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Multiscale Modelling – 1st report

Introduction

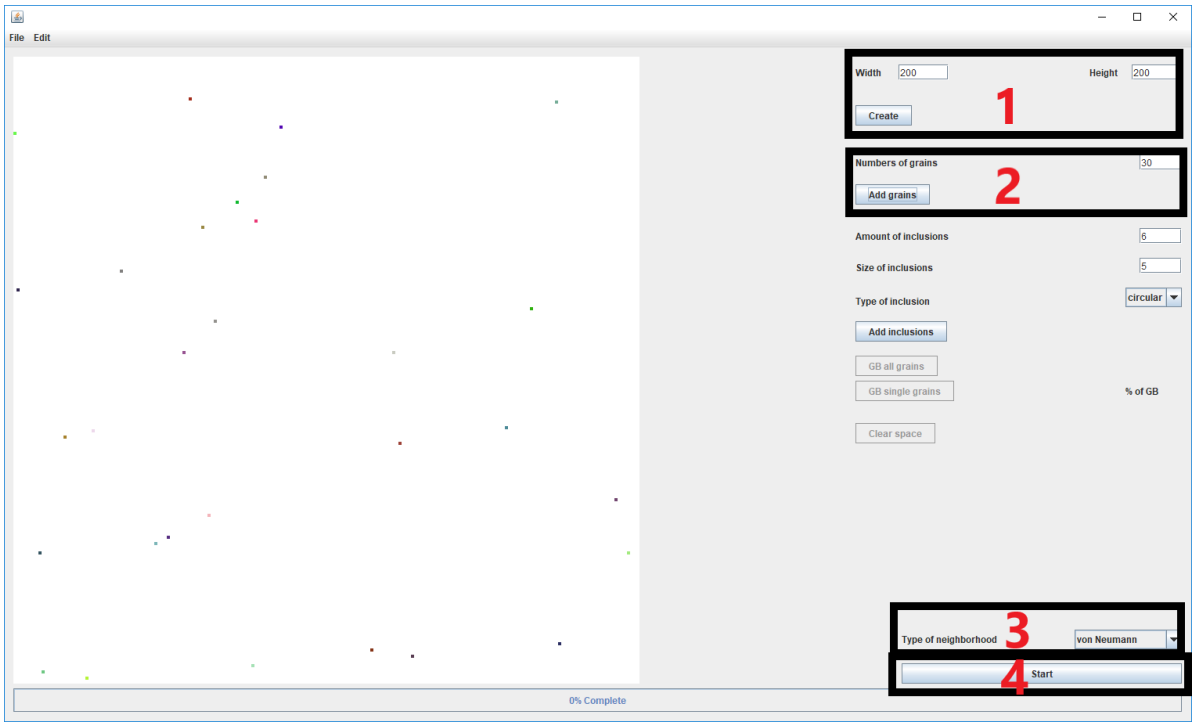
Simple grain growth was implemented by using CA (Cellular Automata). Cellular Automata is a discrete model studied in computer science, mathematics, physics and microstructure modelling. A CA is a model of a system of cell objects with the following characteristics:

- Grid – space where cells live. In this project used 2D though a cellular automaton can exist in any finite number of dimensions.
- Each cell has a state. The number of state possibilities is typically finite. The simplest example has the two possibilities of 1 and 0. In this project used much more possibilities.
- Each cell has a neighbourhood. Neighbourhood describes the closest neighbours of a particular cell. This can be defined in any number of ways. Examples of neighbourhoods types: Von Neumann, Moore, Pentagonal random, Hexagonal random.

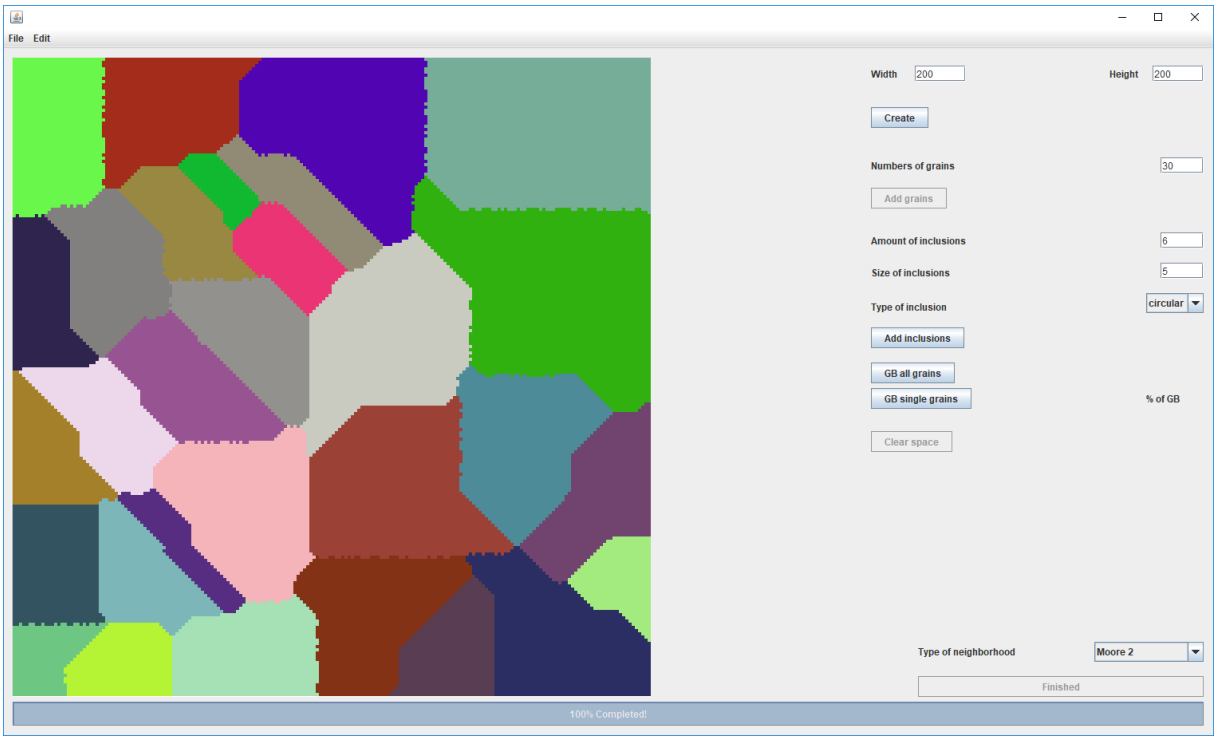
The simulation of simple grain growth was implemented in Java using NetBeans IDE. GUI was created using Java Swing (lightweight GUI toolkit).

First functionality – simple grain growth

User can choose parameters to generate structure. User has to set width and height of grid (**1**) which is display on the panel on the left side of the main window. User can set number of grains and add it by pressing button (**2**) or by clicking on the simulation panel. User can set type of neighbourhood (**3**). It is possible to choose Von Neumann or Moore. In order to run simulation need to click Start button (**4**) It see on the **picture 1**.



Picture 1: Main window, setting up size, adding grains, choosing type of neighbourhood.

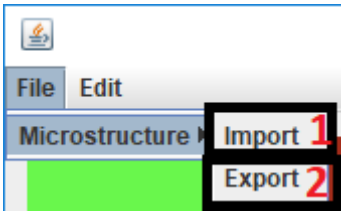


Picture 2: Completed grain growth simulation.

Picture 2 shows the completed grain simulation of the growth of Moore's neighbourhood.

Second functionality – microstructure import/export

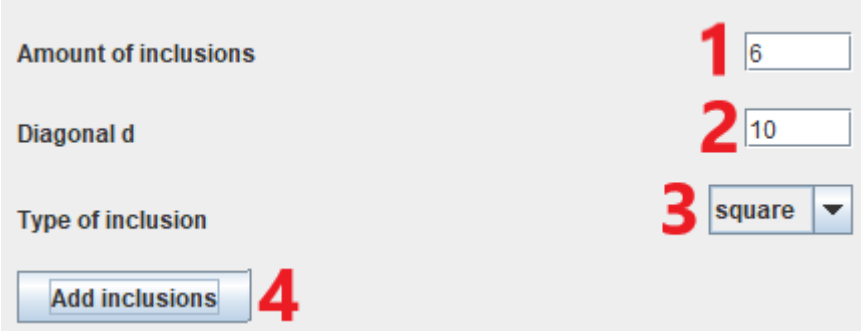
Picture 3 shows how user can import microstructure from text file or BMP file(**1**). Also user can export microstructure to text file or BMP file (**2**).



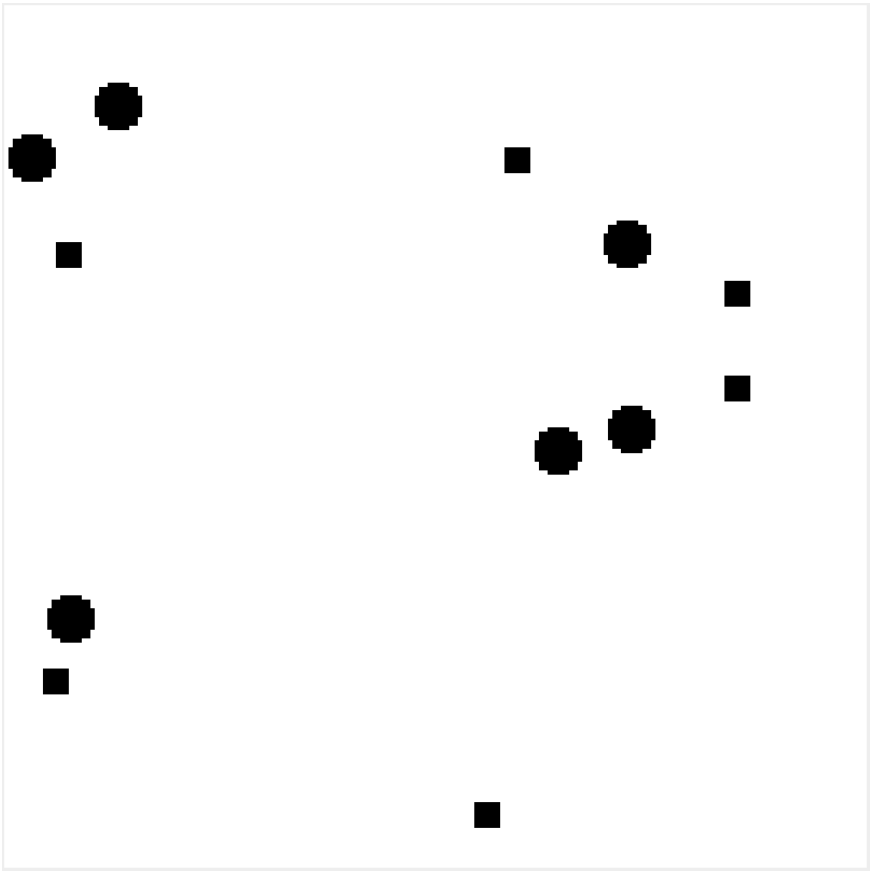
Picture 3: Import/Export.

Third functionality – inclusions

As you can see from the **picture 4** below, in order to add inclusions user has to enter amount of inclusions (**1**), size of inclusions(if type of inclusion is square it is diagonal and if type of inclusion is circle it is circle) (**2**), type of inclusion (square or circle)(**3**). And then click Add inclusions button (**4**).



Picture 4: Inclusions parameters.



Picture 5: Inclusions at the beginning of simulation.

Picture 6: Inclusions after simulation.

Inclusions added after simulation are located on the grain boundaries.

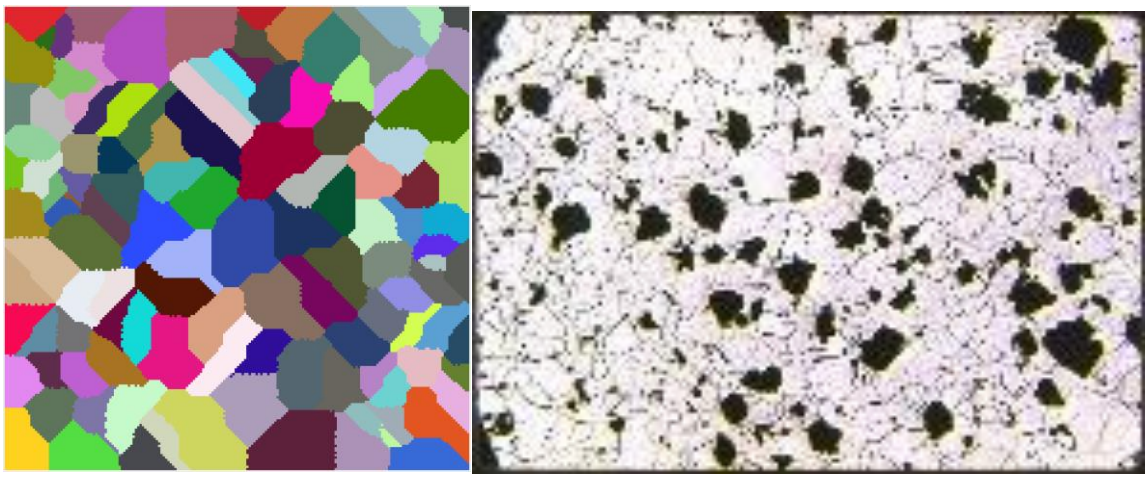
Fourth functionality – boundaries coloring

User can select grain boundaries in two ways presented in the **picture 7** below: all grains (**1**) or single grain (**2**). And then click Clear space button to clear space (**3**).

Picture 7: Boundaries coloring parameters.

Comparison

The following **picture 8** presents a comparison of the microstructure created in the program and the microstructure of a malleable cast iron after conversion to nodular graphite. The growth in the created application is not as accurate as the real one. The microstructure created in the program has a lot of grains in different colors and identifiers.



Picture 8: Comparison of the real microstructure with the microstructure from the program. (Source: https://www.georgesbasement.com/Microstructures/CastIronsHighAlloySteelsSuperalloys/Lesson-1/Specimen03.htm)

Conclusions

In this report have presented software designed to implement simulation of the grain growth. The program is based on the cellular automata method. Cellular automata is algorithm that can implemented in many ways. It can be used in many of different areas such as computer science, mathematics, physics, biology, microstructure modelling.

The software has a lot of functionality such as microstructure import and export (TXT file, BMP file), two types of inclusion (square and circular), time of creation inclusion: beginning of simulation and after simulation (on grain boundaries) ,possibility of change size, two type of neighbourhood (Von Neumann and Moore).