AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Faculty of Metals Engineering and Industrial Computer Science

MULTISCALE MODELLING

"Simple grain growth with cellular automata algorithms"

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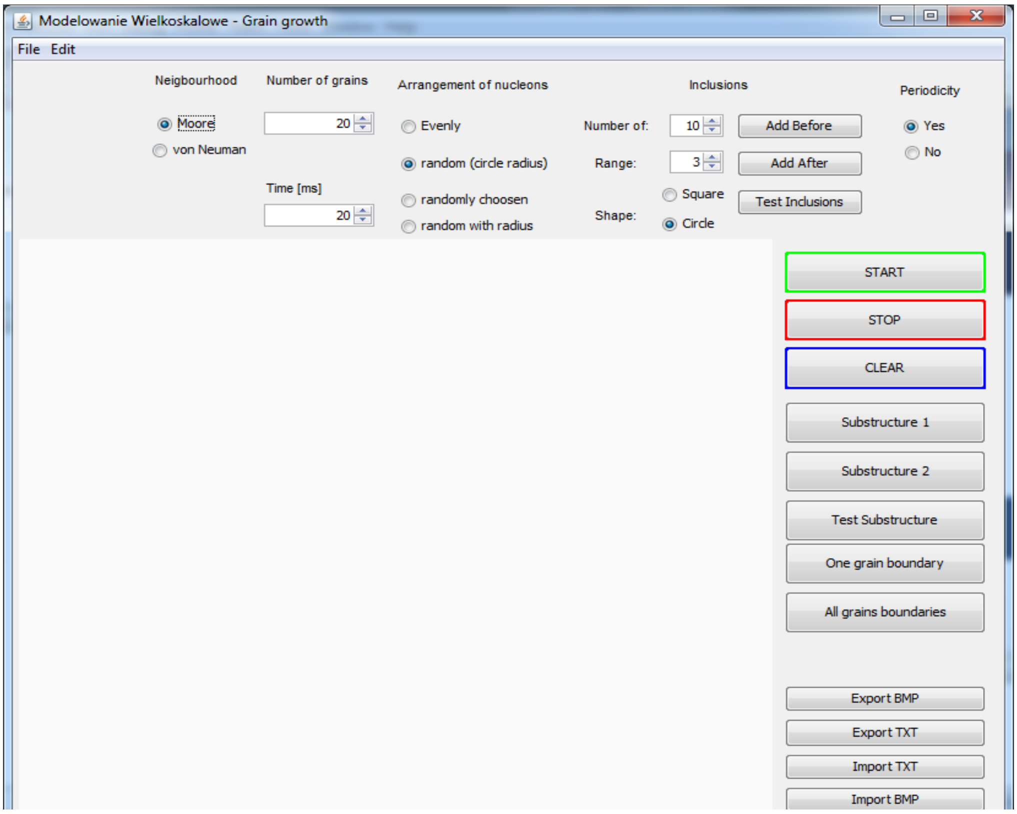
Introduction, GUI and technologies

The idea of the project was to implement simple grain growth algorithms and some other functionalities.

Cellular Automata method was used to implement SGG (simple grain growth). Cells have some specific interaction rules between each other called neighborhood rules – Moore and von Neuman ones.

Project was implemented in Java using NetBeans IDE 8.2 environment because that's a programming language that I know best.



Picture 1 – Graphic User Interface

The main window (picture 1) is divided into three parts. The bottom panel is used to display visualization of grain growth..

The 2nd panel (top one) contains several options:

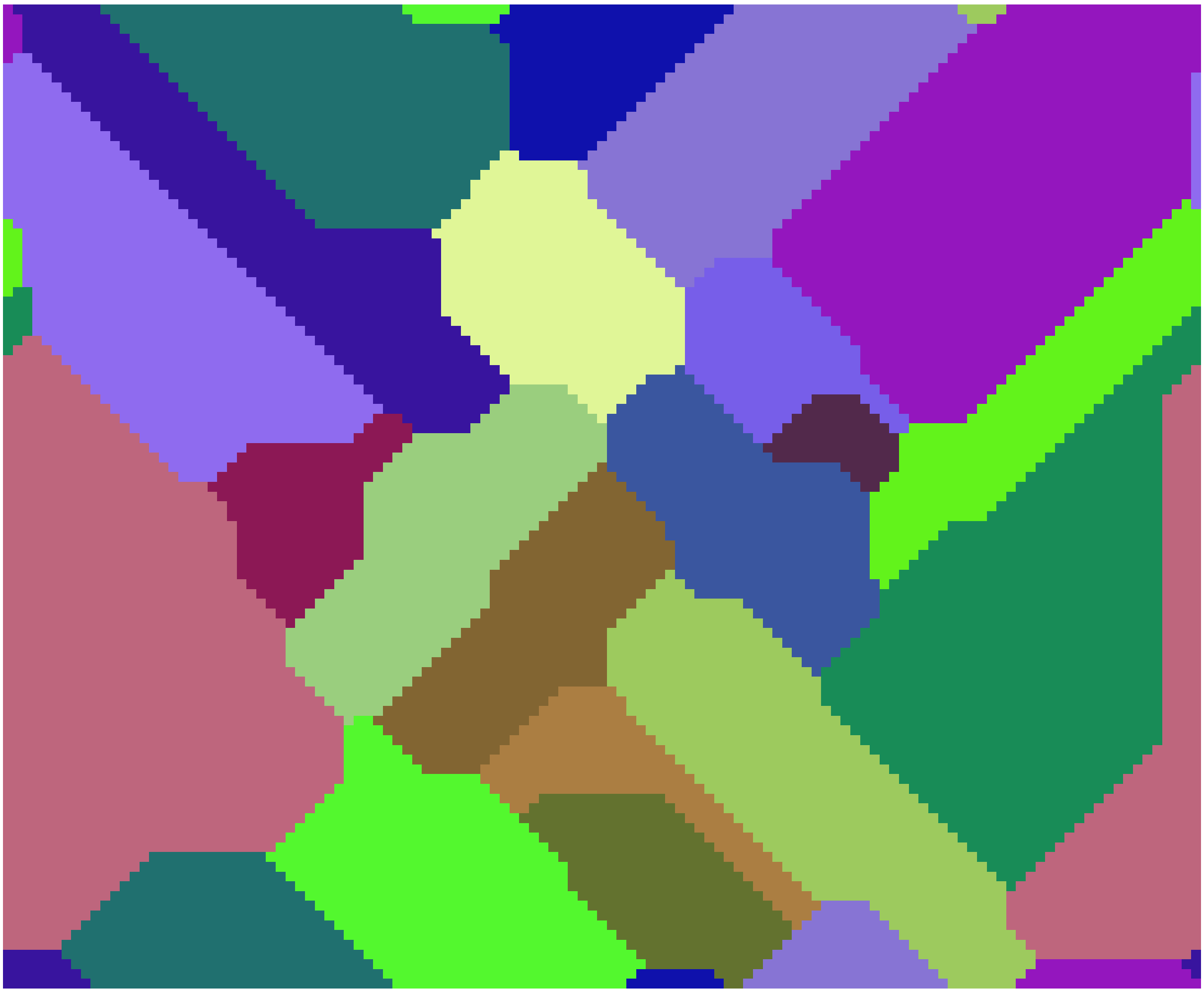
- Neighborhood
- Number of grains
- Time [ms]
- Arrangement of nucleons
- Number, range and shape of inclusions
- Buttons responsible for adding inclusions
- Periodicity condition

The right menu panel contains:

- START/STOP/CLEAR buttons
- Buttons responsible for generating substructures/grain boundaries
- Import/Export buttons

Lab 1: Simple grain growth CA + visualization

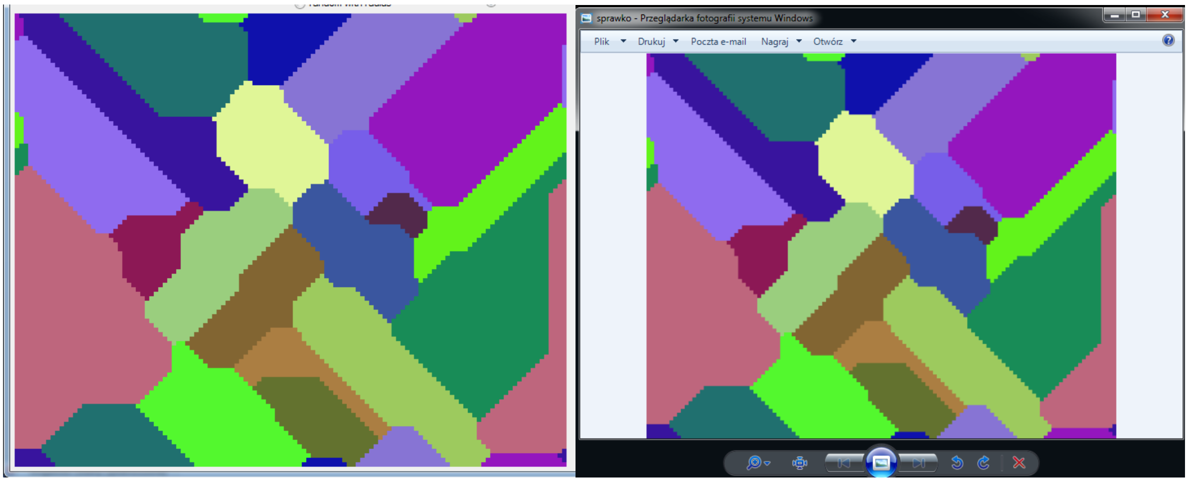
User can choose number and arrangement of grains, neighborhood type, periodicity codition and time of simulation. After clicking start button grains are generated and the visualization is displayed on a panel. Depending on choosen neighborhood type the final visualization of microstructure looks different. Grains can also be placed on the board by clicking anywhere in the area of the board.



Picture 2 – Visualization of Simple Grain Growth

Lab 2: Microstructures export/import to/from txt files, pictures.

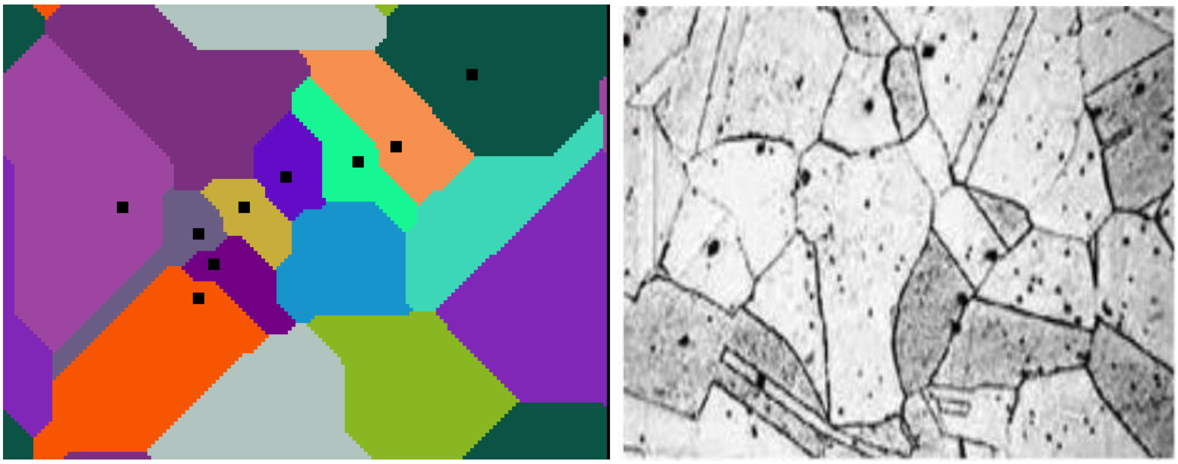
The second part of the project was to implement functionality of importing and exporting data to both text and image format. For exporting pictures users can choose location, name and format of saved file. Picture 3 shows the visualization (on the left) and saved .bmp file (on the right). Txt files are exported with the default name and location.



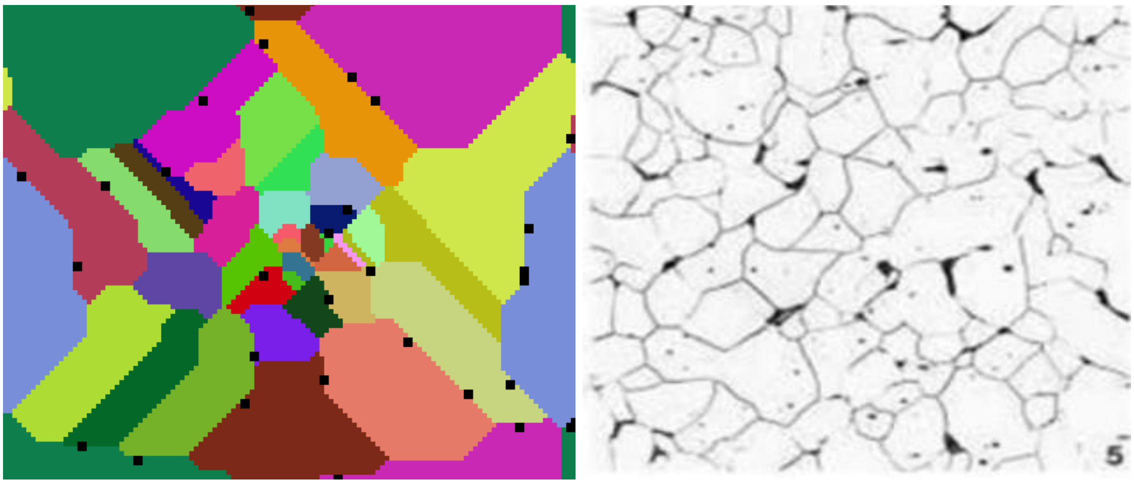
Picture 3 – Exporting visualization to .bmp file

Lab 3: Modification of cellular automata grain growth algorithm - inclusions

The third part of the project was to implement generating inclusions. The inclusions are treated as cells that are not empty, but does not belong to the grain. Inclusions can be added both Before and After Grain Growth and may have an user-defined shape (square or circle) and size.



Picture 4 – Generated microstructure and microstructure of austenitic stainless steel 00H17N14M2



Picture 4 – Generated microstructure and microstructure of austenitic stainless steel AISI/SAE 1010

This is a comparison (picture 4 and 5) of real microstructure and generated by developed application. It could be similar to real microstructure but that depends on how accurate is the written algorithm.

Lab 4: Modification of CA grain growth algorithm - influence of grain curvature

Unfortunately I've not been able to create that part of the Project.

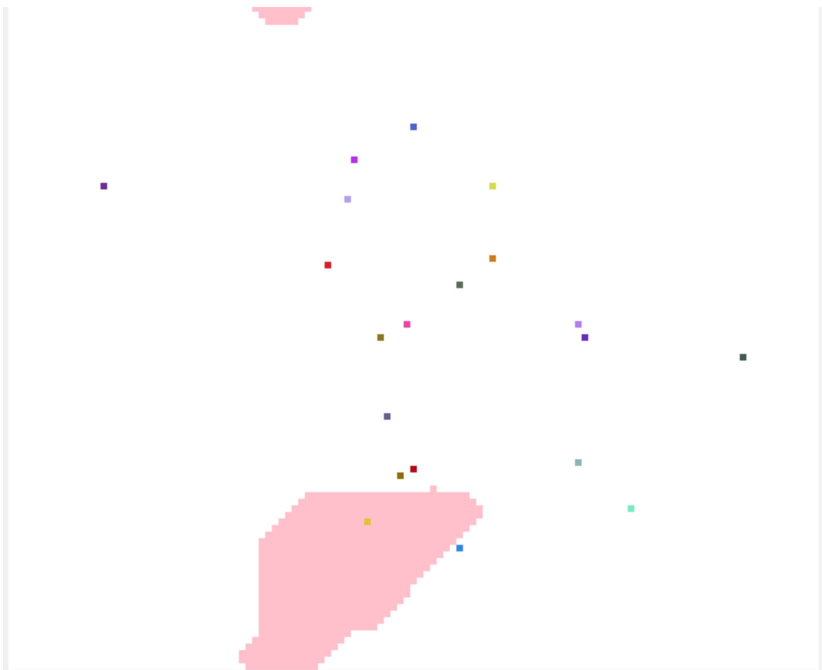
Lab 5: Modification of CA grain growth algorithm - substructures CA

During the implementation, there were some problems with adding this functionalities. However, it works, at least partially.

Picture 6 – Substructure CA -> CA

Picture 7 – Substructure Dual Phase CA -> CA

As a result of encountered problems, it's not fully working – the substructures are generated correctly (Pictures 6 and 7) but I'm not able to rerun the naïve growth with them (Picture 8)

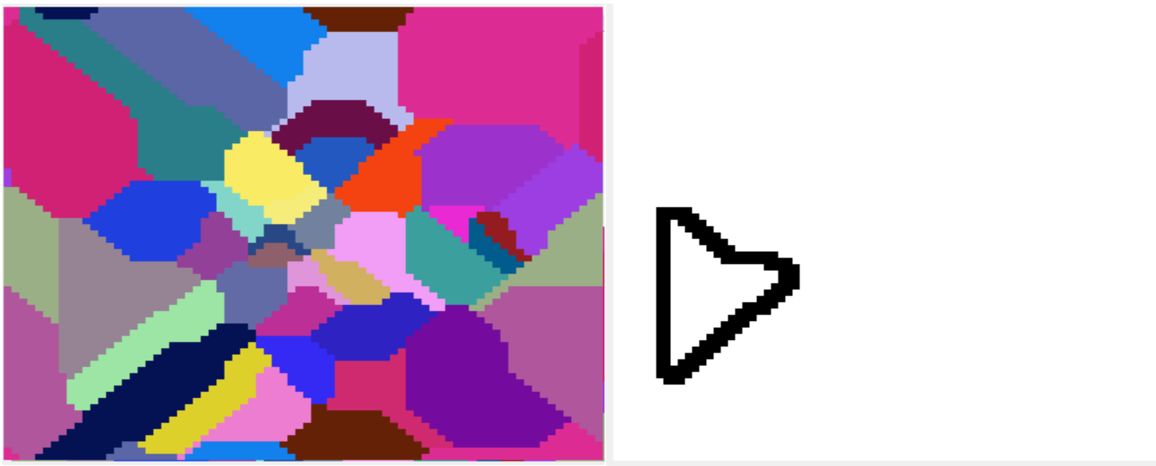


Picture 8 – Substructure "prepared" to rerun.

Lab 6: Modification of CA grain growth algorithm – boundaries coloring

The last part was to display only grain boundaries of generated mictrostructure. The grain boundaries can have different thickness – it's changeable by clicking again the grain boundaries button. Below, it's a comparison of visualization, all grain boundaries and the real steel – HSLA (Picture 9). It could be noticed that there is some similarity between simulation and real steel. Picture 10 shows the only one grain boundary.

Picture 9: Microstructure generated using Moore neighborhood and all grains boundaries, compared with Steel HSLA



Picture 10: Microstructure generated using Moore neighborhood and only one grain boundary

Conclusion

A cellular automata is a collection of colored cells on a grid. The final shape of microstructure depends on chosen neighborhood, number of grains and arrangement of them. It is possible to get different results by using various rules and combinations of options mentioned above.

It is easier to understand grain growth, when it is possible to see simulation of it, how it could look. Of course, it's not perfect visualization but the whole generated structure can be treated as a very loose approximation of a real structure.