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Multiscale modeling - Project Report

GUI DESCRIPTION

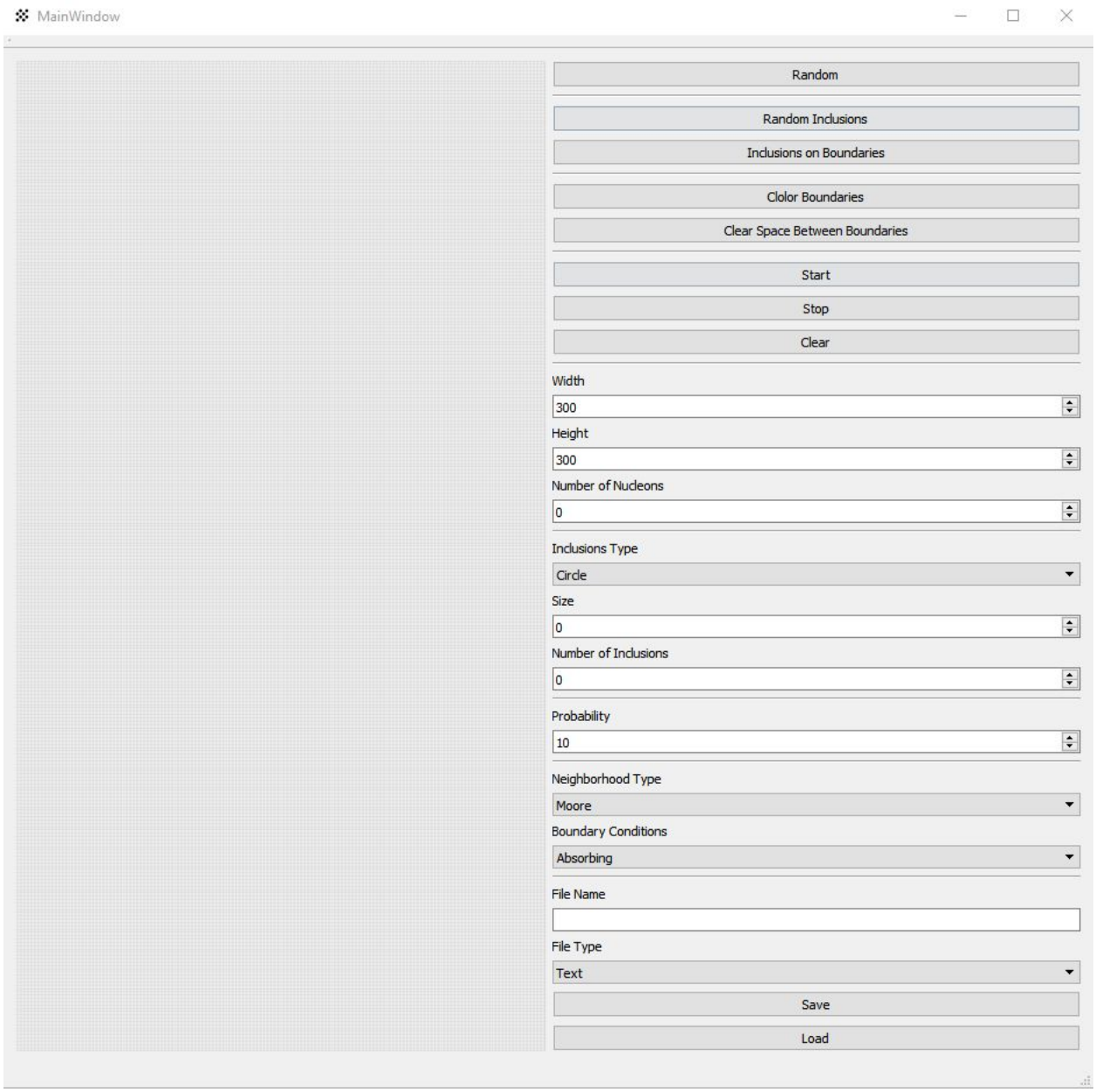

Fig. 1. Graphical User Interface

The left part of the interface is the space on which the microstructure is generated. The right part of the interface is responsible for controlling the application:

- Random button - generates nucleons in random places of space
- Random Inclusion button - generates inclusions in random places of space
- Inclusions on Boundaries button - generates inclusions on grains boundaries
- Color Boundaries button - colors grains boundaries on black
- Clear Space Between Boundaries button - cleans space between boundaries
- Start button - starts simulations
- Stop button - stops simulations
- Clear button - cleans the space
- Width spin box - sets width of the space (range 1-300)
- Height spin box - sets height of the space (range 1-300)
- Number of Nucleons spin box - sets number of nucleons in simulation
- Inclusion Type combo box - chooses type of inclusions (Circle or Square)
- Size spin box - sets size of inclusions
- Number of Inclusions spin box - sets number of inclusions
- Probability spin box - sets probability for rule 4 in “Extension of Moore” neighborhood type
- Neighborhood Type combo box - chooses type of neighborhood (Moore, von Neuman, Extension of Moore)
- Boundary Conditions combo box - chooses type of boundary conditions (Absorbing or Periodic)
- File Name text field - sets the file name
- File Type combo box - chooses type of file (Text, Bitmap)
- Save button - saves the file
- Load button - reads the file

RESULTS

In the first stage of the project, grain growth with the use of the Moor neighborhood was implemented. The result of the simulation with use of this neighborhood is presented below (Fig. 2).

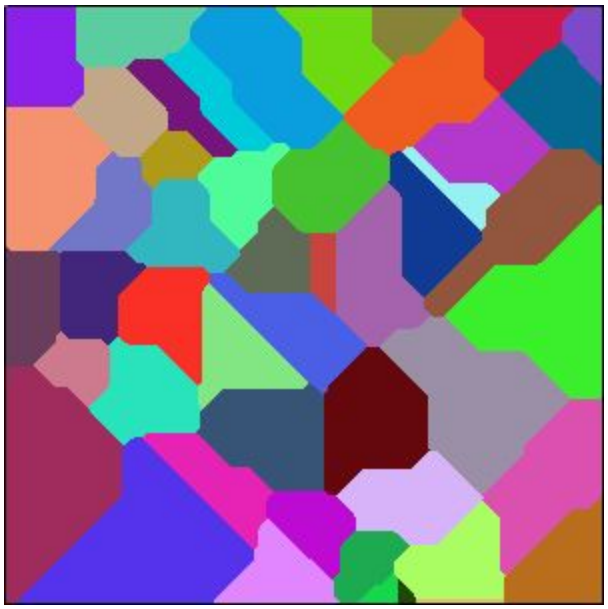

Fig. 2. 300x300 - Moore Neighborhood - 50 Nucleons

Next, von Neuman neighborhood was implemented. Simulations parameters was the same as in the previous example. Result of this simulation is presented below (Fig. 3).

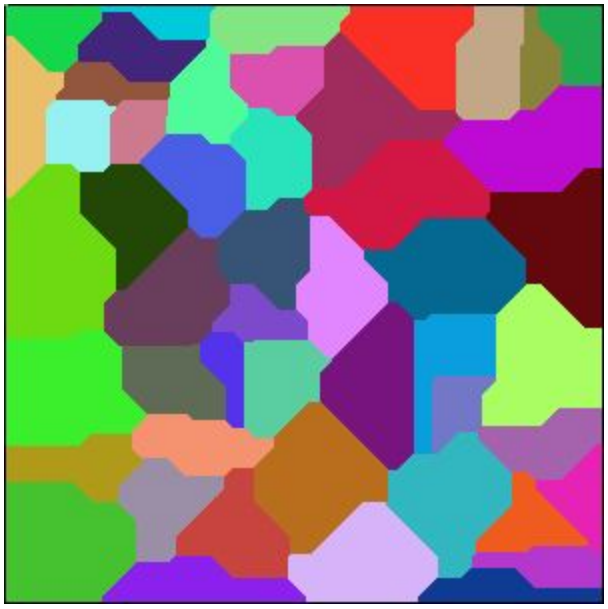

Fig. 3. 300x300 - von Neuman Neighborhood - 50 Nucleons

In the next stage of the project, Moore neighborhood with 4 rules was implemented (in GUI under the name Extension of Moore Neighborhood). As the name suggests, it uses 4 rules that it checks one by one until one of them is fulfilled. The result of the simulation with use of this neighborhood is presented below (Fig. 4). For last rule a 10% probability was used.

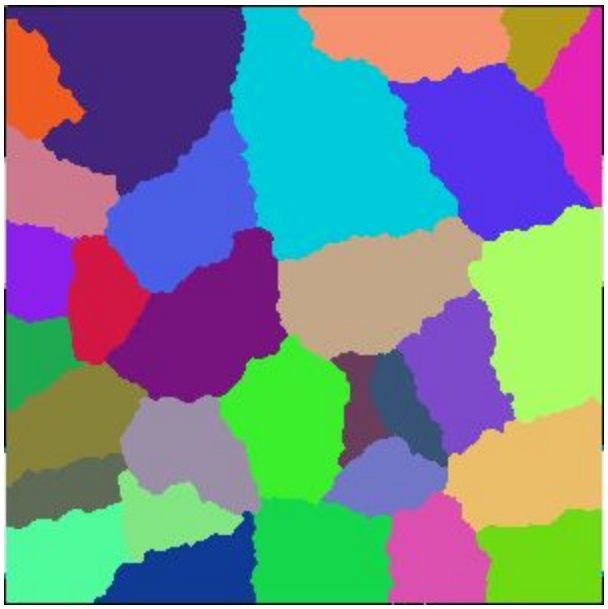

Fig. 4. 300x300 - Extension of Moore Neighborhood - 50 Nucleons - 10% Probability

The next step during the project was to add the possibility of generation of inclusion. Two types of inclusions was implemented: square and circle with the option of choosing their size and quantity. Also the possibility of adding inclusions on the grains boundaries or in random places was implemented. On pictures (Fig. 5 and Fig. 6) below we see results of simulations with with added inclusions on grains boundaries.

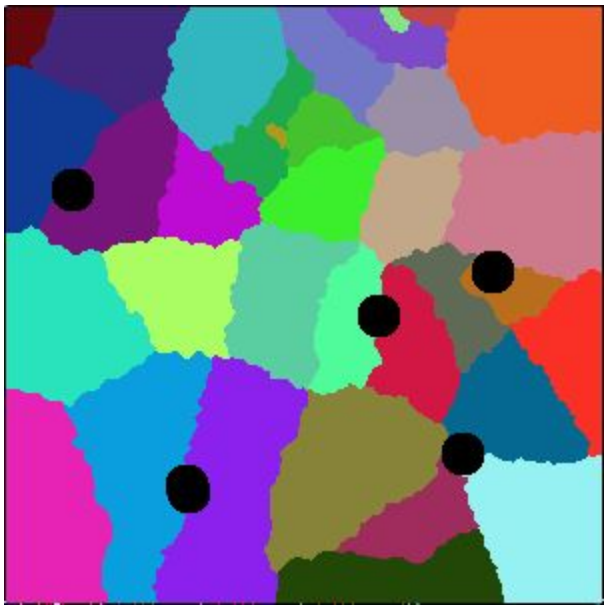

Fig. 5. 300x300 - Extension of Moore Neighborhood - 50 Nucleons - 10% Probability - Inclusions on Boundaries - Circle Type - Number 5 - Size 10

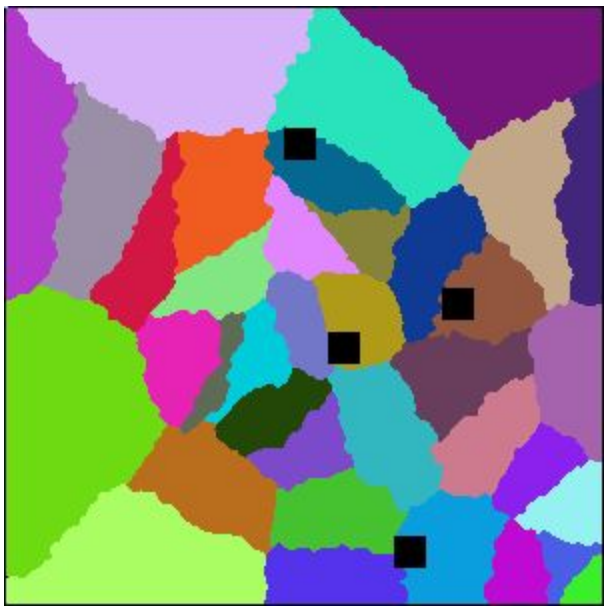

Fig. 6. 300x300 - Extension of Moore Neighborhood - 50 Nucleons - 10% Probability - Inclusions on Boundaries - Square Type - Number 4 - Size 15

On pictures (Fig. 7 and Fig. 8) below we see results of simulations with with added inclusions in random places.

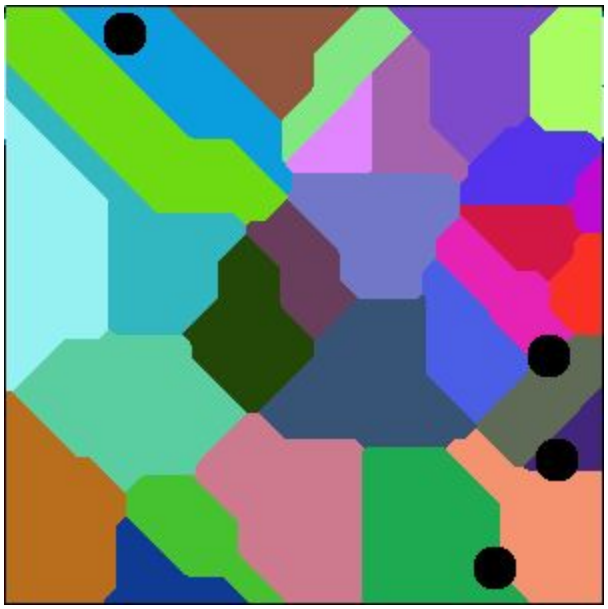

Fig. 7. 300x300 - Moore Neighborhood - 30 Nucleons - Random Inclusions - Circle Type - Number 4 - Size 1

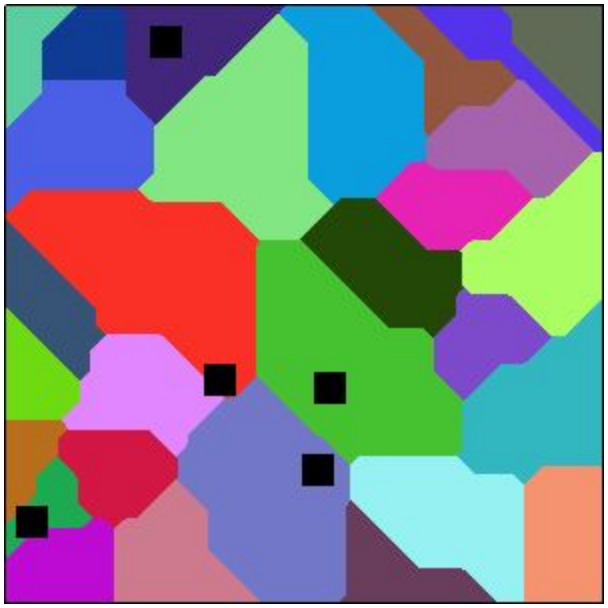

Fig. 8. 300x300 - Moore Neighborhood - 30 Nucleons - Random Inclusions - Square Type - Number 5 - Size 15

The final stage of the project was the implementation of the possibility to mark grain boundaries in black color and to add the possibility to clear the space between them. The results of this stage have been presented below (Fig. 9 and Fig. 10).

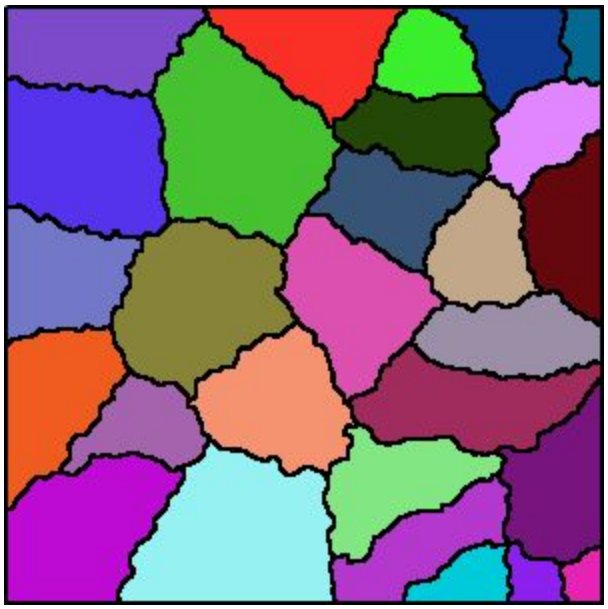

Fig. 9. 300x300 - Extension of Moore Neighborhood - 50 Nucleons - 10% Probability - Color Boundaries

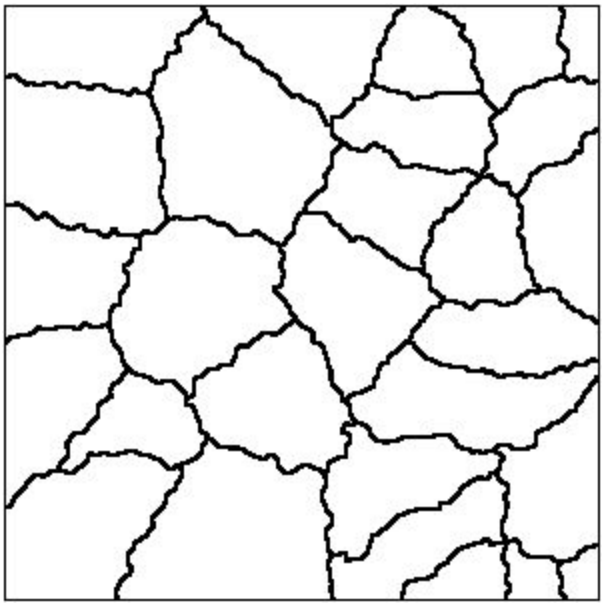

Fig. 10. 300x300 - Extension of Moore Neighborhood - 50 Nucleons - 10% Probability - Color Boundaries with Clear Space Between Boundaries

COMPARISON WITH REAL MICROSTRUCTURES

Real

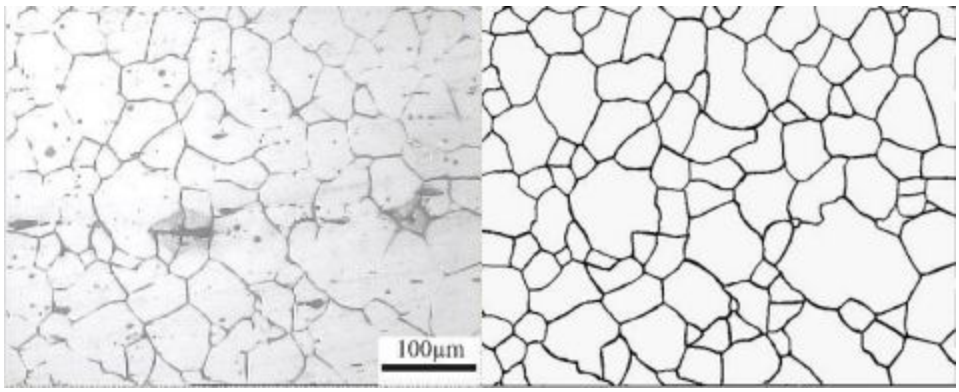

Fig. 11. Real microstructure

Generated

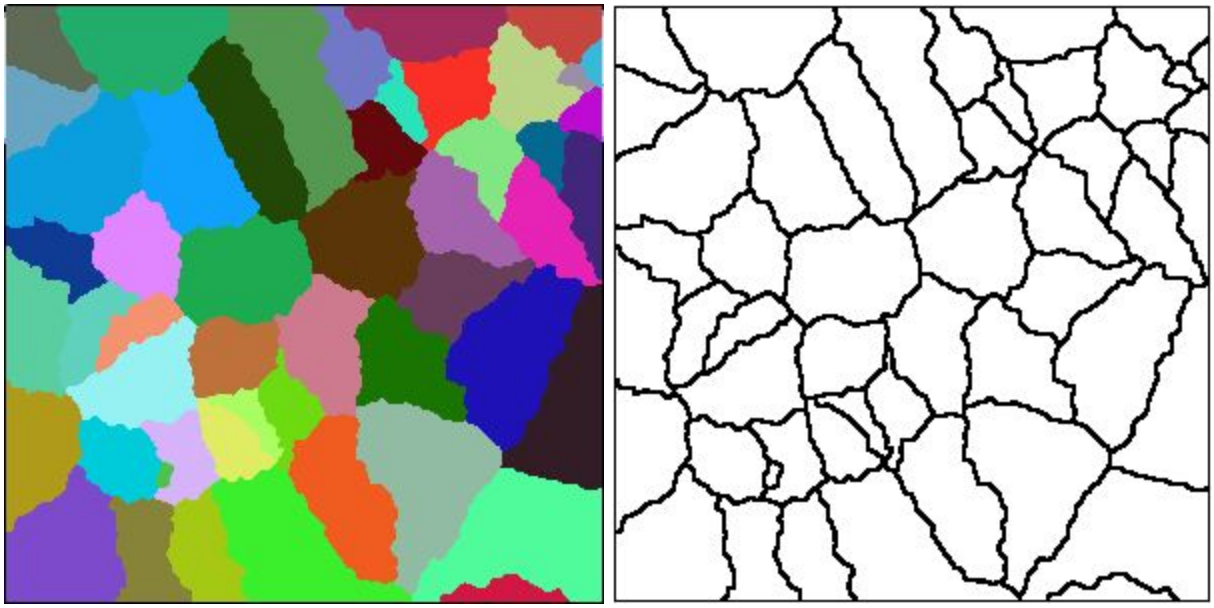

Fig. 12. Generated microstructure

In the pictures above you can see the comparison of the real microstructure (Fig. 11) with the generated microstructure (Fig. 12) with marked grain boundaries and removed space between them for better comparison. As you can see, the generated structure is similar to the real one.

SUMMARY

During the project the following functionalities were implemented:

- generation of space of given size
- random distribution of a given number of nucleons
- simulation with one of the three types of neighborhood (Moore, von Neuman, Extension of Moore)
- possibility of choosing the boundary conditions (Absorbing, Periodic)
- saving simulation results to a txt or bitmap file
- loading simulation results to a txt or bitmap file
- selection of the quantity, size and type of inclusions
- generation of inclusions in random places and at the border of grains
- ability to color grain boundaries and to clear the space between them