Multiscale Modelling – Report no. 1

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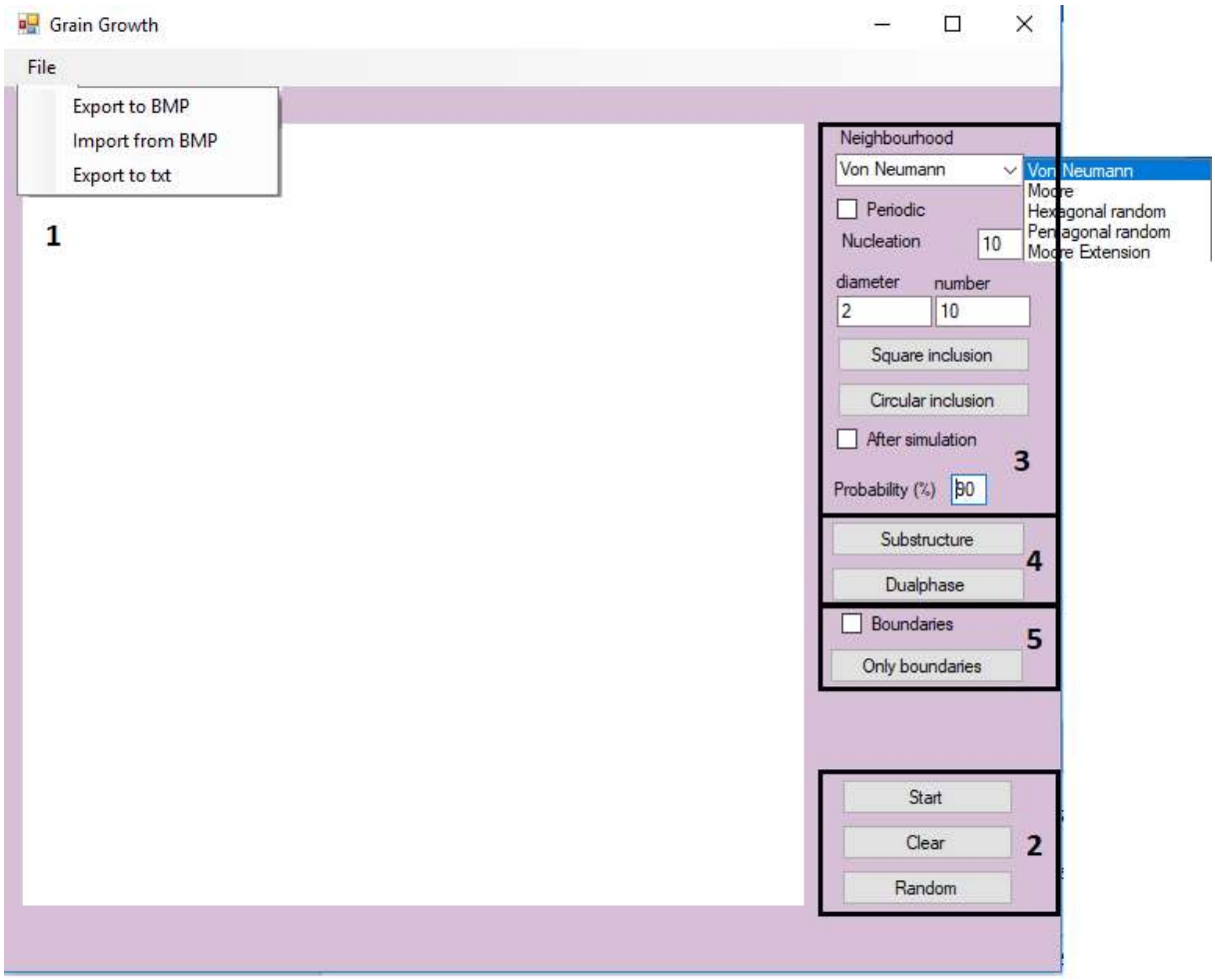
During the classes of Multiscale Modelling I was developing application using .NET Framework to simulate grain growth. It was written with C# language, and is based on cellular automata algorithms of grain growth. UI was built with Windows Forms, and it contains standard Windows controls in order to provide intuitive usage. In next part of this report I will try to present you briefly user interface and functionality of my program on screens and example results of grain growth.

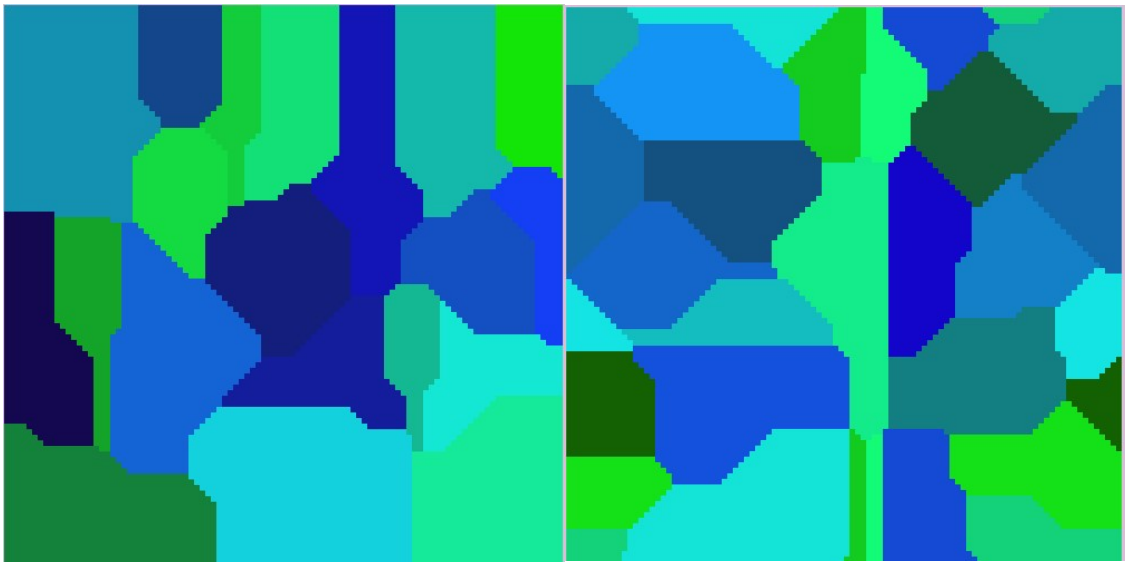


Picture 1 – Main window of application

You can divide main window of application to sections. Description of every section is below.

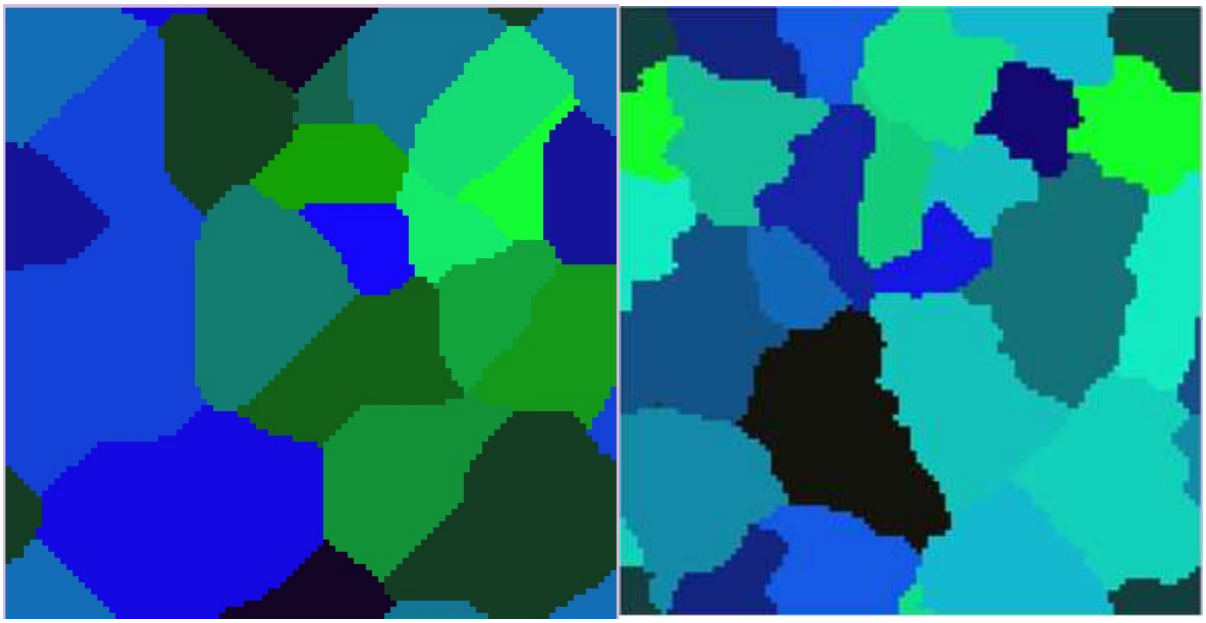
1. PictureBox which will be showing result of grain growth.
2. Buttons to start simulation, clear window and prepare seeds to grow.
3. Part when you can adjust parameters of simulation. You can choose neighbourhood, type of boundary condition (periodic), nucleation, inclusion (and types of inclusions).
4. After every simulation you can choose between Substructure or Dualphase
5. Buttons to operate grains boundaries.

Examples are the best to show the functionality of application. In next part of this report, you can see screens of ended simulations.



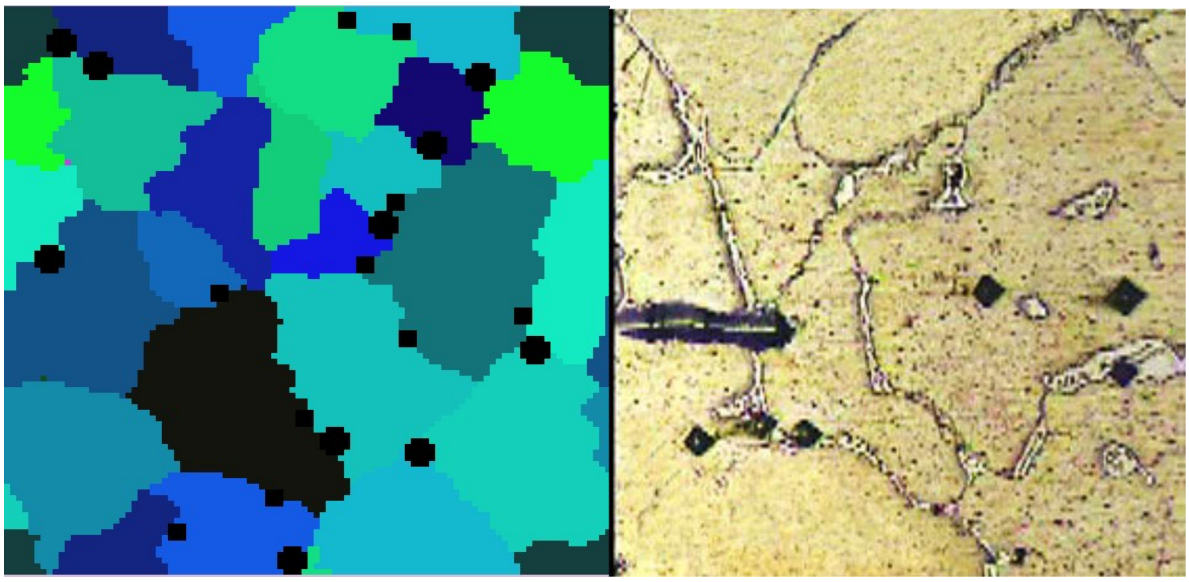
Picture 2 Normal and periodic

Picture 2 shows difference between normal and periodic boundary conditions. Simulations where done with 20 nucleons and Von Neumann neighbourhood.



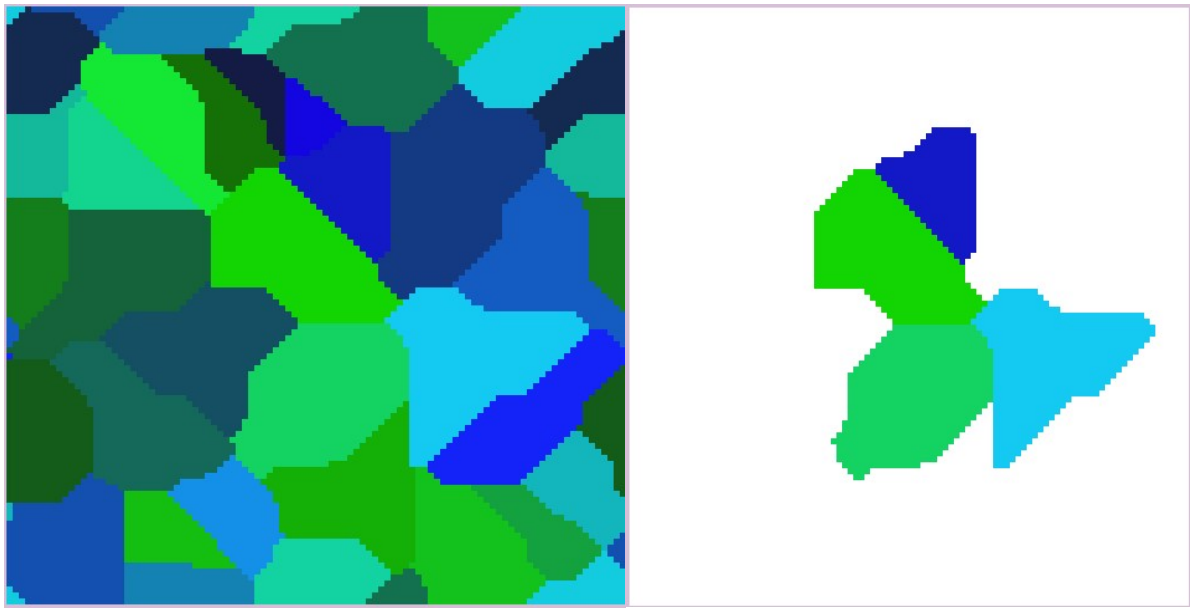
Picture 3 Extended Moore neighborhood

In the picture no. 3 you can see the difference between 20% and 80% probability for rule 4 with extended *Moore* neighbourhood. Picture above confirms that even slight parameter changes have a big impact on the final structure.



Picture 4 Microstructures with inclusions

Picture 4 shows example with generated microstructure containing 20 nucleons and circular and radius inclusions on grain boundaries. Neighborhood used in this simulation was moore extension. On the other side you can see real microstructure of austenitic matrix and network of sigma phase precipitation on grain boundary from Cr-Ni steel[1]. Inclusions similar to examples above can lead to very early failure of high-temperature parts.
You can add inclusion before simulation by clicking Square or Circular Inclusion (you can change Diameter and number of Inclusion)

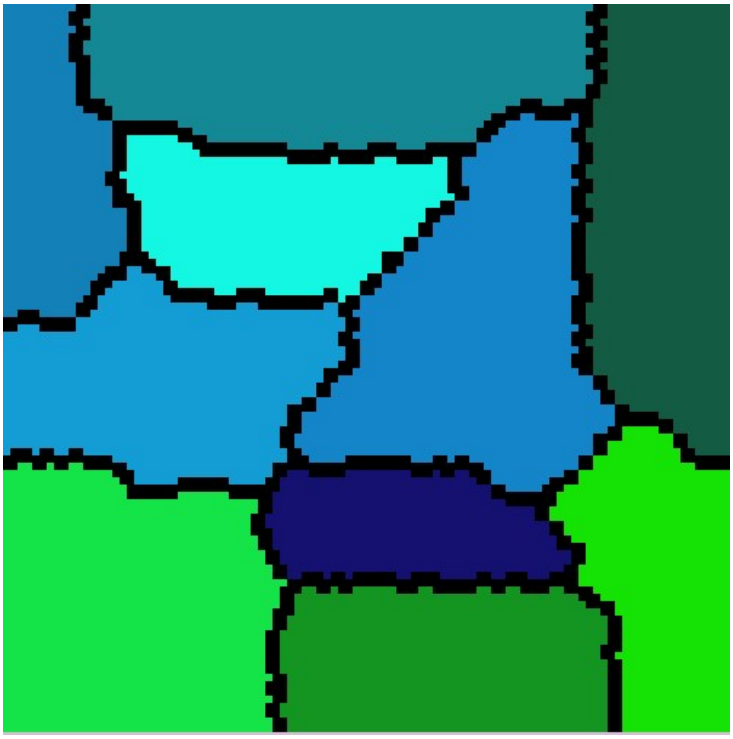


Picture 4 Substructure

After you generate microstructure, click on button Substructure and mark with mouse (by clicking) on grains. Next click on substructure button will clear others grains and clicked before stays. You can generate new microstructure.

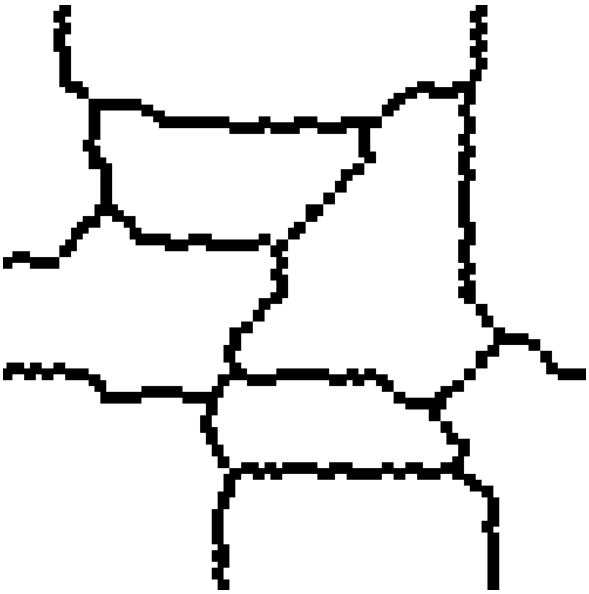
Picture 5 Dualphase

After you generate microstructure, click on button Dualphase and mark with mouse (by clicking) on grains. Next click on substructure button will clear others grains and clicked before stays but change colour. You can generate new microstructure.



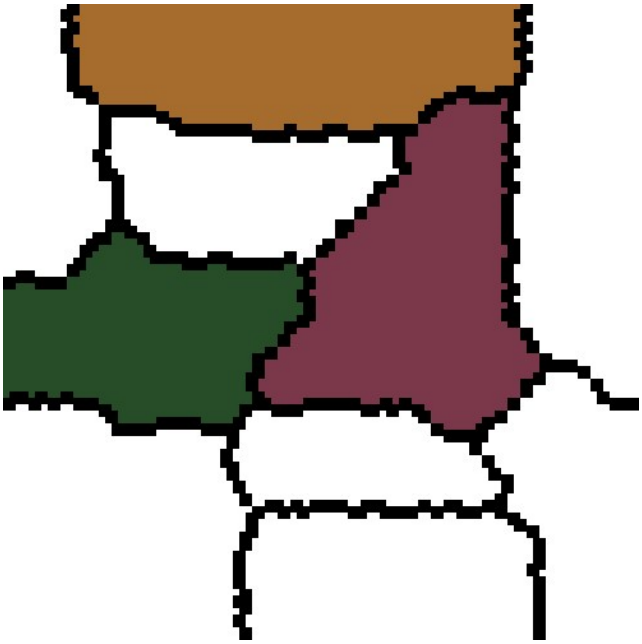
Picture 6 Grains boundaries

Before you generate new microstructure You can mark Boundaries – it will mark in black grains boundaries.
By clicking on Only boundaries button and mark boundaries (click mouse on it) and click again on button space will clear and you can see only grains boundaries



Picture 7 Only grains boundaries

By clicking mouse you can add new nucleons (or click random). They will generate but will be blocked by grains boundaries from previous generated microstructure.



Picture 8 New microstructure blocked by grains boundaries