AGH

UNIVERSITY OF SCIENCE AND TECHNOLOGY CRACOW

Metals Engineering and Industrial Computer Science

Multiscale Modelling 1st Report:

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Repository:	**https://github.com/FabiolaDabros/MultiscaleModeling**
Course:	**Multiscale Modelling**

1. Technology

The application was created using Java, which is a high-level programming language. Java is class-based, object-oriented and designed to have as few implementation dependencies as possible.

Advantages	Disadvantages
- Simple (automatic memory allocation and garbage collector) - Object-oriented - Platform-independent - Multithreaded - Stack allocation system	- Slower and more memory-consuming than natively compiled languages - No unsigned types - No control over garbage collector - No support for low-level programming

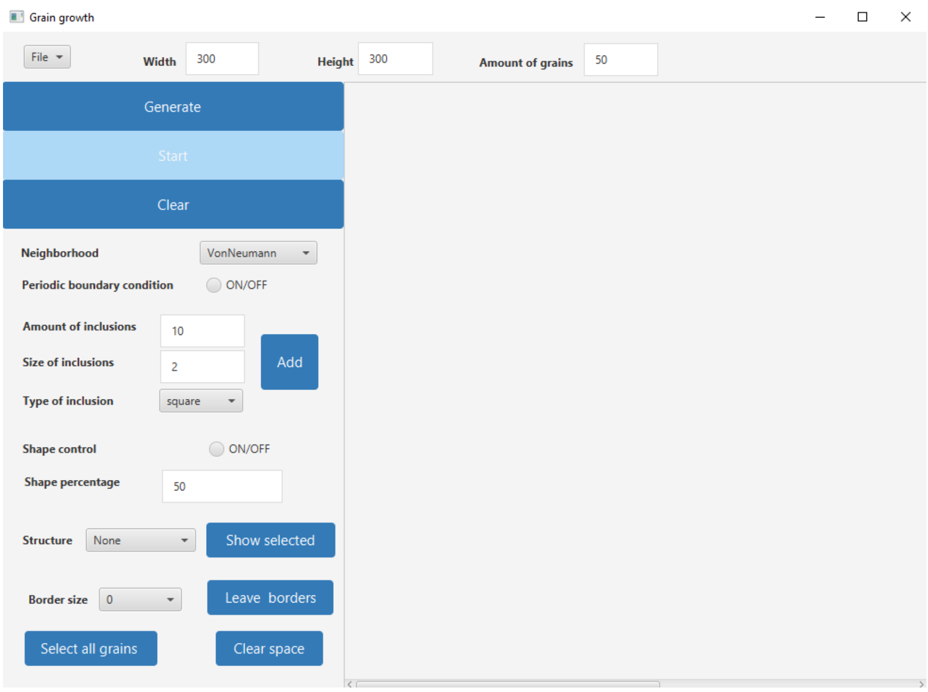
Tab1. Advantages and disadvantages of Java.

The Graphical User Interface was implemented with the JavaFX library, which is a very powerful tool to make GUI based java applications. It can run on cross platform environments and support a different language called FXML, which is only used to define the interface of an application, keeping it completely separate from the code logic.

I have also used IntelliJ Idea and Git VCS.

2. Graphical User Interface

The picture 1 presents the main window of the application.

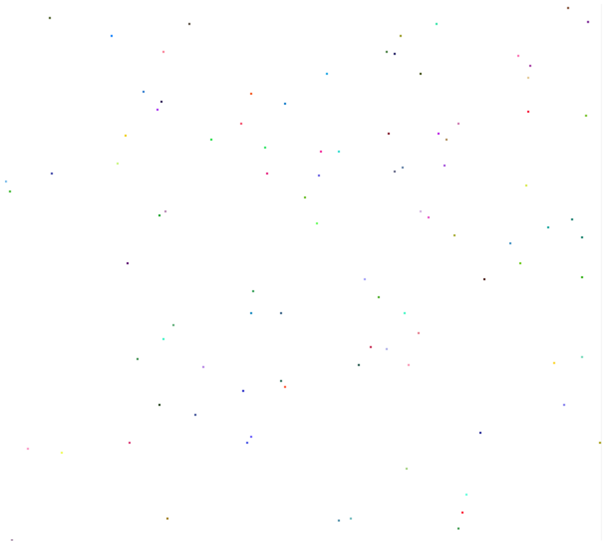


Picture 1. Graphical User Interface - main application window.

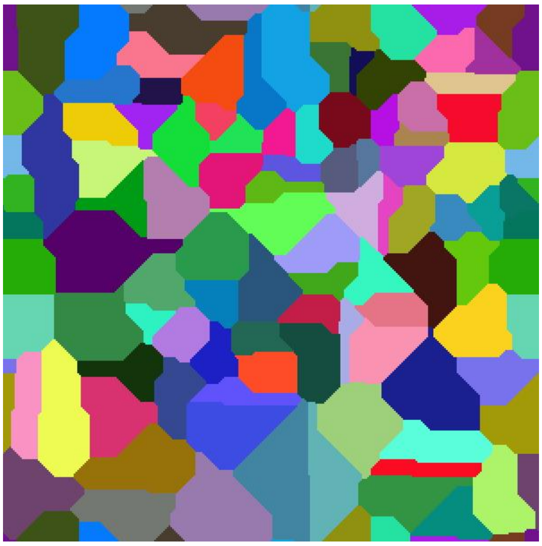
The main window of the application allows the user to make a lot of actions, which are described below. On the empty space appears generated image of the microstructure.

2.1 Simple grain growth CA

To make simple grain growth using Cellular Automata method the user has to set the dimension of the grid by entering width and height data. The minimum size is 300x300 but the user can also define rectangular grid. Another component is a textfield that allows to insert different number of nucleons, which are placed randomly. Next, the user has to choose the type of the neighborhood from the combobox. There is VonNeumann neighborhood, which looks for 8 neighbors around the grain and Moore neighborhood, which looks for 4 nearest neighbors. The last step is optional – the user can check periodic boundary condition. After setting all of the options the user has to press "Generate" button to generate random positions of nucleons and "Start" button to start the process of growth. There is also "Clear" button which allows the user to clear the grid. Pictures 2 and 3 show results of these actions.



Picture 2. Nucleons placed randomly.



Picture 3. Microstructure with periodic boundary condition and VonNeumann neighborhood.

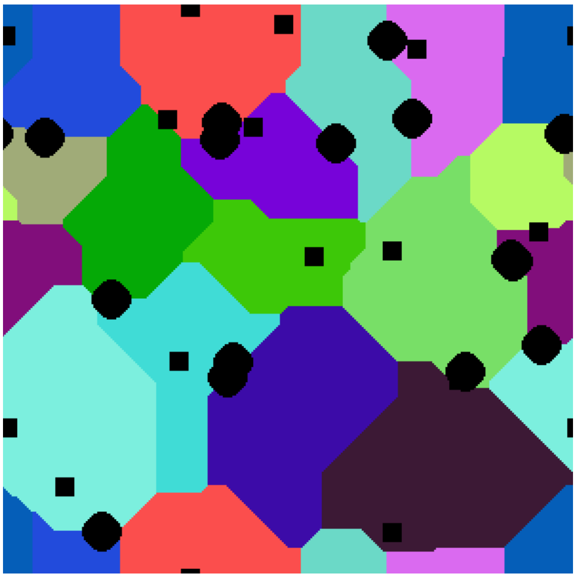
2.2 Microstructure import/export

Another feature is import and export of generated microstructure as a text or bitmap file. After clicking "File" button, which is placed at the top of application, user can select one of these options. After that appears a file dialog that allows the user to choose a file from the file system or to find a place where the user can save generated microstructure.

2.3 Inclusion

The next group of components is responsible for inclusion creation. The user has to choose the type of inclusion: circle or square, the size of inclusions and the amount of inclusions. There are also two times of creation – at the beginning of simulation or after the simulation. The first option is adding inclusions in random places, whereas the second option is adding them on the grain boundaries. Pictures 4 and 5 show different options of inclusion creation.

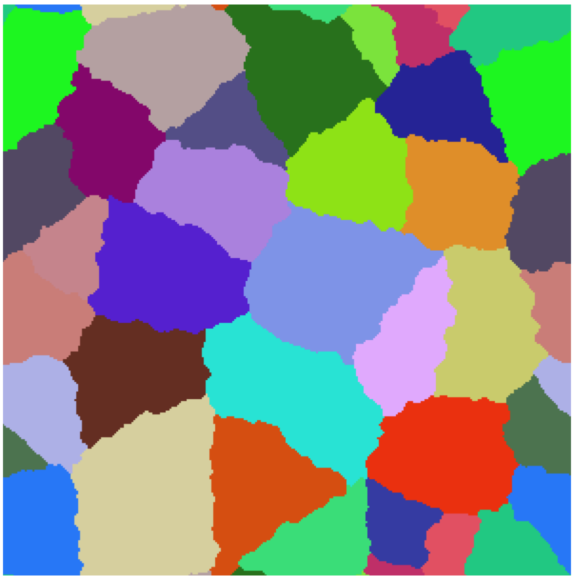
Picture 4. Microstructure with square inclusions added at the beginning.



Picture 5. The same microstructure as at picture 4. with circle inclusions added after simulation.

2.4 Control of grain boundary shape

The user can use this feature after turning on the “Shape control” option with certain percentage of probability. This option is related to the extension of Moore neighborhood. The algorithm goes through the 4 rules which check the Moore neighbors, the nearest Moore neighbors, the furthest Moore neighbors and at the end if none of these three rules are completed, the shape is determined by global probability defined by the user. Pictures 6 and 7 show microstructures generated with different percentage of probability.



Picture 6. Microstructure with 15% shape control.

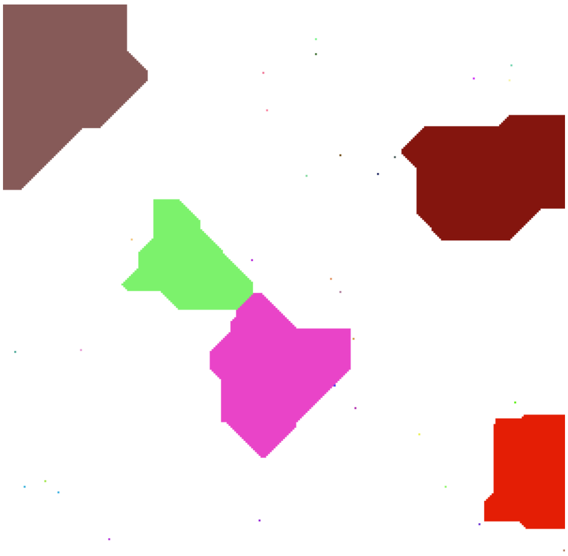
Picture 7. Microstructure with 90% shape control.

2.5 Different microstructure type

When the process of growth is finished, the user can choose the type of structure – substructure (selected grains are separated – they have different ids and colors) or dual phase (selected grains are united – they have the same id and color). After that the user has to select unlimited number of grains by clicking on them. What is more, the user can unselect selected grain by clicking on this grain again. When the user selects all the grains which he wants, he has to press the “Show selected” button which makes the non selected grains deleted. After that the user can start the process of growth again. Pictures 8, 9, 10, 11, 12, 13, 14 and 15 show the full process of creating substructure and dual phase.

Picture 8. Microstructure after grain growth.

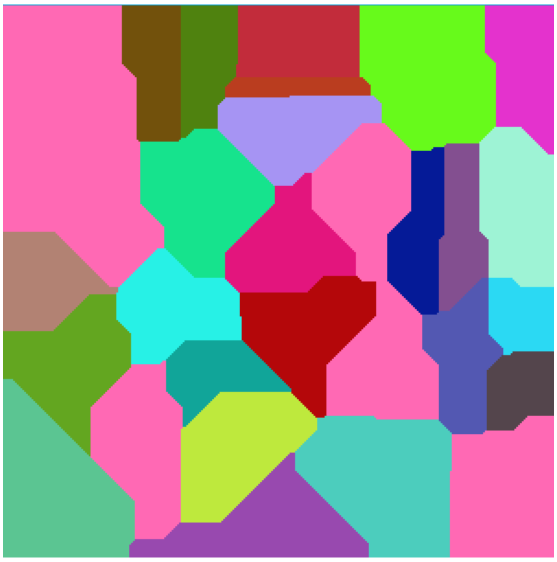
Picture 9. Selected grains for substructure.



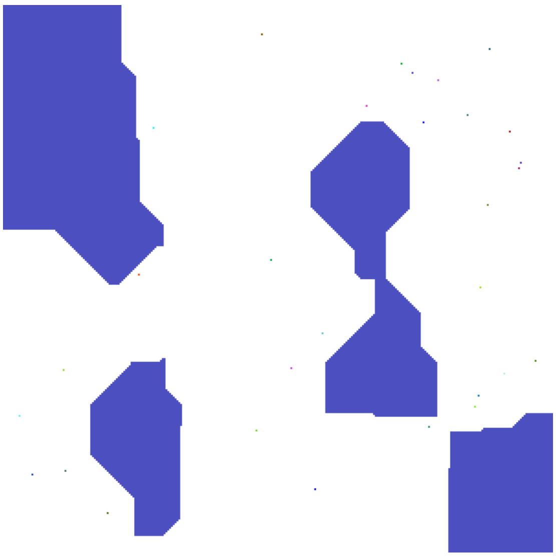
Picture 10. Substructure before regrowth.

Picture 11. Substructure after regrowth.

Picture 12. Microstructure after grain growth.



Picture 13. Selected grains for dual phase.

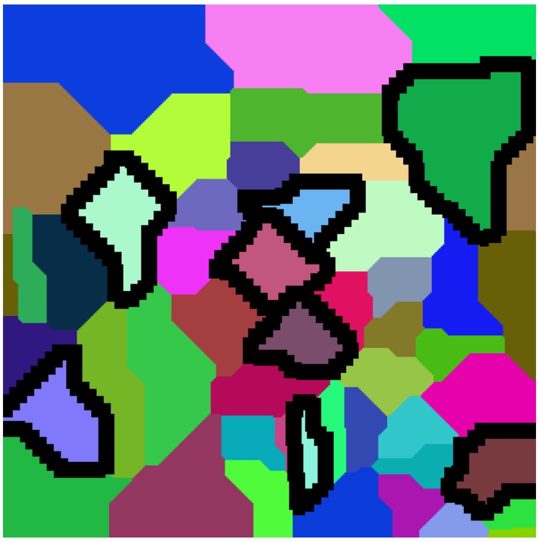


Picture 14. Dual phase before regrowth.

Picture 15. Dual phase after regrowth.

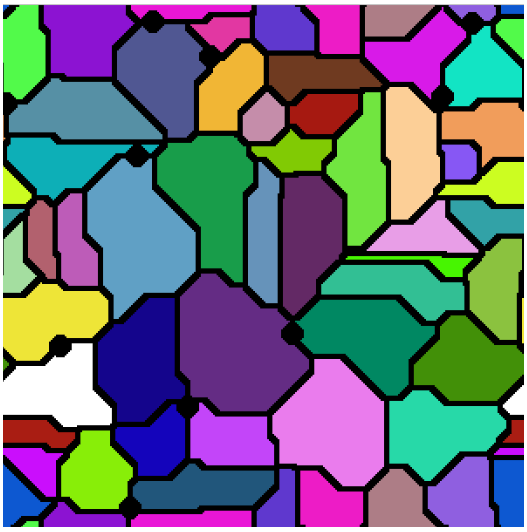
2.6 Grain boundary selection

The last feature allows the user to leave only the boundaries of each selected grain of the microstructure. To start this process the user has to select the borders size from the combobox and then click the “Leave borders” button. If the user wants to select all of the grains he can press the “Select all grains” button. After that it is possible to clear all colors from the microstructure and leave only black boundaries and inclusions. The user can also read the information about the percentage of covering the grid. Pictures 16, 17, 18, 19 show the result of grain boundary selection.

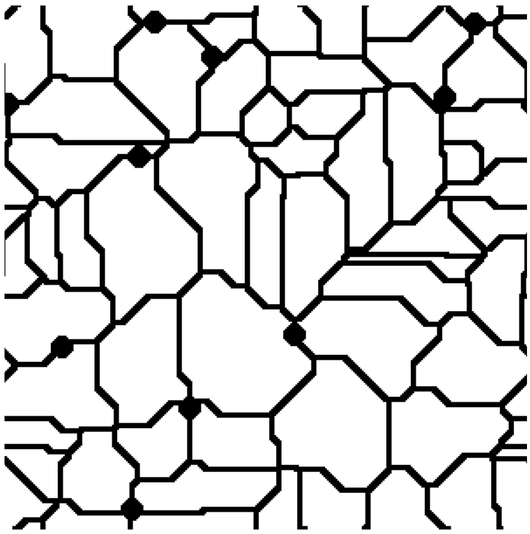


Picture 16. Microstructure with borders (4th size) on selected grains before cleaning the colors.

Picture 17. The same microstructure as at picture 16. after leaving only boundaries, which cover 15,02% of the grid.



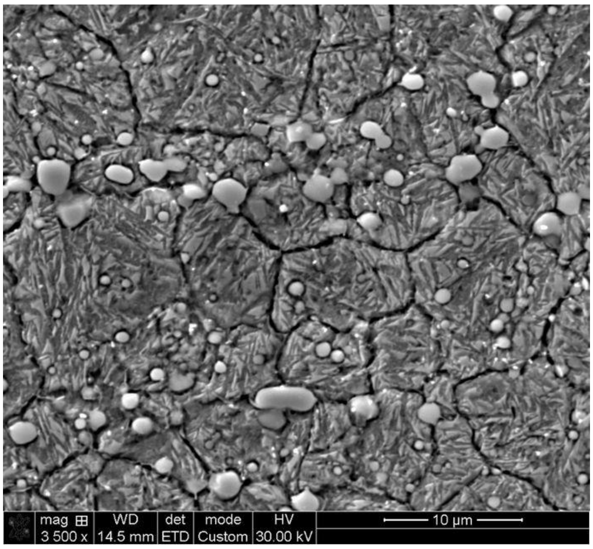
Picture 18. Microstructure with inclusions and borders (1th size) on all of the grains before cleaning the colors.



Picture 19. The same microstructure as at picture 18. after leaving only boundaries and inclusions, which cover 17,74% of the grid.

3. Summary

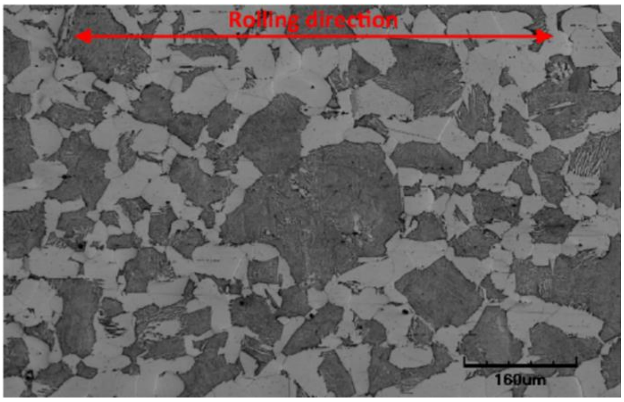
The application allows the user to generate many different microstructures. In fact, the real-life microstructures are very similar to them. Pictures below show the comparison between the program results and genuine microstructures.



Picture 20. Microstructure of high speed steel [1].

Picture 21. Microstructure with circular inclusions added before and after simulation.

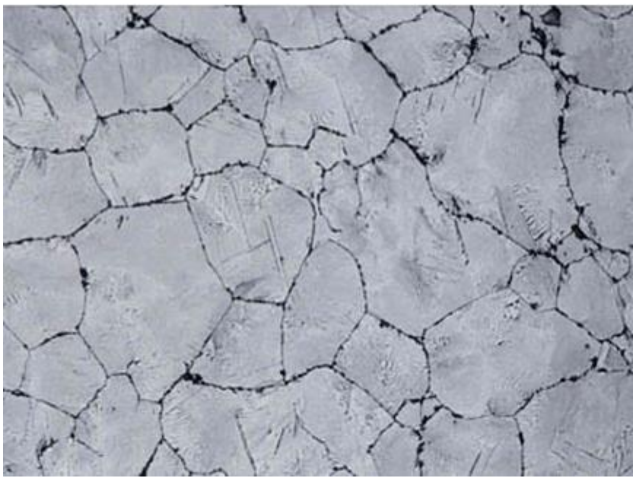
Picture 21. was generated by using VonNeumann neighborhood with inclusions added before as well as after the growth process. We can conclude that presented structures are very similar. The microstructure clearly present circular inclusions and what is more grain boundaries are clearly marked in both cases.



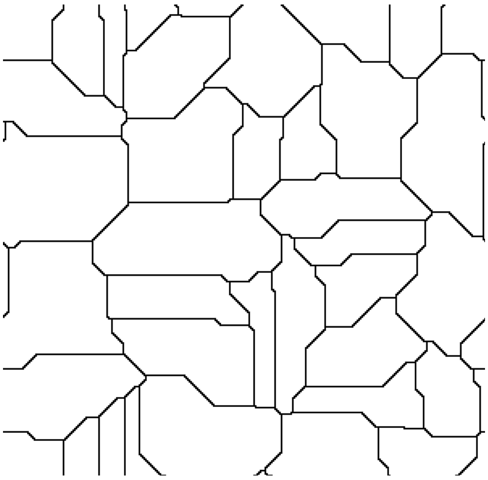
Picture 22. Microstructure of dual phase steel [2].

Picture 23. Dual phase after regrowth.

Picture 23. was generated with the dual phase option. I have selected same grains and then I have started the growth process again. The likeness to the real-life structure is marvelous.



Picture 24. Microstructure of cementite during cooling from hot rolling [3].



Picture 25. Microstructure after process of grain boundary selection.

Picture 25. was generated with the grain boundary selection. I have selected all of the grains and then I have selected the smallest borders size. The generated microstructure is very similar to the genuine microstructure.

4. References

[1] http://www.ur.edu.pl/wydzialy/matematyczno-przyrodniczy/jednostki-organizacyjne/centrum-innowacji-i-transferu-wiedzy-techniczno-przyrodniczej/struktura-centrum/1-laboratorium-technologii-materialow-dla-przemyslu/1-2-pracownia-mikroskopii-elektronowej-i-preparatyki

[2] https://www.researchgate.net/figure/Microstructure-of-the-dual-phase-steel_fig1_272050203

[3] http://www.georgevandervoort.com/revealing-prior-austenite-grain-boundaries-in-heat-treated-steels-article/