MULTISCALE MODELING

Report 2

„*Application for simple grain growth with cellular automata algorithm*”

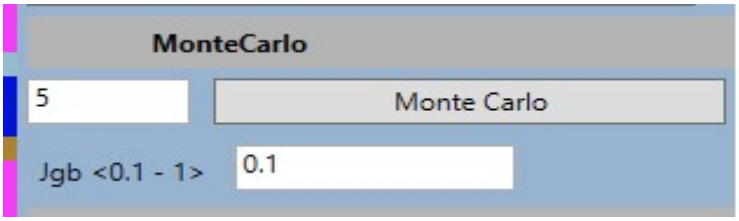
Marcin Combik

II rok, II st. WIMiIP

1. Introduction:

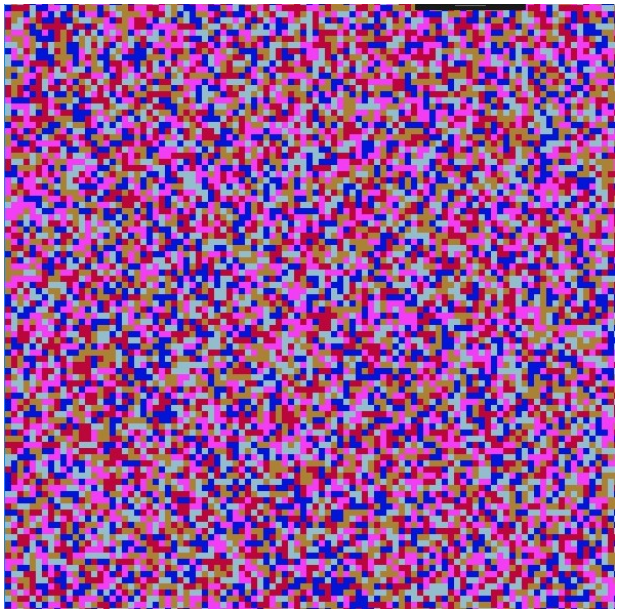
Second part of implementation was Monte Carlo grain growth algorithm. Cellular automata structures from previous part of application was helpful. Grains choose in algorithm has state. Example with two possibilities has two states: on and off. Algorithm uses RGB colors which represent states.

2. Monte Carlo growth:

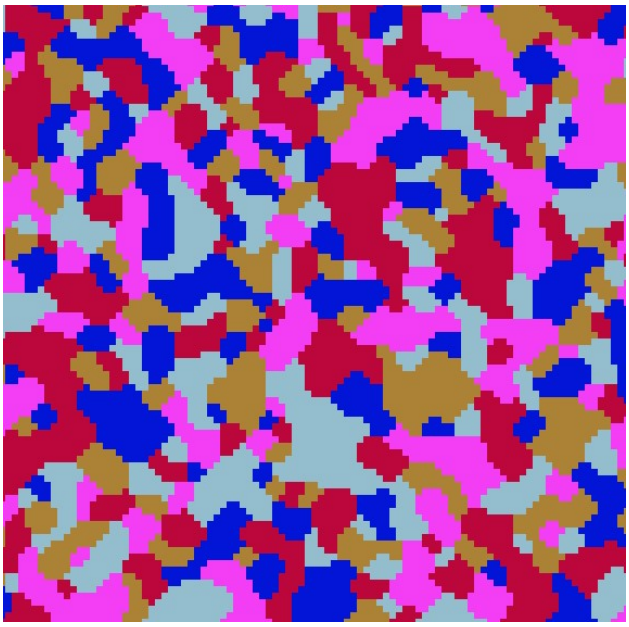


User is able to set number of nucleons type in textbox which are connected with grid. After set number (it's nucleons size), and click Monte Carlo [nucleons], algorithm creates a list of possible coordinates to choose one from it randomly and calculate the energy for that cell. The process ends when there are no empty cells left.

After choose Monte Carlo radio button and click start in interface , algorithm runs. When the process of calculating energy for that cell is finished, the coordinates of that cell are deleted from the list. The loop continues until the list isn't empty which ensure that all of the nucleons will be chosen. Algorithm end when all of calculated energies replace old grid.



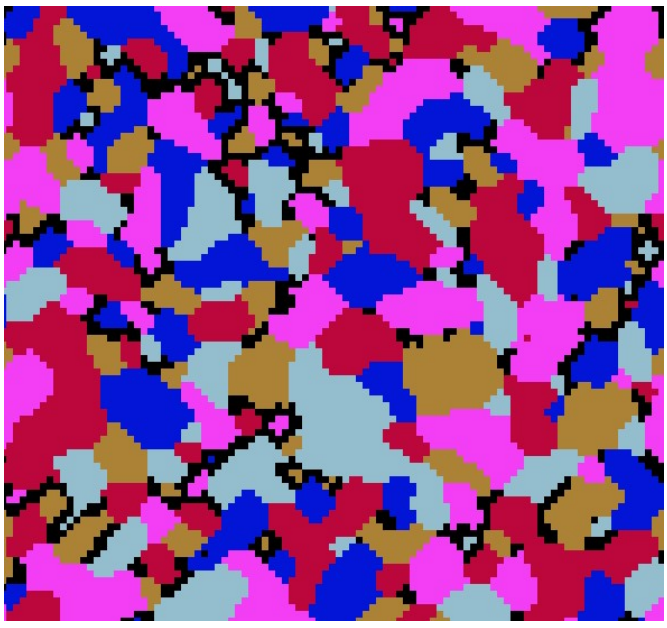
Picture 1 First step of Monte Carlo Algorithm



Picture 2 Monte Carlo algorithm result

3. Dual phase:

Interface provide to user grids which block nucleons. Grains wont participate in second and next grain growth.



Picture 3 Monte Carlo with borders

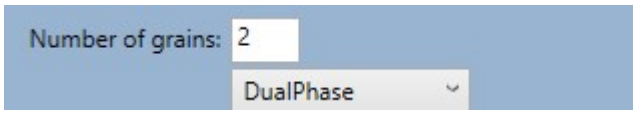
Step 1:

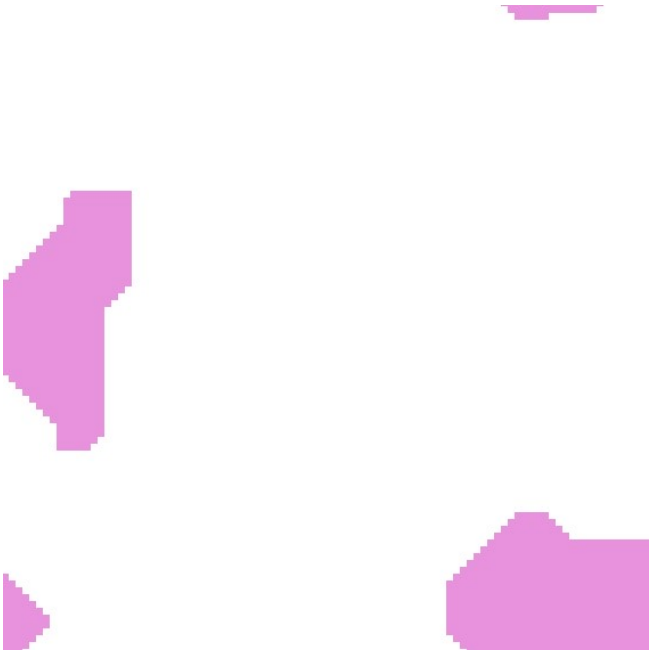
Based on documentation first step for Dual Phase was start simple grain growth CA:

Picture 4 CA with Von Neumann simulation growth

Step 2:

Next we can select grains: (e.g two grains)

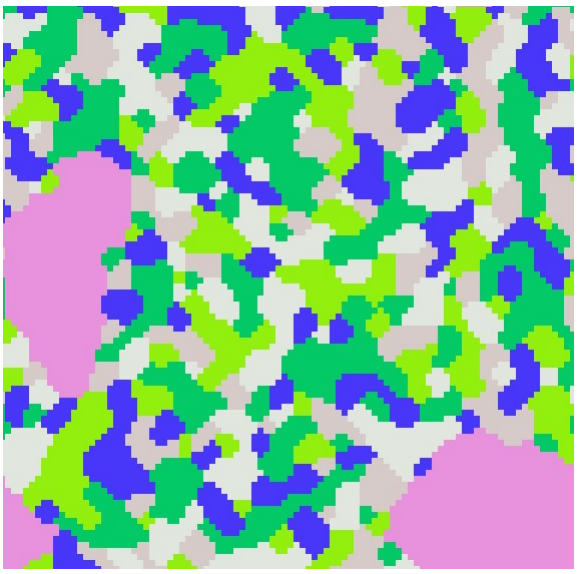




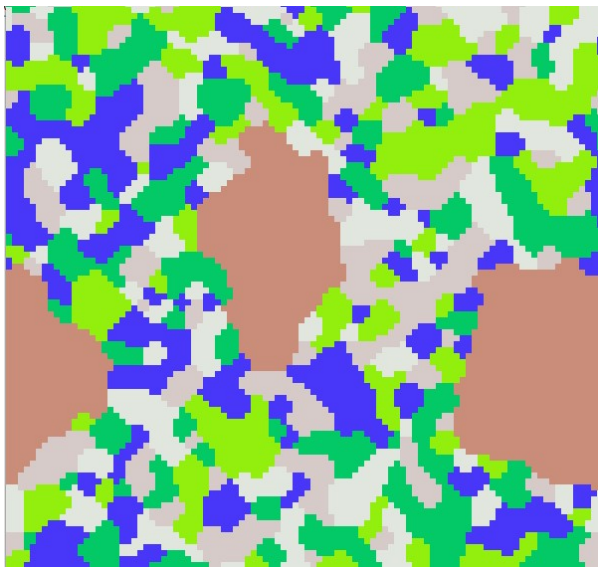
Picture 5 Two selected grains

Step 3:

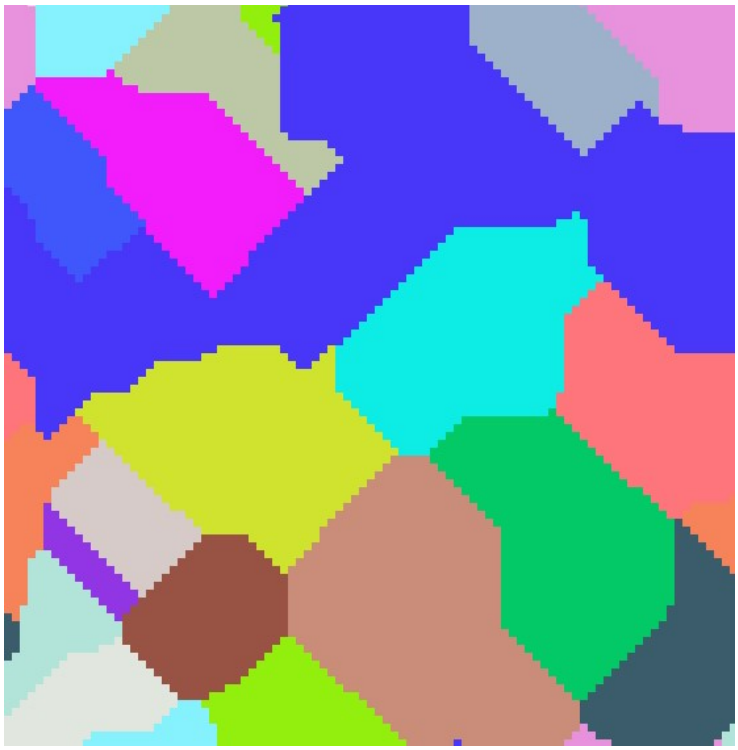
In third step we have two path: one is CA simulation and second is MC simulation:



Picture 6 Example of CA simulation, grain dual phase selection (2 grains) and MC simulation in result



Picture 7 Second example of CA simulation, grain dual phase selection (2 grains) and MC simulation in result

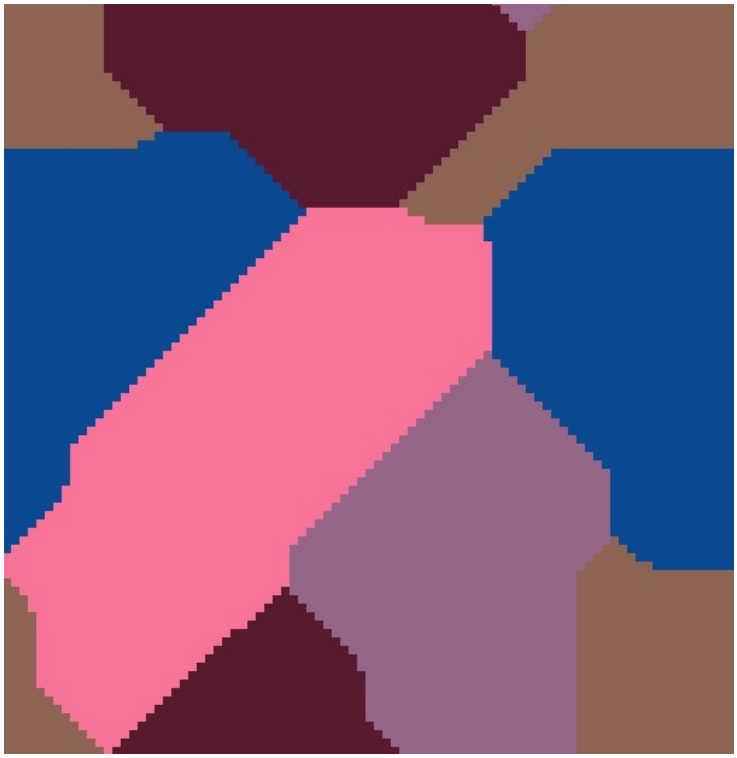


Picture 8 Example of CA simulation based on 20 grains, 4 grains dual phase selection and first step repetition (20 grains, CA)

Monte Carlo SRX:

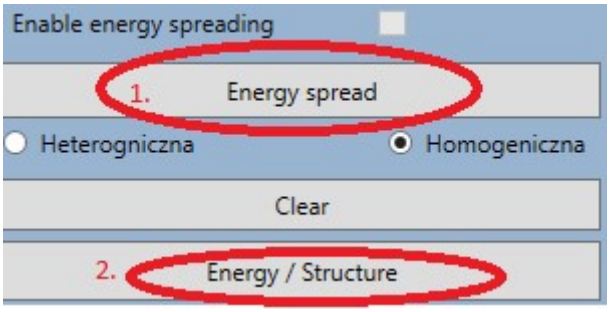
Step 1:

Initial metal morphology:



Picture 9 CA, 5 grains, Moore neighbourhood

Step 2:



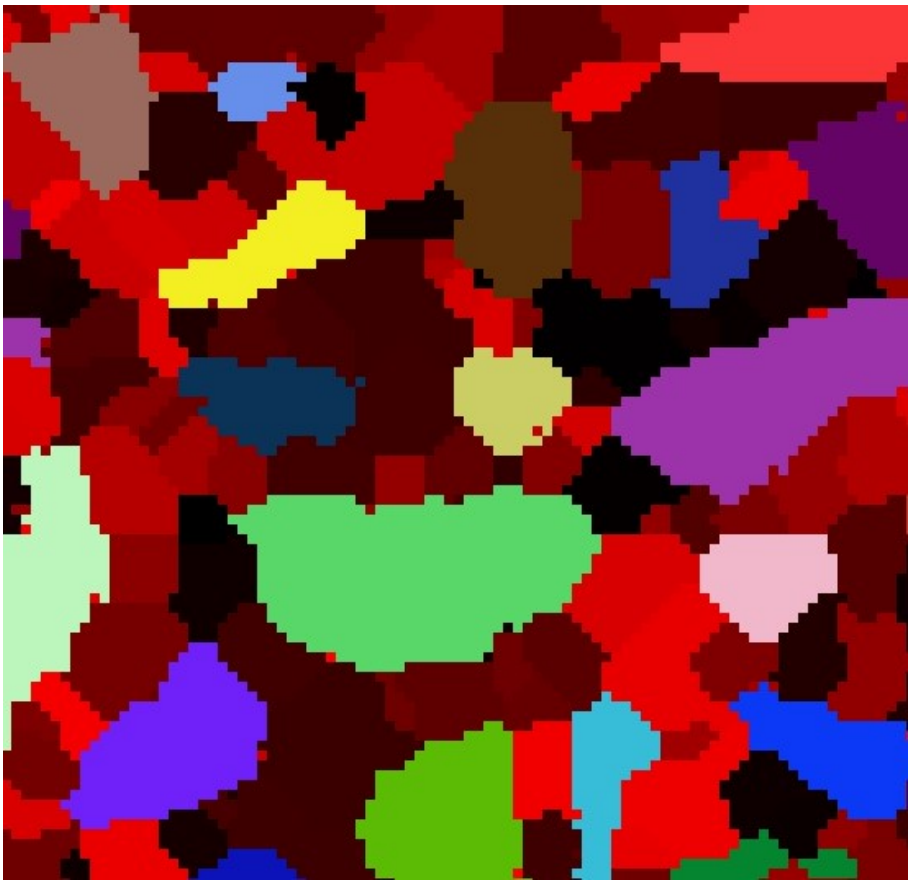
After generate morphology we calculate energy between nucleons. To do this, user should click on 1. “Energy spread” button and next click on 2. “Energy / Structure” button. Result below:

Picture 10 Energy states

Dark parts represent high energy states.

4. Grain Growth Algorithm – Monte Carlo SRX:

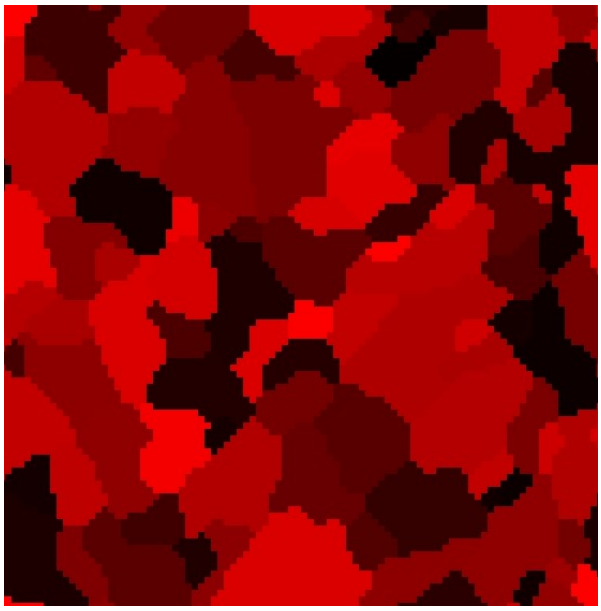
After generate morphology and calculate energy we can run SRX simulation. For that we should choose size of nucleons. Without it algorithm show empty grid – nothing happened.



Picture 11 SRX result with nucleon size set on 20

Other examples:

Result for MC algorithm, heterogenic energy spread and constant size set to 10:



5. Conclusion

This report presents the application designed to handle process of the microstructure simulation. The application using Monte Carlo grain growth logic is based on cellular automata. Application provide implementations like CA, MC algorithm, dual phase subtracter, SRX algorithm.