AGH

AKADEMIA GÓRNICZO-HUTNICZA
IM. STANISŁAWA STASZICA
W KRAKOWIE

Multiscale modelling

1st report: Grain Growth Cellular Automata

Katarzyna Fornal
WIMiIP, IS, 2nd grade
MiTI, gr. 4

INTRODUCTION

Simple grain growth simulation was implemented using CA (Cellular Automata). It's a model of a system of cells with the following attributes:

- grid – in this project it's the 2D set of cells,
- state of cell - each of the grains has a different value of state,
- neighbourhood of cell - describes the closest neighbours of a particular cell.

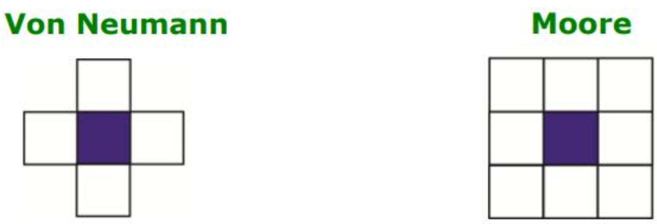
The simulation of simple grain growth algorithm was implemented in C# using Microsoft Visual Studio. GUI was created using Windows Forms Application. Program contains simulation of simple grains growth, microstructure import/export, inserting nucleons, generating different microstructure types and grains boundaries colouring.

FUNCTIONALITY

1. SIMPLE GRAIN GROWTH

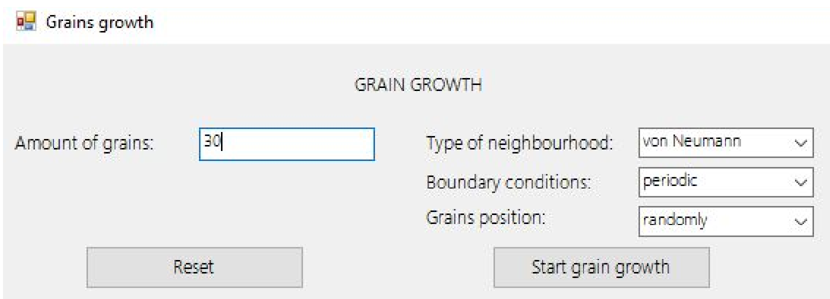
To start simulation of grains growth user has to input amount of grains and decide how grains will grow (picture 2). There are three types of conditions:

- grains position - user decides whether grains will be located randomly or regular
- boundary condition - periodic and absorbing, in case of absorbing boundary conditions, the state of cells located on the edges of the CA area is determined using 0 as a state of missing neighbour. In case of periodic boundary conditions, state of missing neighbour on the edges is define by the state located on subsequent edge of the CA space
- neighbourhood condition - von Neumann and Moore - user decides which and how many states of neighbours grain will be used to determine the state of grain (picture 1).



Picture 1: Neighbourhood types

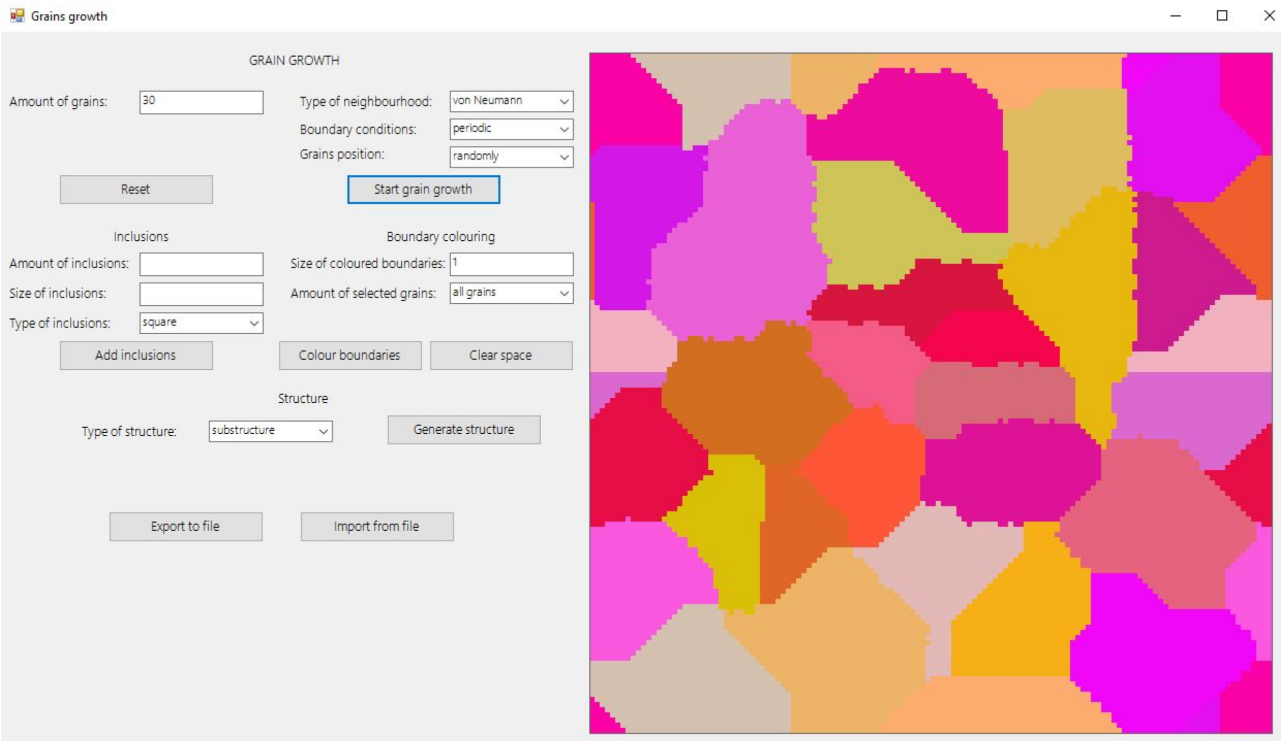
In order to run simulation user has to click 'Start grain growth' button. Generated simulation is shown in the picture 3.



Picture 2: Grain growth algorithm parameters

SIMPLE GRAIN GROWTH ALGORITHM

Defined amount of grains is located by chosen position boundary. Algorithm goes through the CA grid, cell by cell, checking whether the state of cell is defined. If it is undefined, algorithm examines states of neighbour cells, according to chosen neighbourhood condition. The state of undefined cell gets the value as a neighbour with the highest cell count or chooses randomly between those which appeared the most. When all of the cells are checked, image of the CA grid is updated and next iteration begins. The simulation is running until all states of cells are defined.

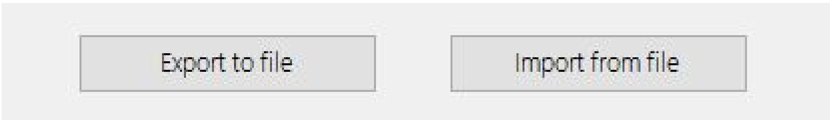


Picture 3: Simple grain growth CA grid visualization

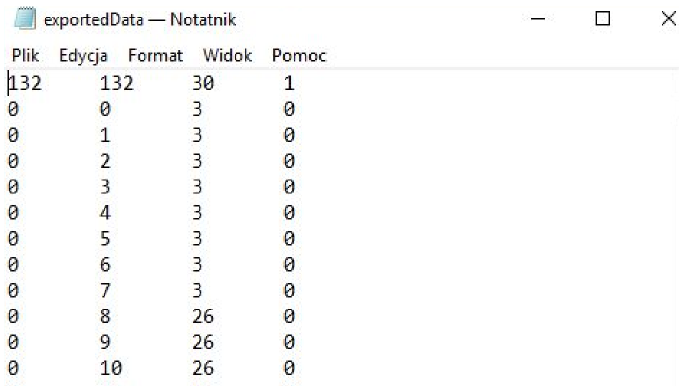
In addition, there is a 'Reset' button to stop the simulation and clear the CA space.

2. MICROSTRUCTURE IMPORT & EXPORT

After generating the CA grid, user can export it to .txt (picture 5) and .bmp (picture 6) file by clicking 'Export to file' button (picture 4).

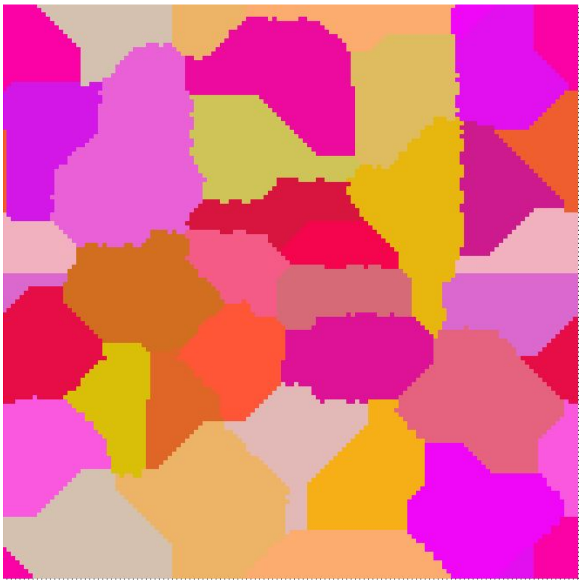


Picture 4: Import/export buttons



Picture 5: Exported text file

In exported text file (picture 5), in first line user has an information about height, width, amount of grains and phases. Next there is position, state and phase of each cell.

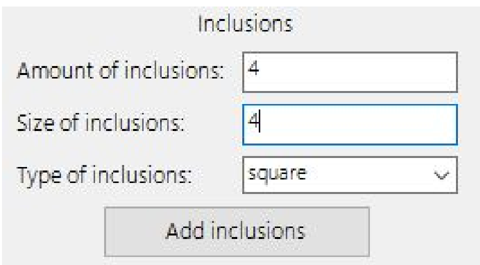


Picture 6: Exported .bmp file

In addition, by using text file with data format like in exported text file, user can import these data, generating the CA grid by clicking 'Import from file' button (picture 4).

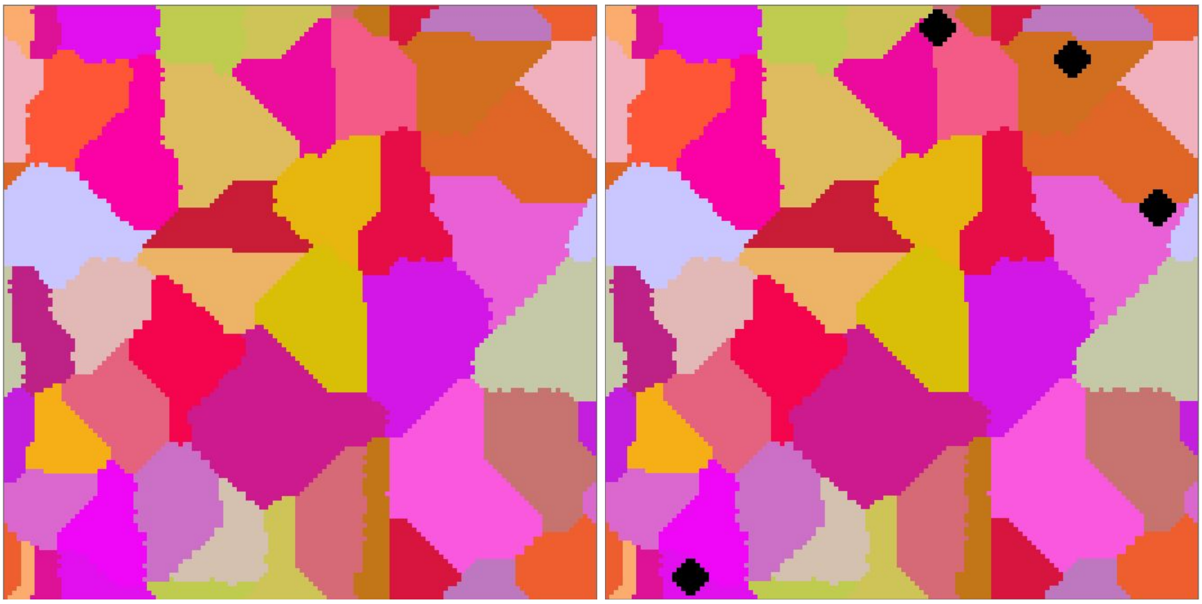
3. INCLUSIONS

Every CA structure can include some inclusions. To present them in generated CA grid, user has to input amount, size and type of inclusions - square or circular (picture 7). The inputed size is a radius of circular shaped inclusion and length of the side in square inclusions.

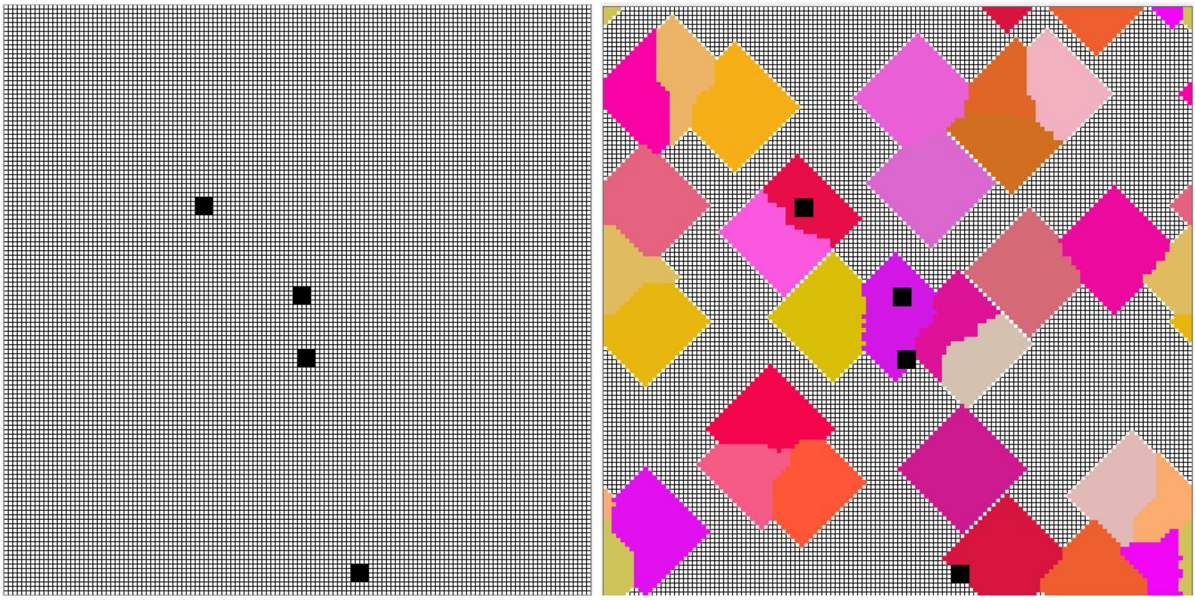


Picture 7: Inclusion parameters

Inclusions are added after clicking ‘Add inclusions’ button. There are two options - user can add them after (picture 9) or before grain growth simulation (picture 8).



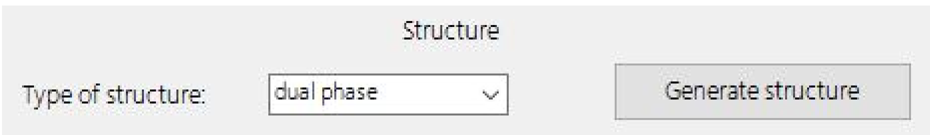
Picture 8: Circular inclusion at the beginning of simulation



Picture 9: Square inclusion after the simulation

4. DIFFERENT MICROSTRUCTURE TYPE

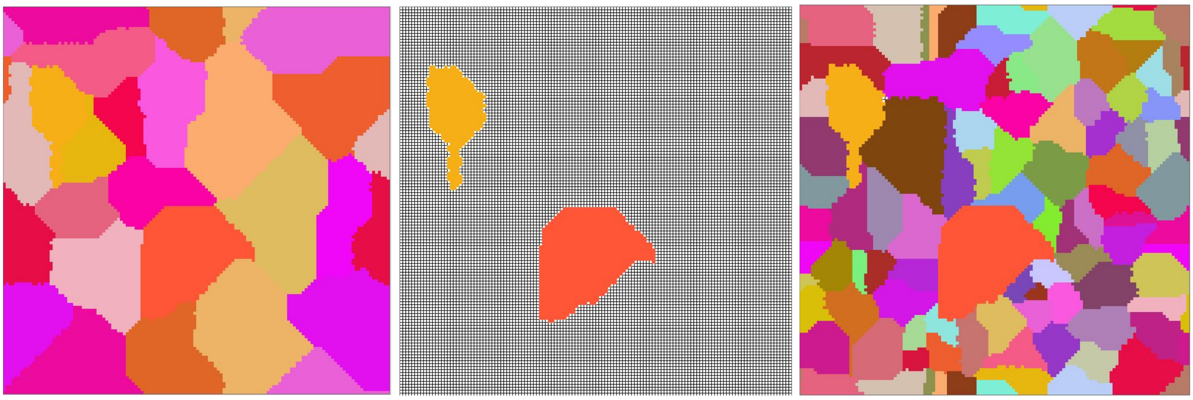
To achieve different microstructure type, user needs to only click on chosen grains of generated CA grid, select type of structure and click ‘Generate structure’ button (picture 10).



Picture 10: Microstructure type parameters

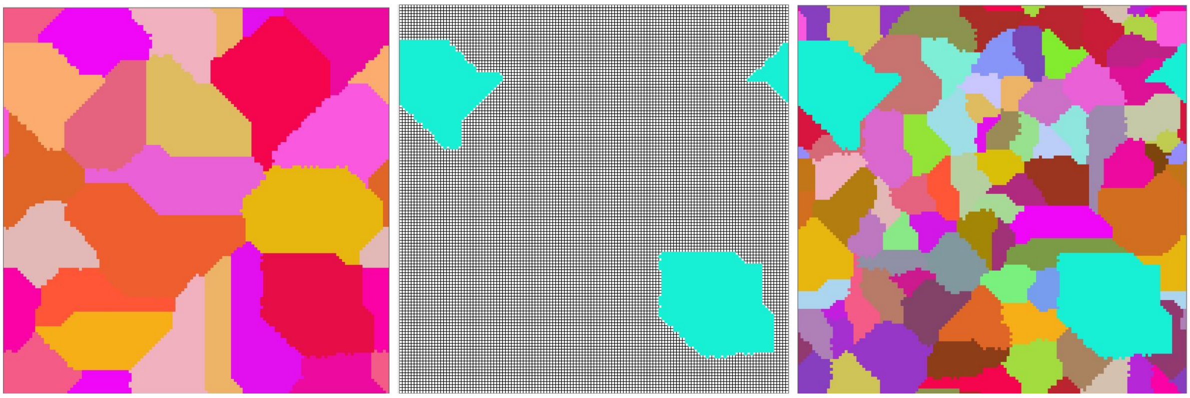
In addition, the phase value of chosen grains increase. Under the generated structure user can start a new simulation. Picture 11 presents grains growth (11a), generated substructure (11b) after choosing two grains, by clicking on them, then generating new structure under the substructure (11c). Picture 12 presents similar operation, but after grains growth (12a), dual phase structure is generated (12b) and then new structure under the dual phase (12c).

Picture 11: Substructure



a. grains growth **b. generated substructure** **c. grains growth under substructure**

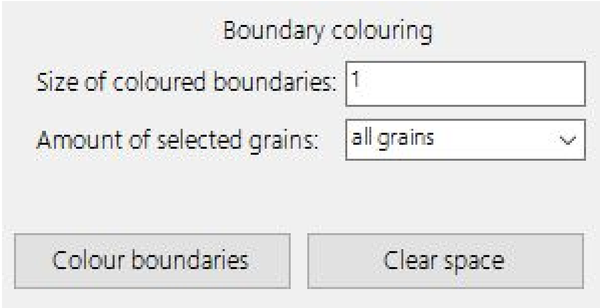
Picture 12: Dual phase



a. grains growth **b. generated dual phase** **c. grains growth under dual phase**

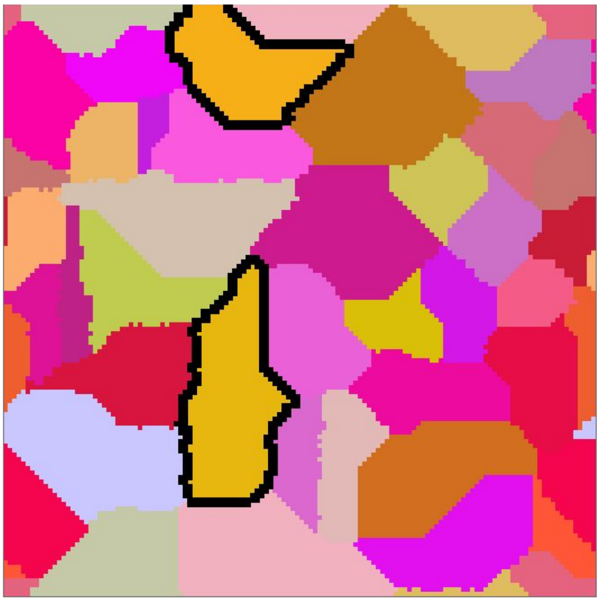
5. GRAIN BOUNDARIES SELECTION

In case of grain boundary colouring, user inputs size of coloured boundaries and selects whether all grains boundaries will be coloured or only chosen ones, by clicking on them (picture 13). To colour boundaries, user needs to press the ‘Colour boundaries’ button. ‘Clear space’ button is used for clearing the CA grid, leaving only coloured boundaries (picture 13).

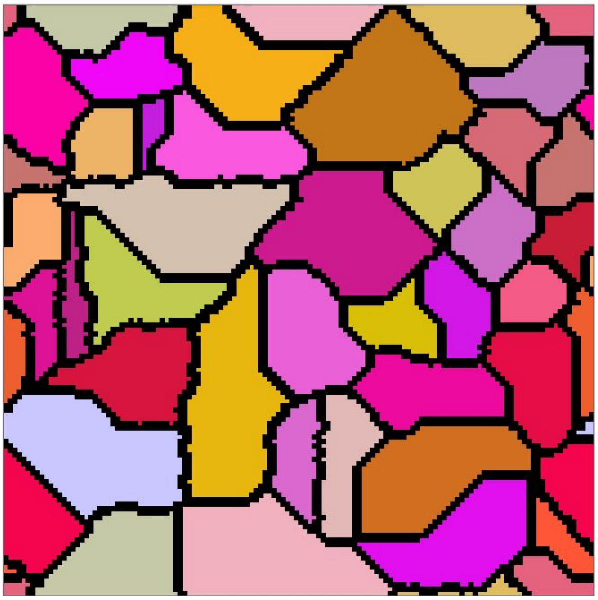


Picture 13: Boundary colouring parameters

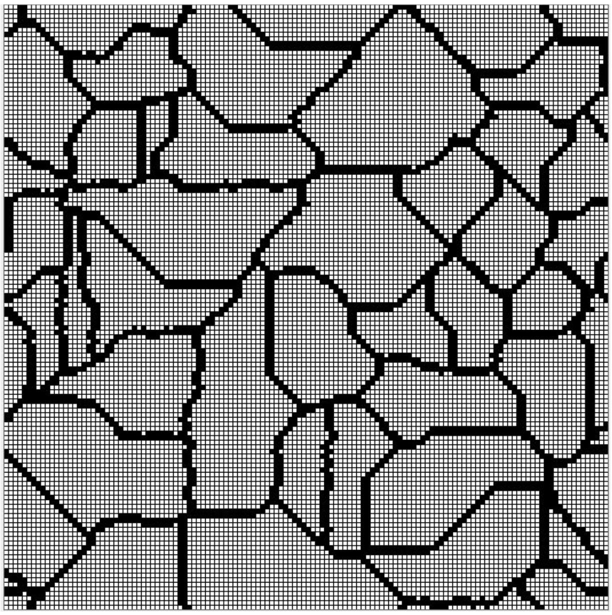
Picture 14 presents chosen grains boundary colouring operation. Picture 15 shows that all grains have theirs boundaries coloured. After clicking on ‘Clear space’ button when all of the grains boundaries are colored, user gets structure like in the picture 16.



Picture 14: Boundary colouring of selected grains



Picture 15: Boundary colouring of all grains

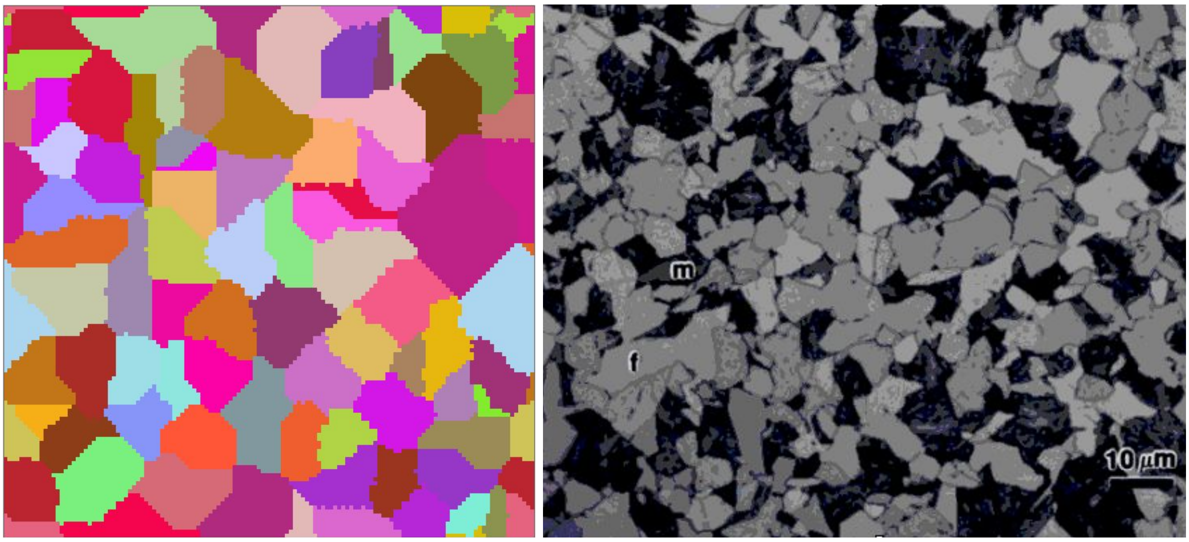


Picture 16: Cleared space

COMPARISON OF REAL AND SIMULATED MICROSTRUCTURES

In the picture below (picture 17), there is comparison between the CA microstructure generated by program (17a) and the microstructure of a malleable cast iron after conversion to nodular graphite (17b). The simulated structure seems to match the real one, especially the shape and size by inputting correct amount of grains. However, user can't differentiate properly between ferrite and martensite grains.

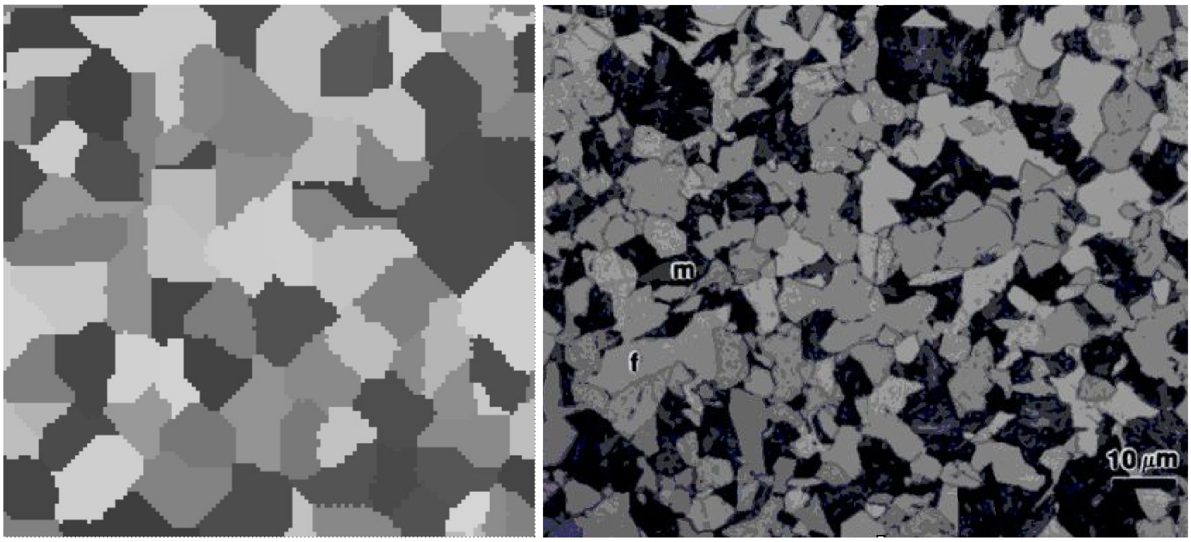
Picture 17: Comparison of generated CA microstructure vs. real microstructure



a. Generated CA microstructure **b. Real microstructure**

To solve this problem, image of generated microstructure was displayed in grayscale (18a).

Picture 18: Comparison of grayscale, generated CA microstructure vs. real microstructure



a. Grayscale, generated CA microstructure **b. Real microstructure**

Grayscale, generated image of the CA microstructure (18a) seems to be similar to real microstructure (18b). By adding more conditions, decreasing the size of grains or adding inclusions, user can achieve more similar simulated version to the real one.

This report presents a software, designed to implement simulation of the simple grain growth with additional features such as generating other microstructures or adding nucleons.
Program is based on the cellular automata algorithm, which can be used in many of different areas such as computer science, mathematics, physics, biology, microstructure modelling.