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Technical Computer Science

Multiscale Modelling report

Project: CA grain growth algorithm

1. Graphical user interface

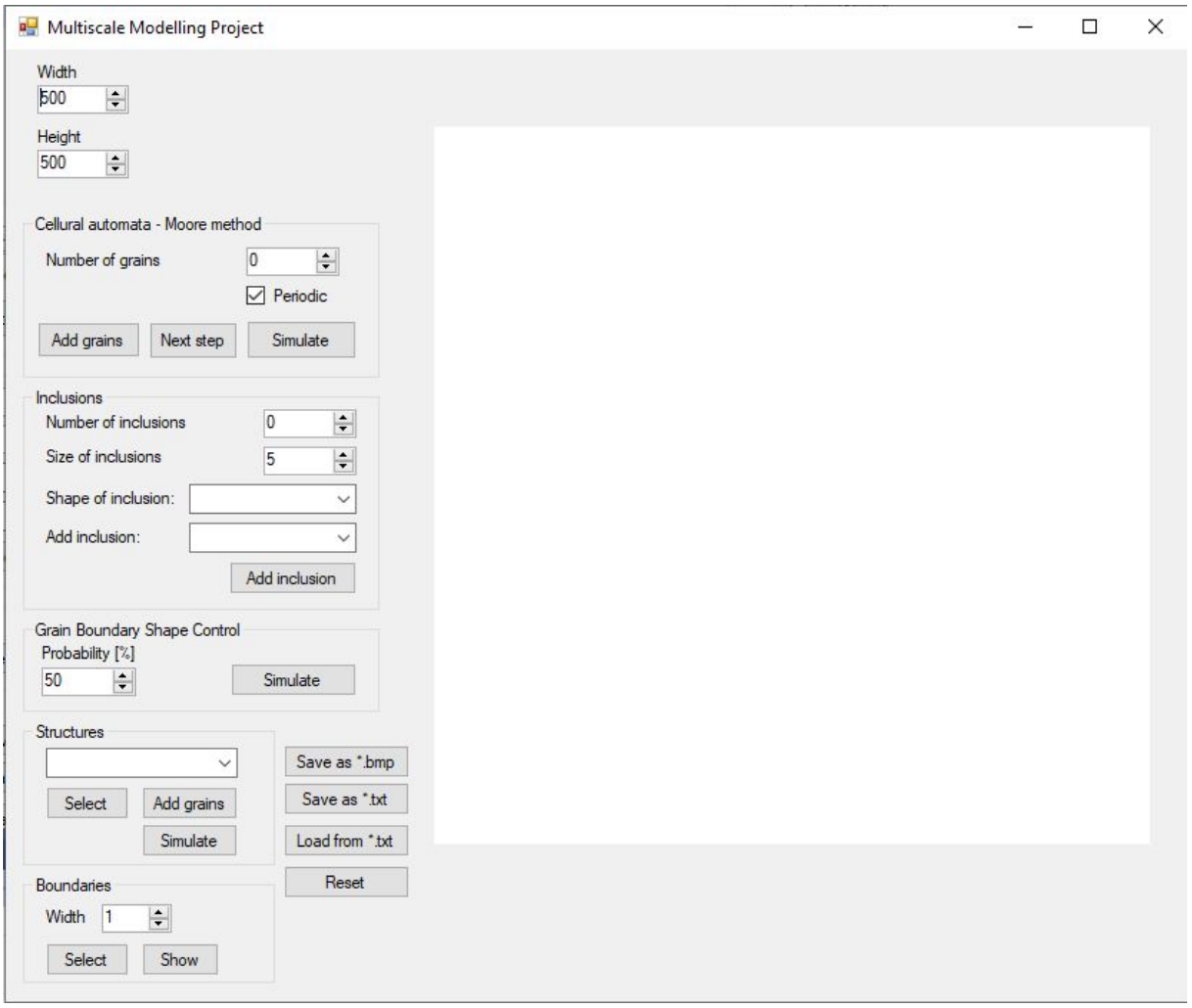

Figure 1. Application's window at startup.

- Width numeric up down – board's width (in pixels)
- Height numeric up down – board's height (in pixels)
- Number of grains numeric up down – defines number of new grains
- Add grains button – adds new grains
- Next step button – single step in cellular automata algorithm
- Simulate button – automated cellular automata algorithm

- Number of inclusions numeric up down – defines number of inclusion(s)
- Size of inclusions numeric up down – defines size of inclusion(s) (in circular inclusions – r; in square inclusions – a)
- Shape of inclusions combo box – defines shape of inclusion(s) (circle or square)
- Add inclusion combo box – defines where to add inclusions (randomly or on the grain boundary)
- Add inclusion button – adds inclusions on the board
- Probability numeric up down – defines probability for rule 4 in grain boundary shape control
- Simulate button – cellular automata algorithm with grain boundary shape control included
- Structure combo box – defines substructure or dual-phase for select button underneath
- Select button – selects grains to become dual-phase or substructure
- Add grains button – add grains for substructures
- Simulate button – simulates the substructure
- Width numeric up down – defines width of boundary
- Select button – select grains to show their boundaries
- Show button – shows boundaries of all grains
- Save as *.bmp button – saves board as bitmap
- Save as *.txt button – saves board as text file
- Load from *.txt button – loads board from text file
- Reset button – resets board's properties

2. Functionality

Application can generate various types of microstructure based on cellurar automata algorithm. Depending on arguments given to the program simulation can take few to several dozen seconds.

To define board's size you need to enter width and height and click reset button.

To start cellular automata algorithm you need to enter number of grains, click add grains button and then simulate. If you want to use grain boundary shape condition you need to enter probability and click simulate button beside it.

After the simulation you can add inclusions by selecting number, size, shape of inclusions and position of them then clicking add inclusions.

Dual-phase or substructures can be obtained by selecting one of them in structure combo box, then by clicking select and selecting grains on the board. After selection you need to click select button second time, then you can proceed with second grain growth.

To show boundary of specific grain you need to click on select button in boundaries group box, then on the grain(s) and click one more time on select button. To show boundaries of all grains you need to click show button.

3. Examples

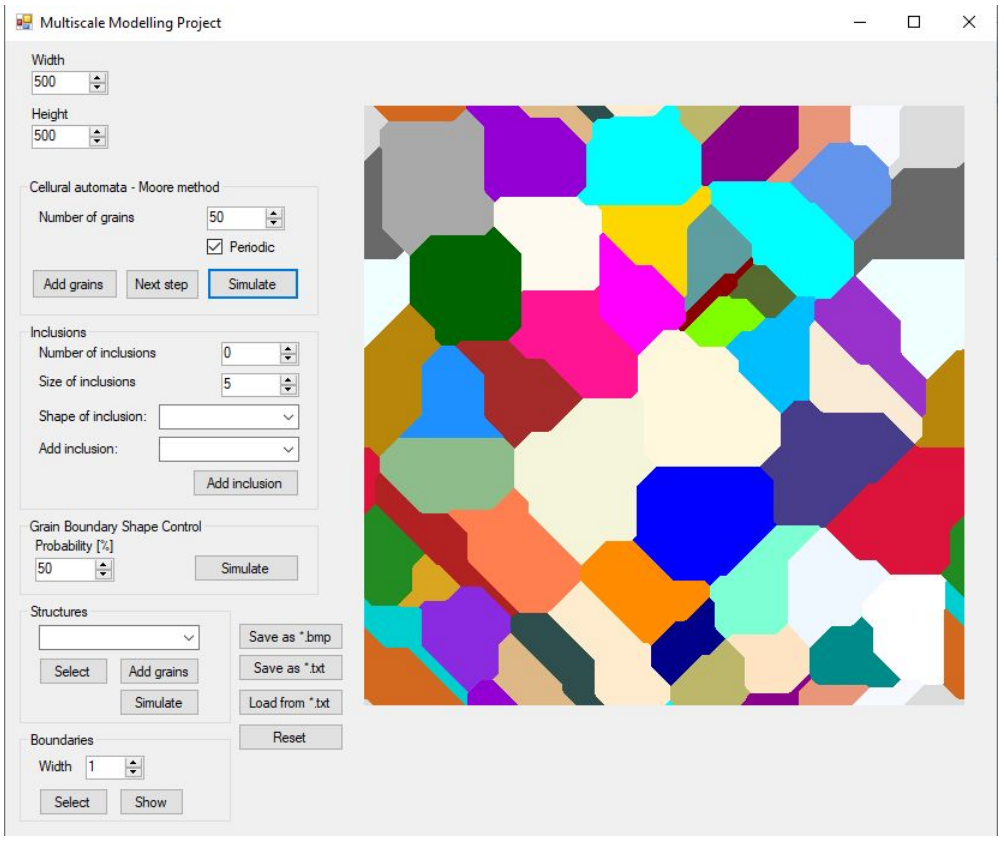

Figure 2.Exemplary microstructure based on Moore neighbourhood.

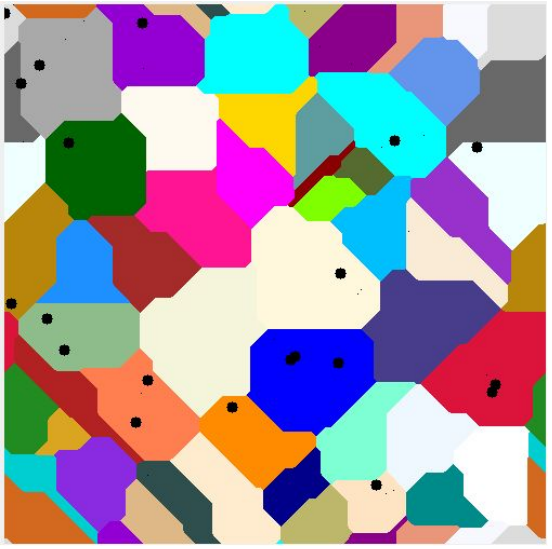

Figure 3.Exemplary microstructure based on Moore neighbourhood with inclusions.

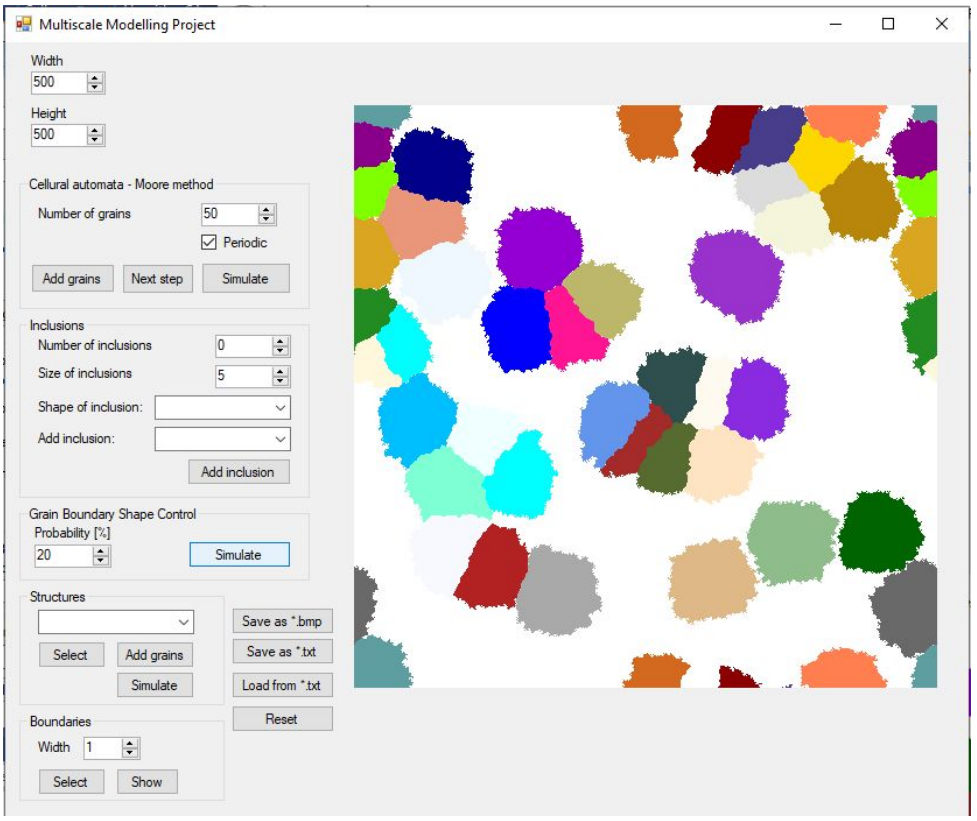

Figure 4. Growth based on grain boundary control with 20% probability for rule 4.

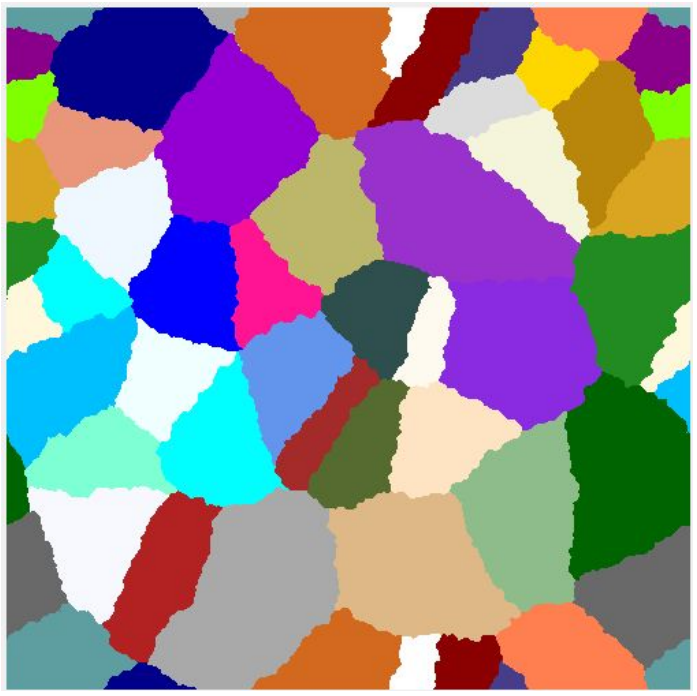

Figure 5. Fully grown grains based on grain boundary control with 20% probability for rule 4.

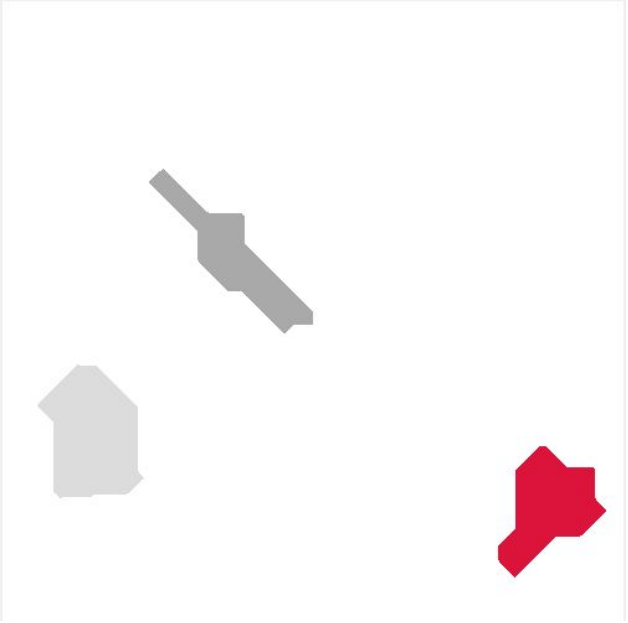

Figure 6. Selected grains for substructure condition

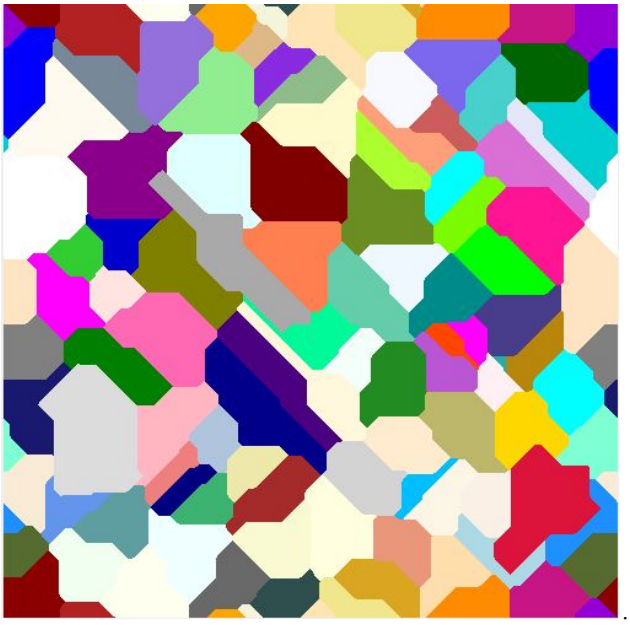

Figure 7. Microstructure after second growth

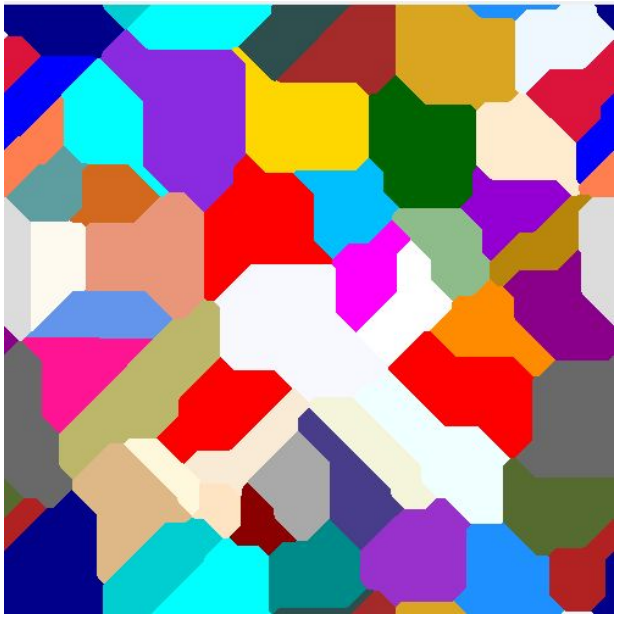

Figure 8. Microstructure with chosen dual-phase grains (in red)

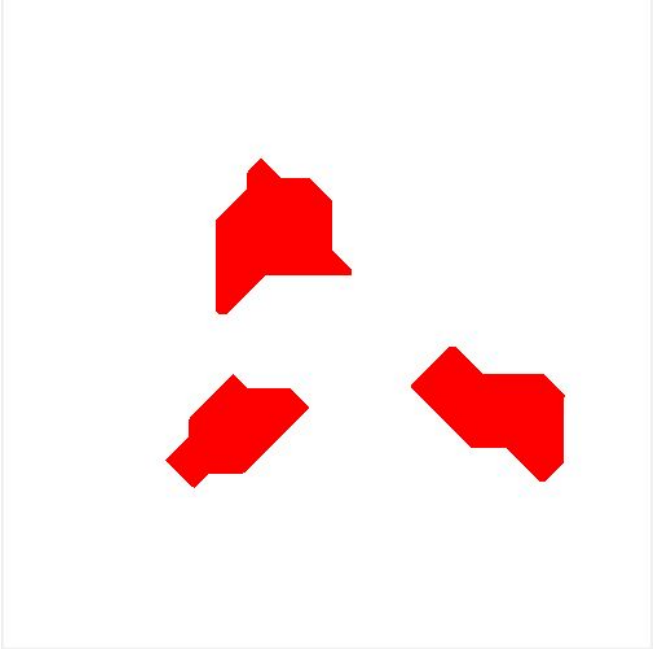

Figure 9. Microstructure with chosen dual-phase grains before second growth

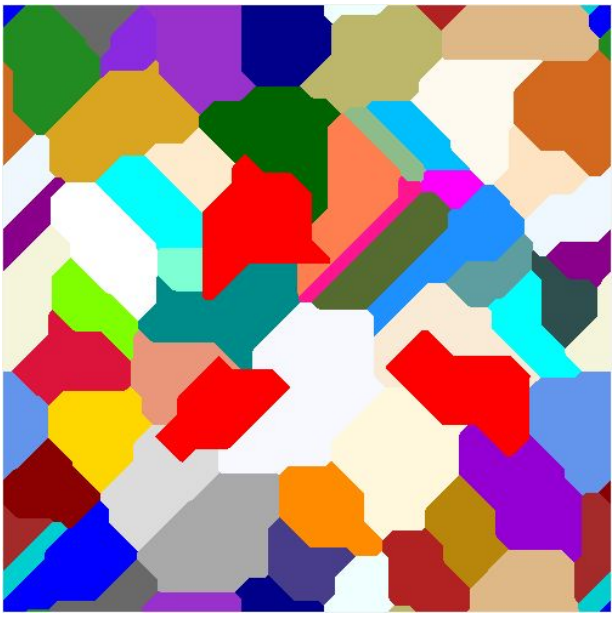

Figure 10. Microstructure with chosen dual-phase grains after second growth

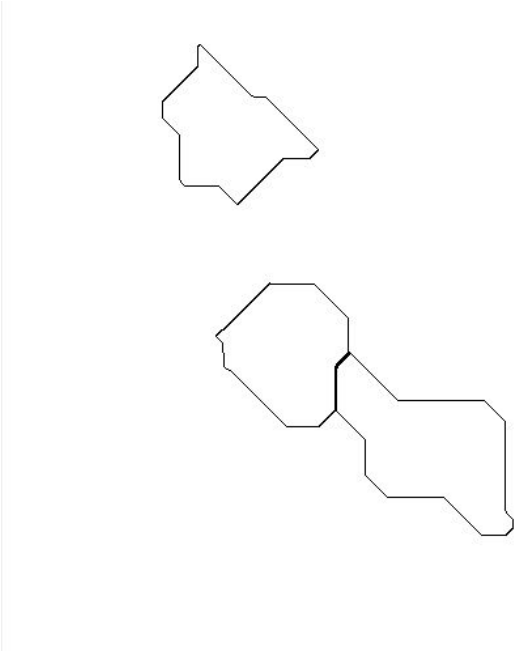

Figure 11. Boundaries for selected grains

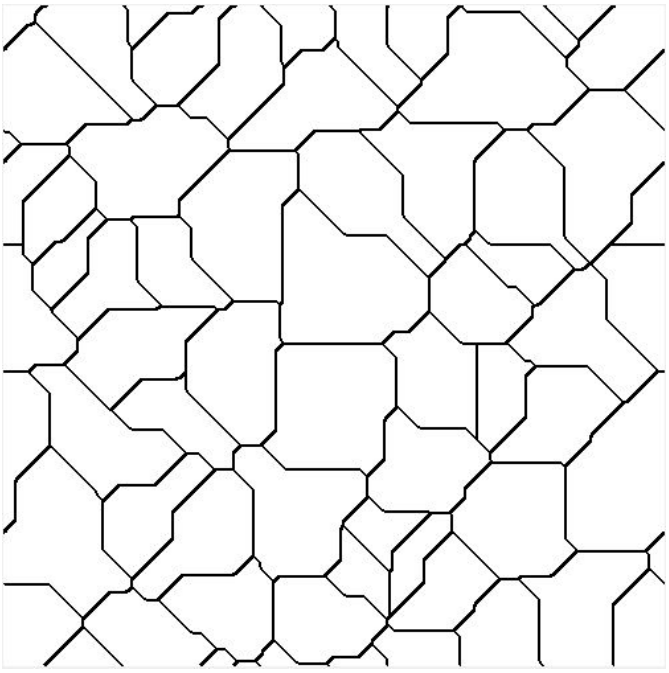

Figure 12. Boundaries for all grains

4. Summary

Cellular automata algorithm efficiently and effectively simulates grain growth in the microstructure. It is simple tool to simulate grain growth for educational purposes.