated using CA method, and dual-phase for MC regrowth.

Pic. 32 shows microstructure for steal MY 3200 during the Quantitative metallography study. There are different grain sizes that can be distinguished by different colors. Pic. 23 shows the mappings generated by the application. For this purpose, the microstructure was generated by the CA method for 200 grains, and subsequently the grains were selected using the dual-phase structure, and the structure was subsequently generated by the Monte Carlo method for 5 grains in 30 steps.



Pic.33 Microstructure of an ordinary construction steel(SS1312).



Pic.34 Microstructure with nucleation on boundaries for 6 steps.

On Pic. 33 is shown a microstructure, on which dark elements are visible at the grain boundaries. Pic. 34 maps this structure. It is a microstructure created using the CA method, energy distribution homogenous and nucleation at the boundaries for 6 steps.

5. References

1. https://www.researchgate.net/figure/Microstructures-and-grain-sizes-of-the-ULC-steel-specimens-after-the-annealing-cycle-of_fig2_286969008
2. http://www.mse.mtu.edu/~drjohn/my3200/index.html
3. http://www.hhallberg.com/?tag=grain-boundaries