Multiscale Modelling – Second report

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Introduction

This application has been expanded for creating microstructure by using Monte Carlo method. New functionalities have been added to the interface. The program provides backward compatibility - the user can mix solutions form the first and the second part of the project. It is possible to create a part of the microstructure by simple grain growth and next expand by the newly added methods.

Interface

In Figure 1, we can see the main view of the interface. On the board, there are text boxes for customizing the process of simulation. Buttons are responsible for the run process and triggers additional actions. To the interface have been added new buttons conform to grain growth by Monte Carlo method and energy distribution.

New features:

- Grain growth by Monte Carlo method - every grain gets an energy, which is randomly set from the range set by user (Figure 1).
    - Field **State Count** lets the user enter a maximum range of energy which will be set for grains.
    - **MCS** field lets the user enter how many iterations will be set for the simulation run.
- Checkboxes **Energy inside** and **Energy on edges** with **Add energy** button allow to add points with zeroth energy (Figure 2 – black points).

- Energy Distribution – lets the user set a range for energy values in grains and boundaries with a 10% approximation error (Figure 3).

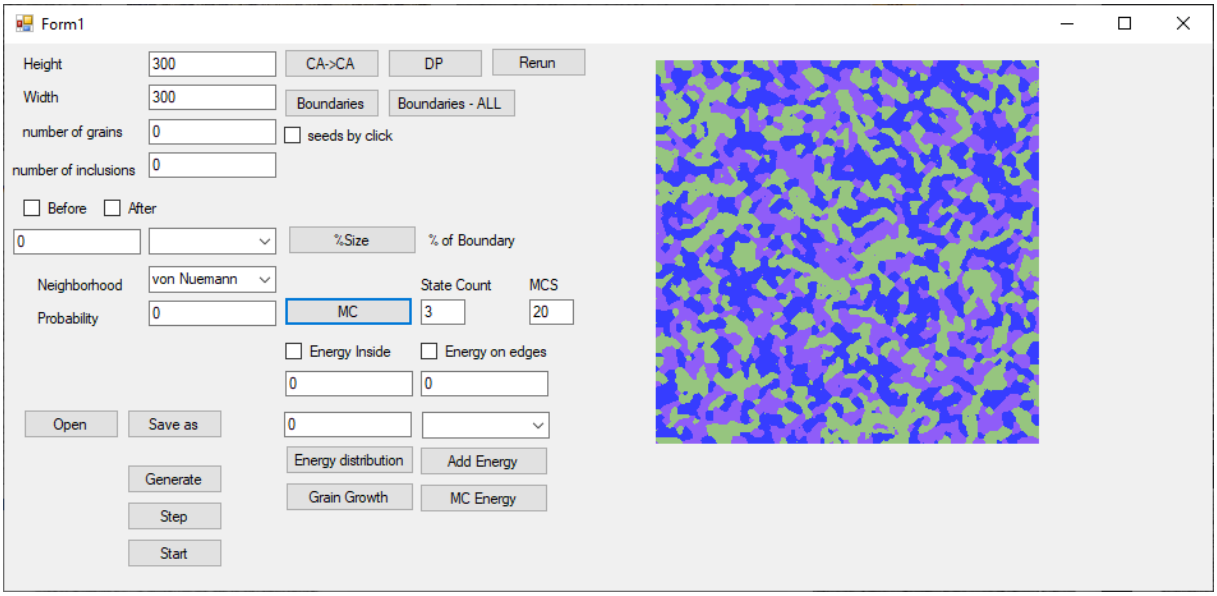

Figure 1 Created microstructure by using Monte Carlo

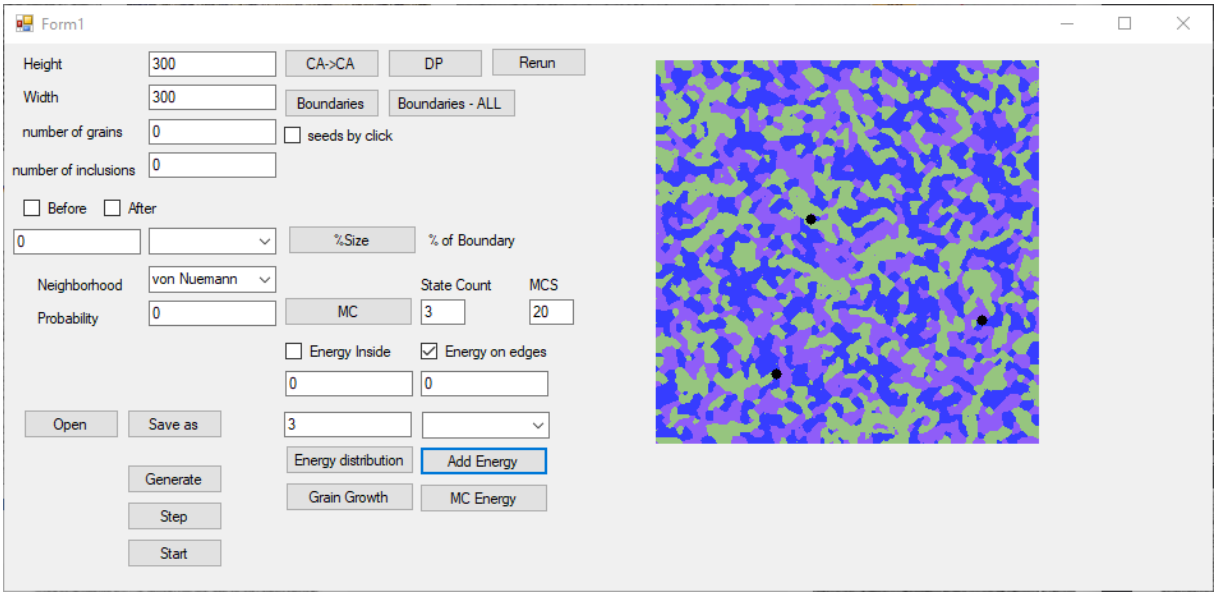

Figure 2 Added places with zeroth energy to microstructure

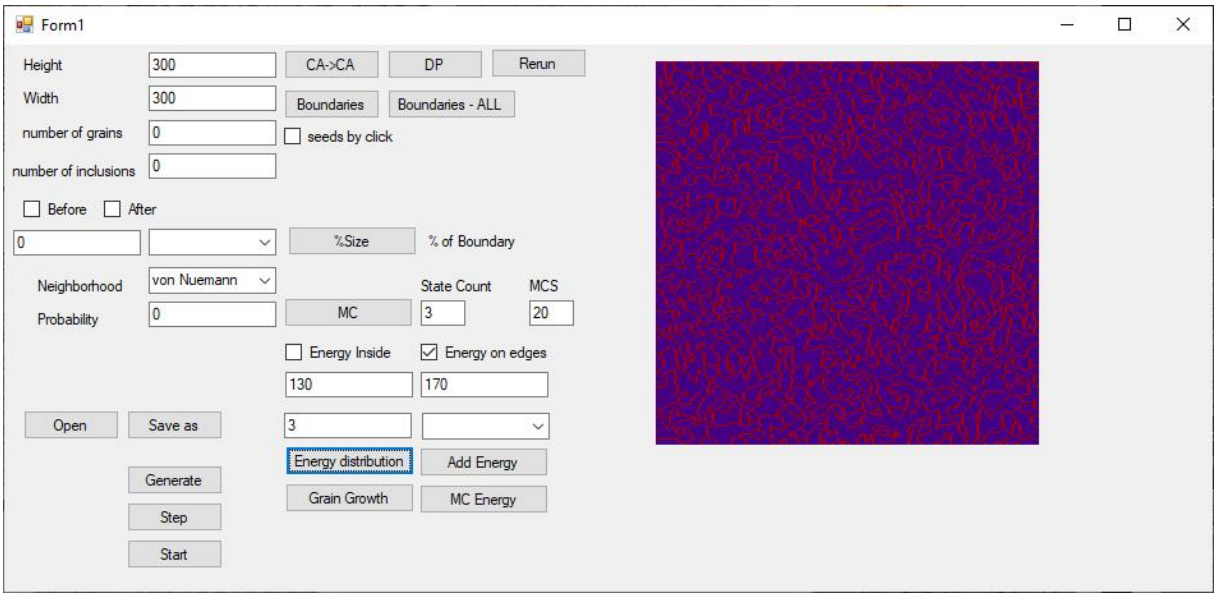

Figure 3 Energy distribution in microstructure

Figure 4 shows following scenario simulation:

First Part

1. 300x300 board size
2. Number of grains at the beginning of simulation = 30
3. Number of inclusions = 0

Second Part

1. Energy inside the grain = 90
2. Energy on the edge of grain = 160
3. State Count = 3
4. MCS = 20

Before execution second part, from the first simulation three, the biggest grains have been chosen as a dual-phase for the next simulation.

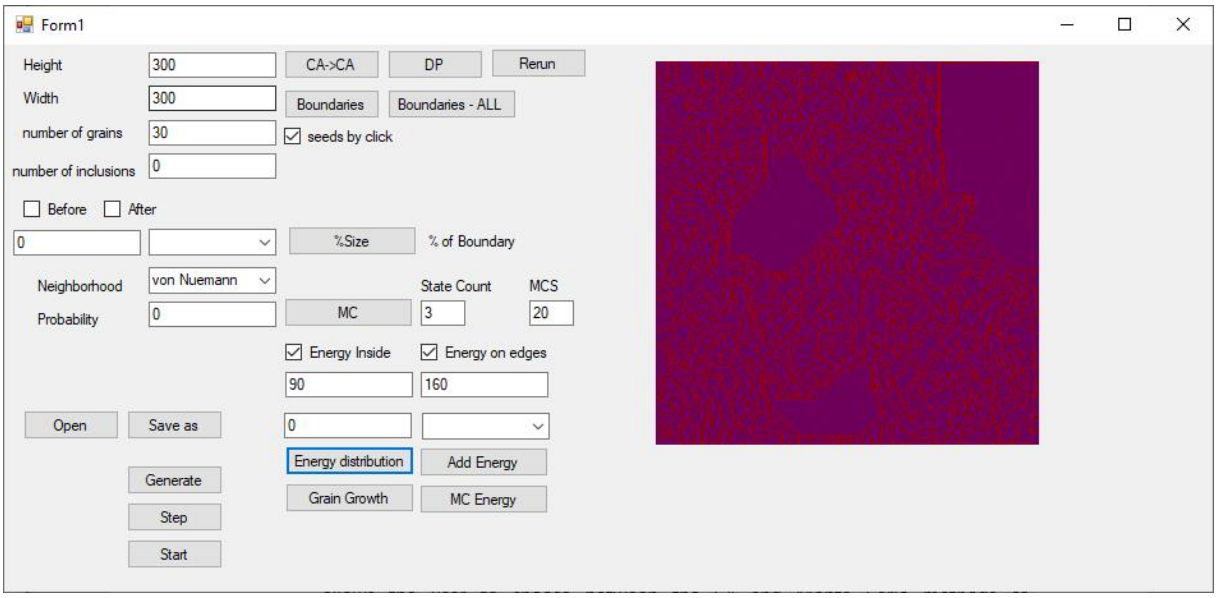

Figure 4 Example microstructure generated by application

What has been done

- Monte Carlo grain growth
- Dual-phase microstructure: CA -> MC or CA | MC -> CA or MC
- Energy distribution
- Nucleation

Comparison and conclusion

In comparison Figures 5 - 7 we can see that generated microstructure is similar to real. Shapes and sizes of grains are very close to real microstructure. For the analysis, the quality of the generated microstructure should be enough. Monte Carlo allows to generate more complicated shapes, which is more natural than Cellular Automata. Connection of both these methods can create more realistic structure. The biggest advantage of the Monte Carlo method is the possibility to create round shapes, more unpredictable which is not possible with Cellular Automata. Monte Carlo method in cooperation with Cellular Automata can create dual-phases areas with different shapes, with inclusions and surrounded grains by others.

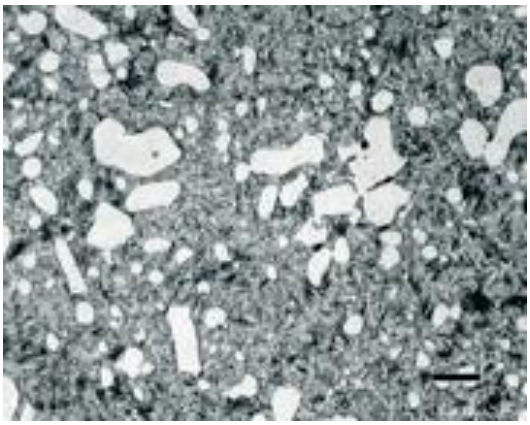

Figure 5 Microstructure of niolox-steel

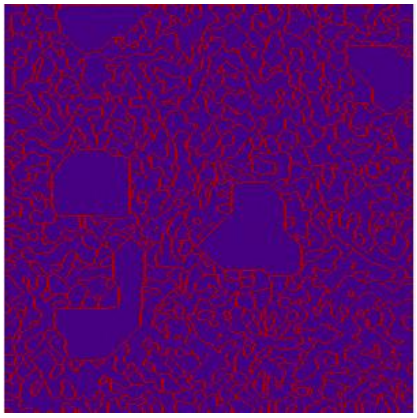

Figure 6 Generated microstructure by Monte Carlo

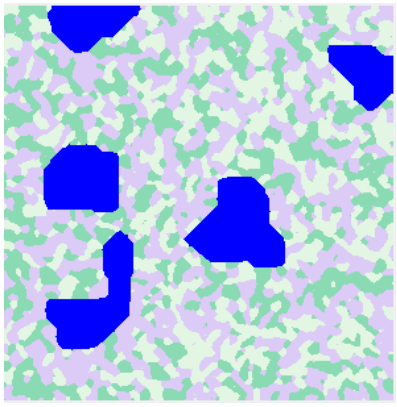

Figure 7 Generated microstructure by Monte Carlo – different view

Monte Carlo method has some disadvantages. First of all, it is impossible to control how many grains will be generated. Shape control is impossible. Monte Carlo method is much slower than Cellular Automata. The energy of the cell is counted randomly only once per simulation. The Monte Carlo method relies on random which is not good as a reference to draw conclusions. Because of uncontrolled grain growth, it is important to put many restrictions into simulation. To make proper research it is needed to add more information about structure, material and chemical composition. Unfortunately, this application does not allow to make simulation more realistic.

Overall, the application meets almost all the requirements except recrystallization which was not done because of wrong design core functions. Thanks to this application, it is possible to create a draft model of microstructure, which is very similar with realistic. For visual purpose this program is more than enough.