AGH University of Science and Technology

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Monte Carlo
grain growth algorithm

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Multiscale modelling

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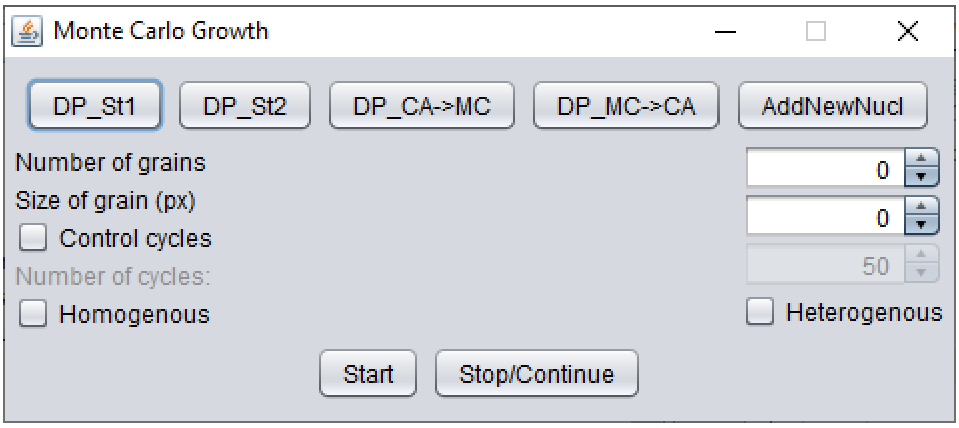
1. Monte Carlo grain growth algorithm

GUI has some specific functions responsible for different features (**Picture 0**)
Neigborhood: Moore (not visible, by default)
Number of Grains: possibility to choose how many grains we need to simulate
Size of Grain: possibility to choose how many pixels each grain has
Control cycles: possibility to choose how many cycles the simulation will take
DP_St1, DP_St2 – buttons responsible for substructures MC-MC
DP_CA->MC - buttons responsible for dual phase CA-MC
DP_MC->CA - buttons responsible for dual phase MC-CA
AddNewNucl - buttons responsible for showing energy visualization/microstructure view
Homogenous/Heterogenous - buttons responsible for energy distribution



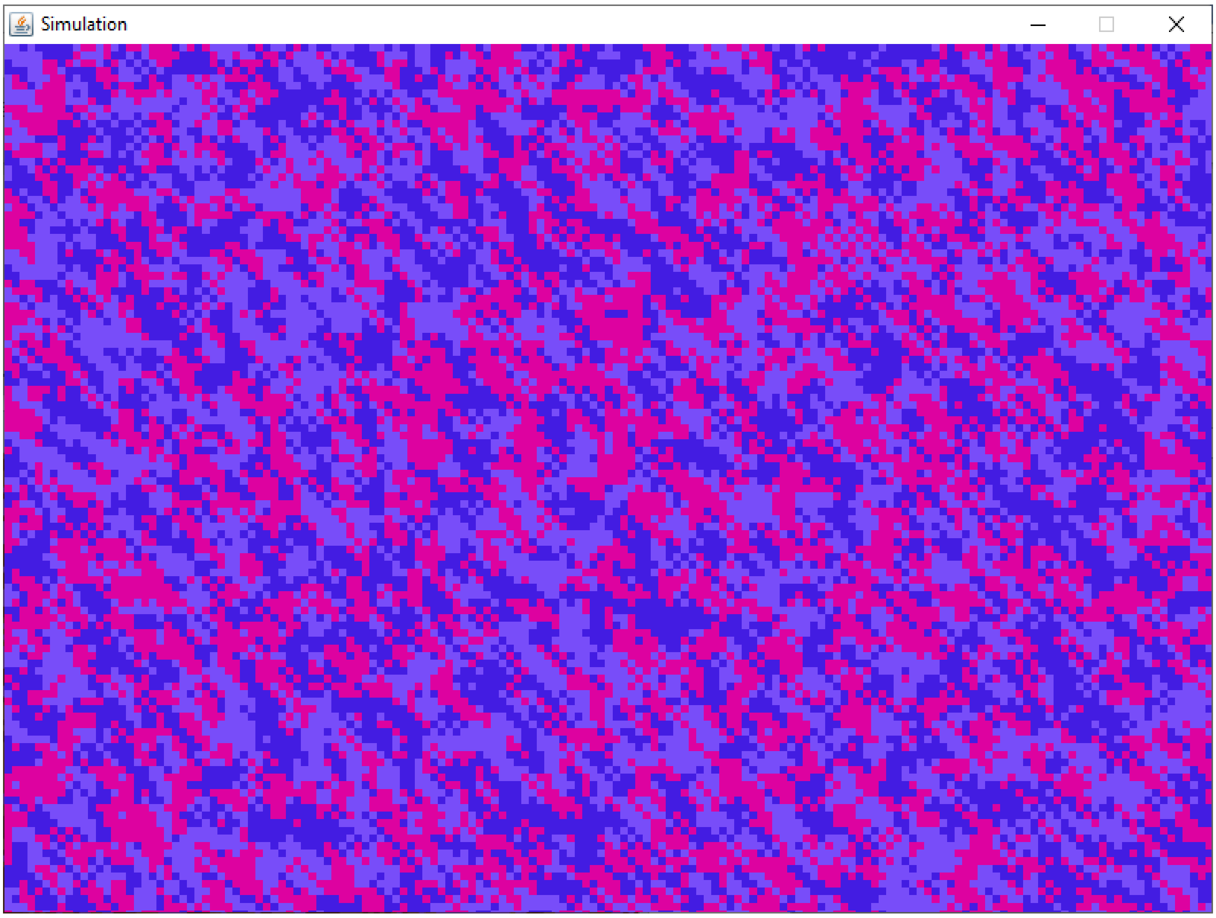
Picture 0 – Control Panel

Whole project can be find on GitHub Project Repository: https://github.com/procesor777

1.1 Example of Monte Carlo grain growth

Number of grains: 3
Size of grains (px): 5
Number of cycles: 50

Example below (**Picture 1.).**

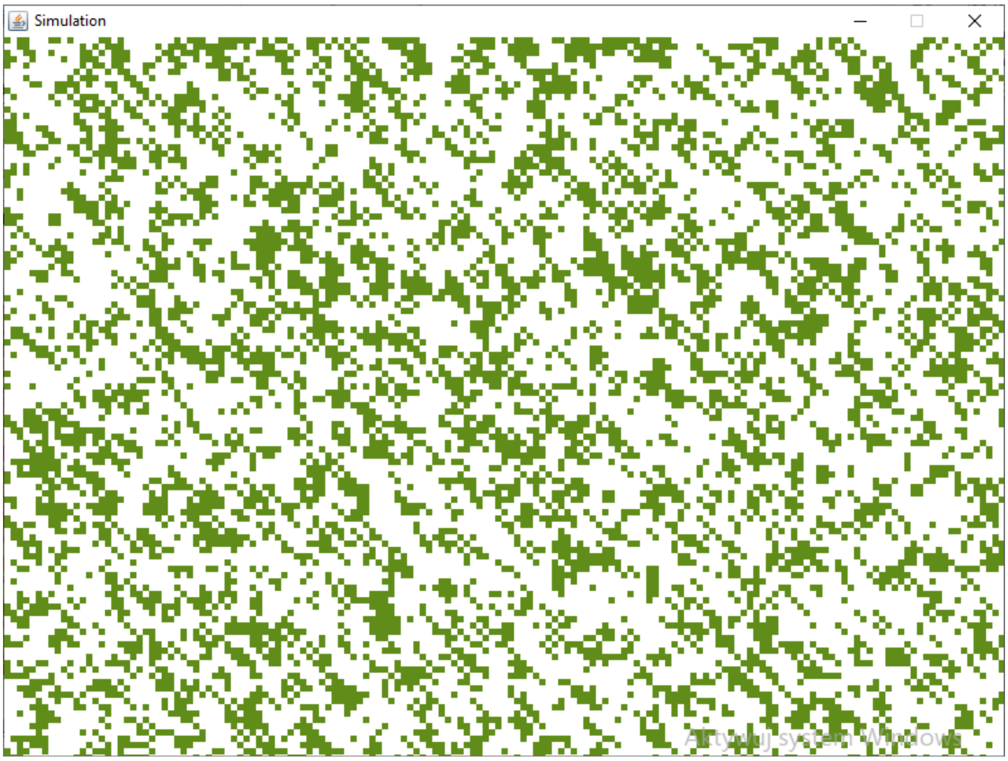


Picture 1 Example of Monte Carlo grain growth

2. Modification of MC grain growth algorithm - substructures CA, MC

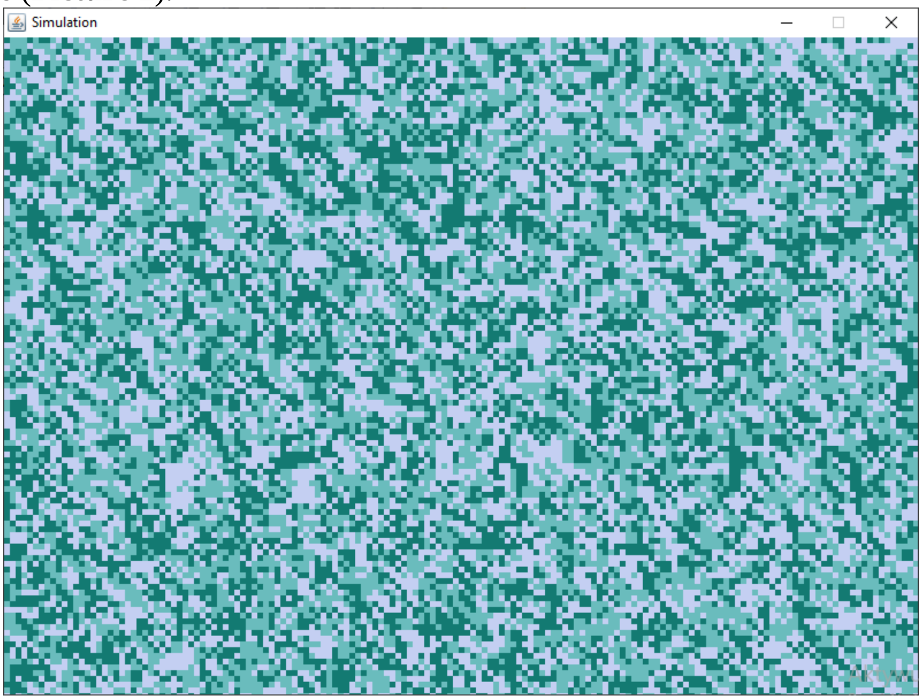
2.1 MC -> MC

On the picture below (***Picture 2***) we can see the randomly choosen cells which will be used as the substructure in next simulations.



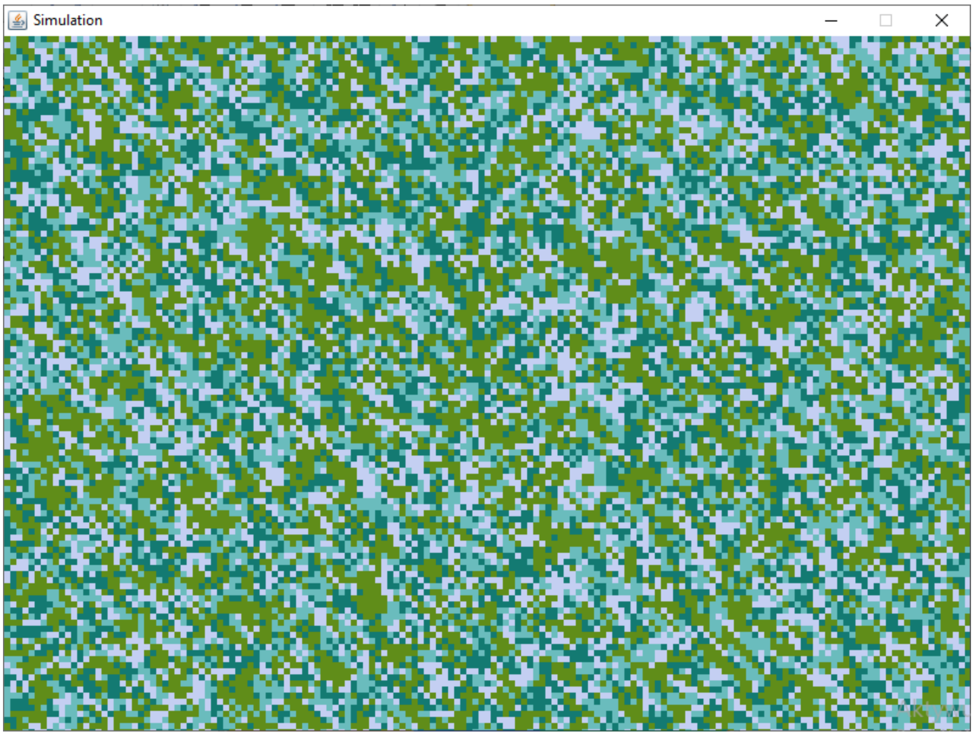
Picture 2 Example of randomly choosen one type of grains from Monte Carlo simulation

Next simulation of Monte Carlo grain growth (**Picture 3**), on which we will add the substructure (**Picture 2**).



Picture 3 Example of another Monte Carlo simulation

And after the adding the substructure, we can see the result on the picture below (**Picture 4**).

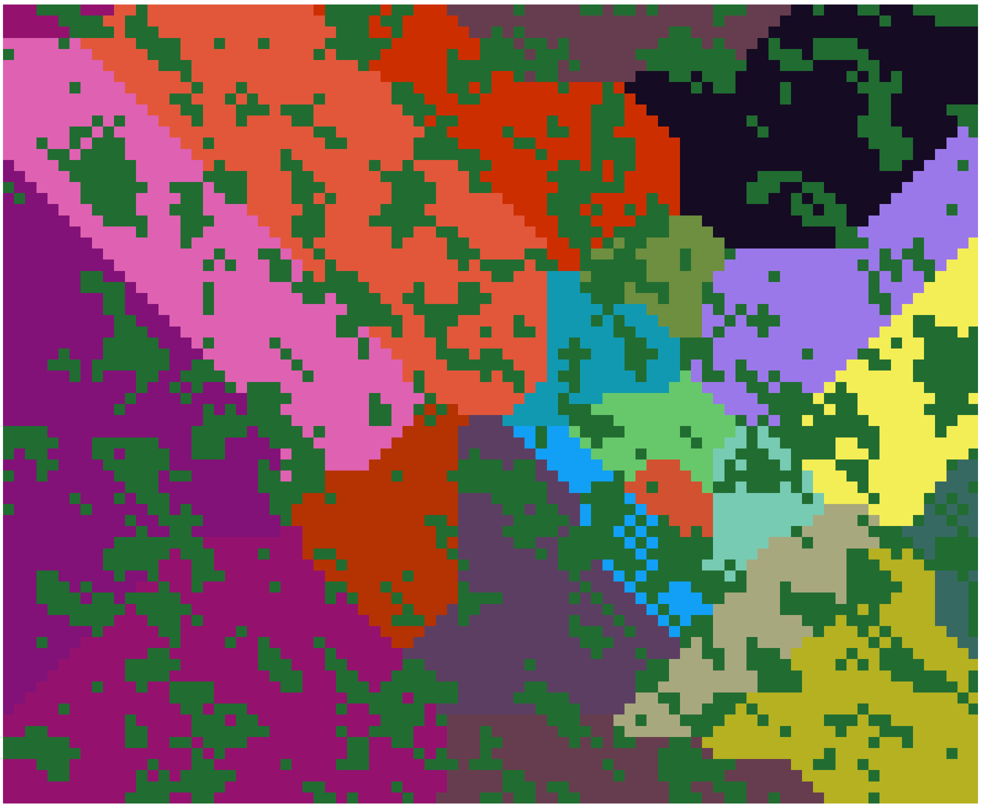


Picture 4 Example of added substructure to MC simulation

2.2 MC->CA

We will use the substructure from the **Picture 2**. And on the **Picture 5** we can see the randomly generated Cellular Automata Grain Growth, on which we will add substructure (**Picture 6**).

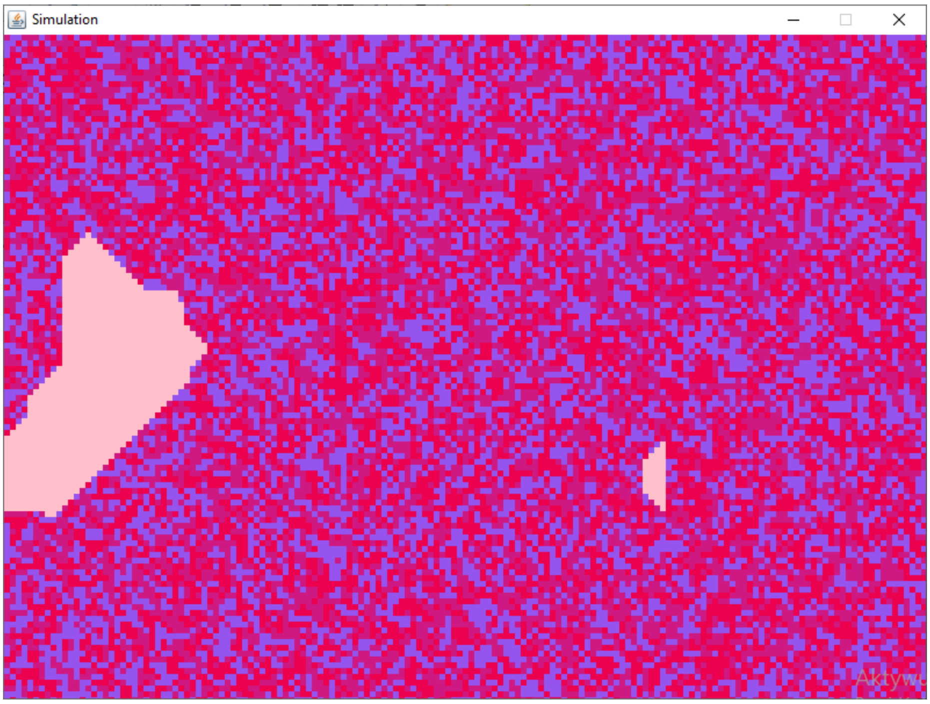
Picture 5 Example of Cellular Automata grain growth


Picture 6 Example of added substructure to Cellular Automata Grain Growth

2.3 CA->MC

On the picture below (**Picture 7**) we can see randomly choosen grain, which will be later added as substructure to the Monte Carlo simulation (**Picture 8**).

Picture 7 Example of substructure from Cellular Automata



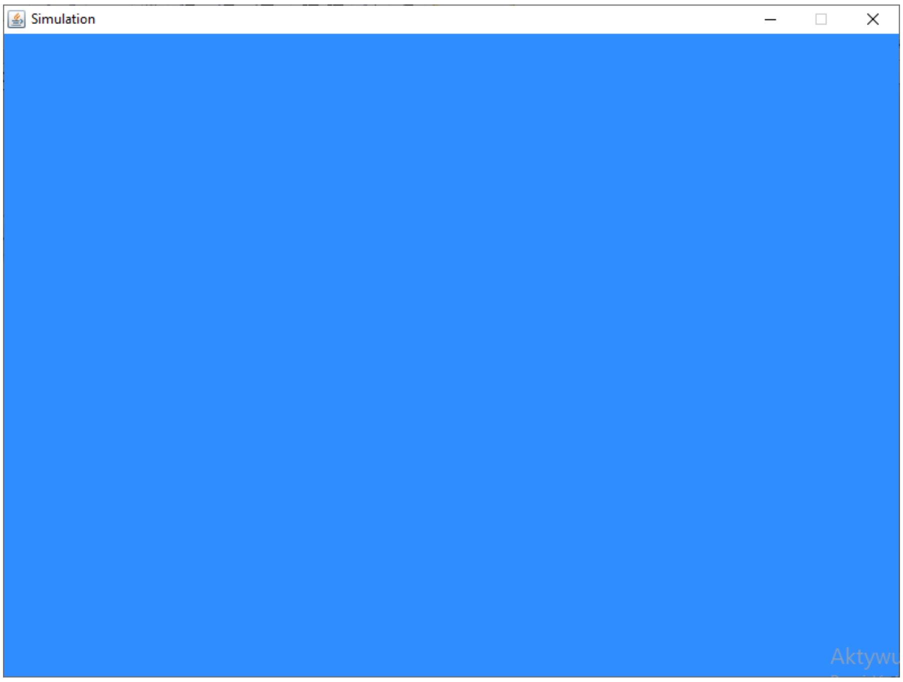
Picture 8 Example of added substructure from Cellular Automata to Monte Carlo.

3. SRX MC: energy distribution, nucleation, growth

3.1 MC static recrystallization algorithm - energy distribution

3.1.1 Homogenous

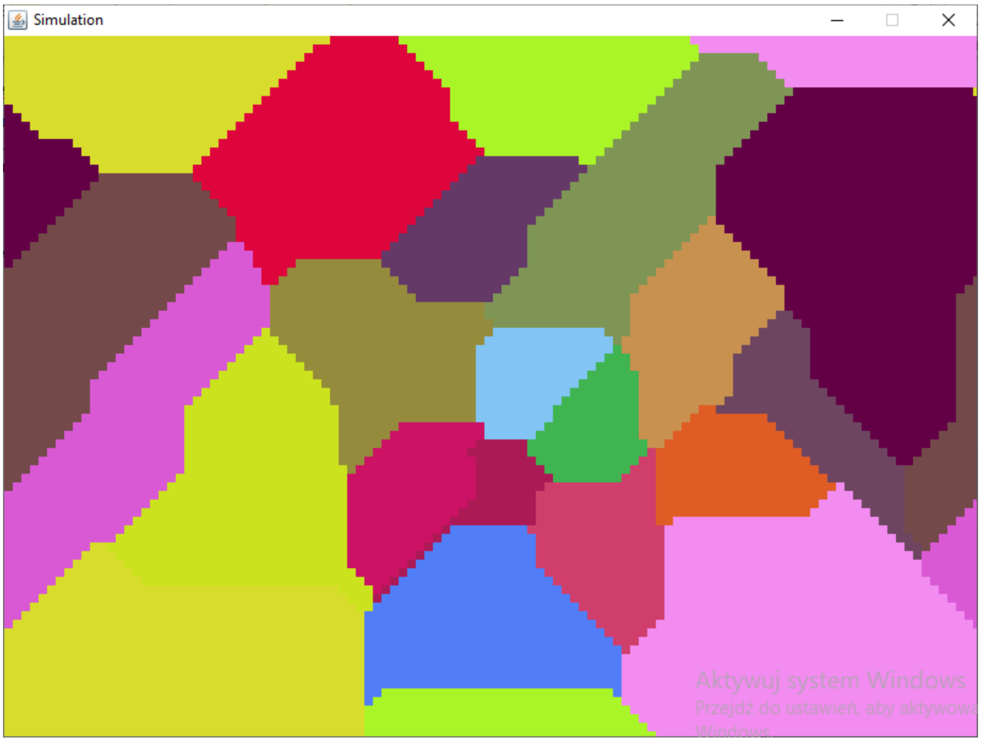
On the picture below (**Picture 9**), we can see the example of homogonous energy distribution. Each cell have also set the energy H to H=5.



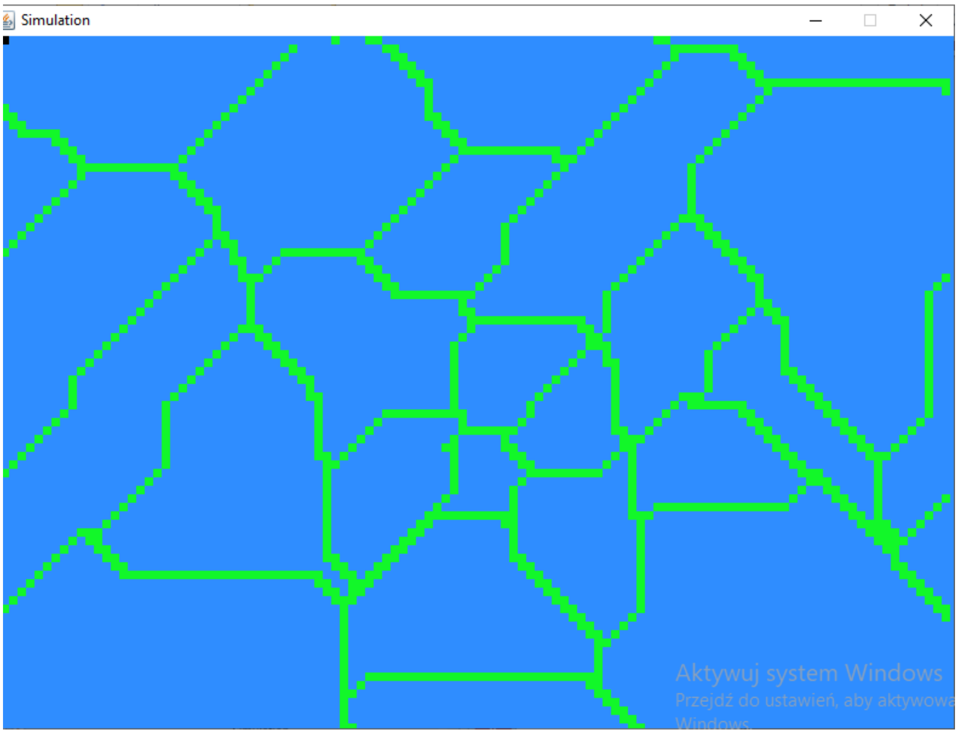
Picture 9 Example of homogenous energy distribution.

3.1.2 Heterogenous

On the **Picture 11**, we can see the example of heterogenous energy distribution.
Below (**Picture 10**) we can see the Cellular Automata simulation.
Each cell on the boundary have also set the energy H to H=5 and each cell in the middle between the boundaries have the energy set to H=2;



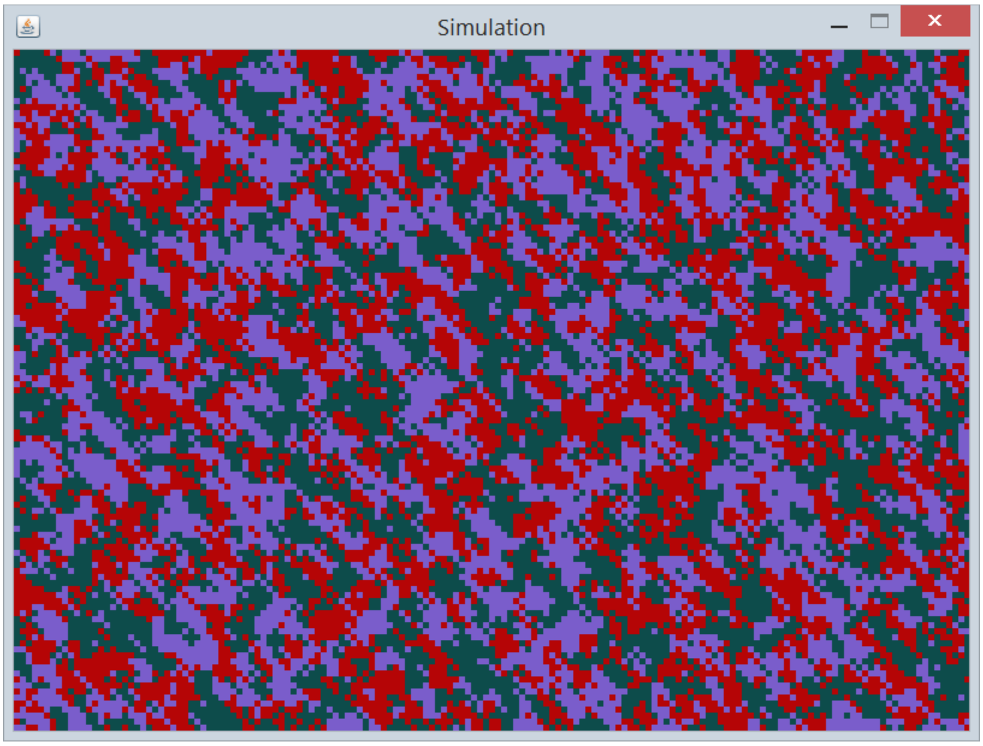
Picture 10 Example of Cellular Automata simulation used for heterogenous distribution of energy



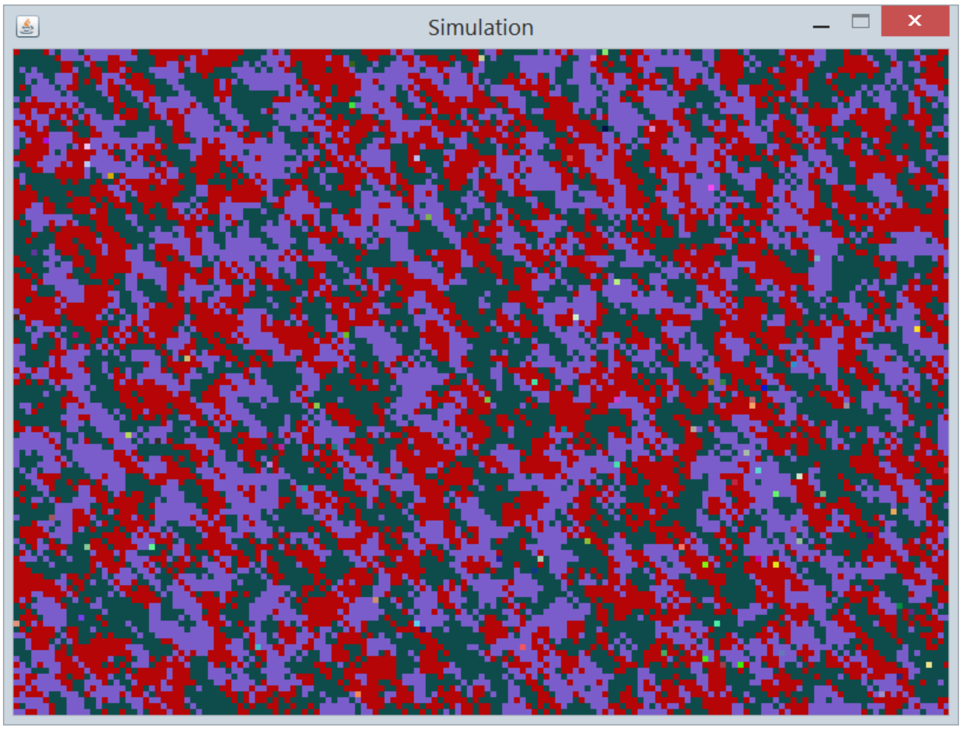
Picture 11 Example of heterogenous energy distribution

3.2 MC static recrystallization algorithm – nucleation

On the **Picture 13** we can see the example of adding 100 new nucleons to finished simulation (**Picture 12**).

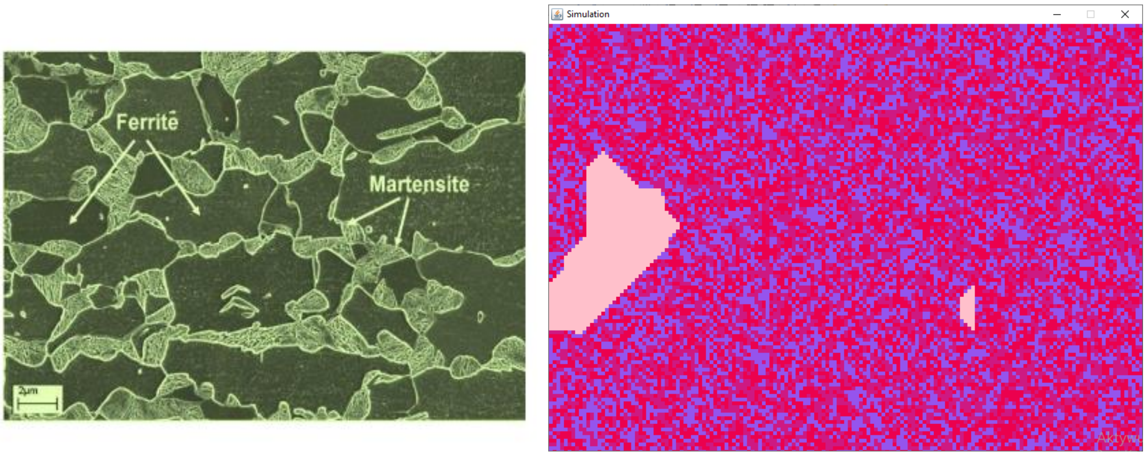


Picture 12 Example of another Monte Carlo simulation

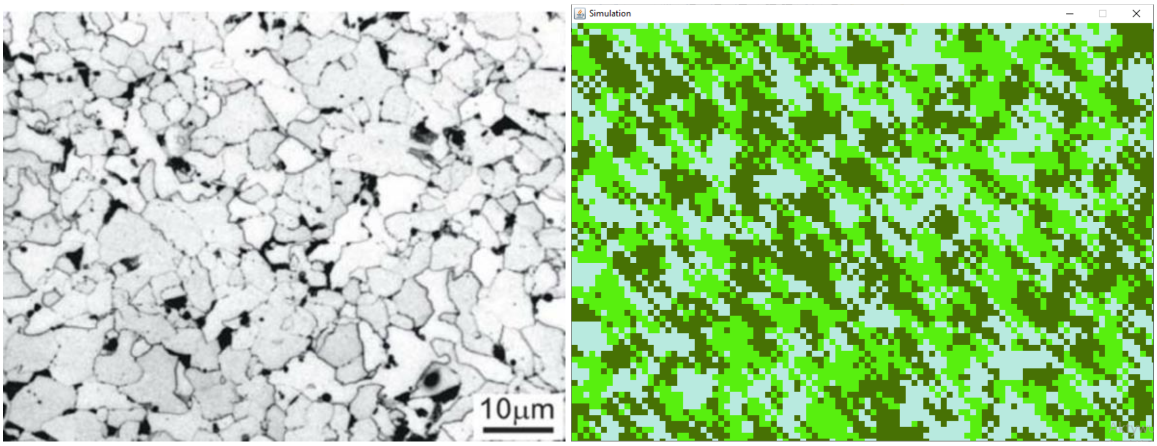


Picture 13 Example of adding new nucleons to already finished simulation

4. Comparison to real microstructure



Picture 14 – Comparison od real DP steel and generated one
(http://ispatguru.com/dual-phase-steels)



Picture 15 – Comparison of real mictrostructure (Steel V-N) and generated one
(https://www.researchgate.net/figure/Optical-micrograph-showing-the-ferrite-and-pearlite-microstructure-in-the-final-strip-for_fig1_29814367)

5. Conclusions

- Making this project allowed us to learn how the Monte Carlo method works.
- The main disadvantage of Monte Carlo mehod is that it takes quite long to make a calculation
- Generated microstructures differ a lot from real ones – that's caused by an imperfect implementation of model
- It allowed us also to train more the programming language which we choose for this project.
- Despite adding many features, you can still develop and improve this project.