



AGH

Multiscale Modelling

Simple Grain Growth Cellular Automaton

Boundaries

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Short introduction

The goal of this project was to implement application simulating grain growth of steel microstructure with use of Cellular Automata methods. Application allows modification of few simulation parameters, for example dimensions or number of initial grains. Report below contains:

- actual look of application with description of user interface
- a few kinds of results of example simulation

Used technology

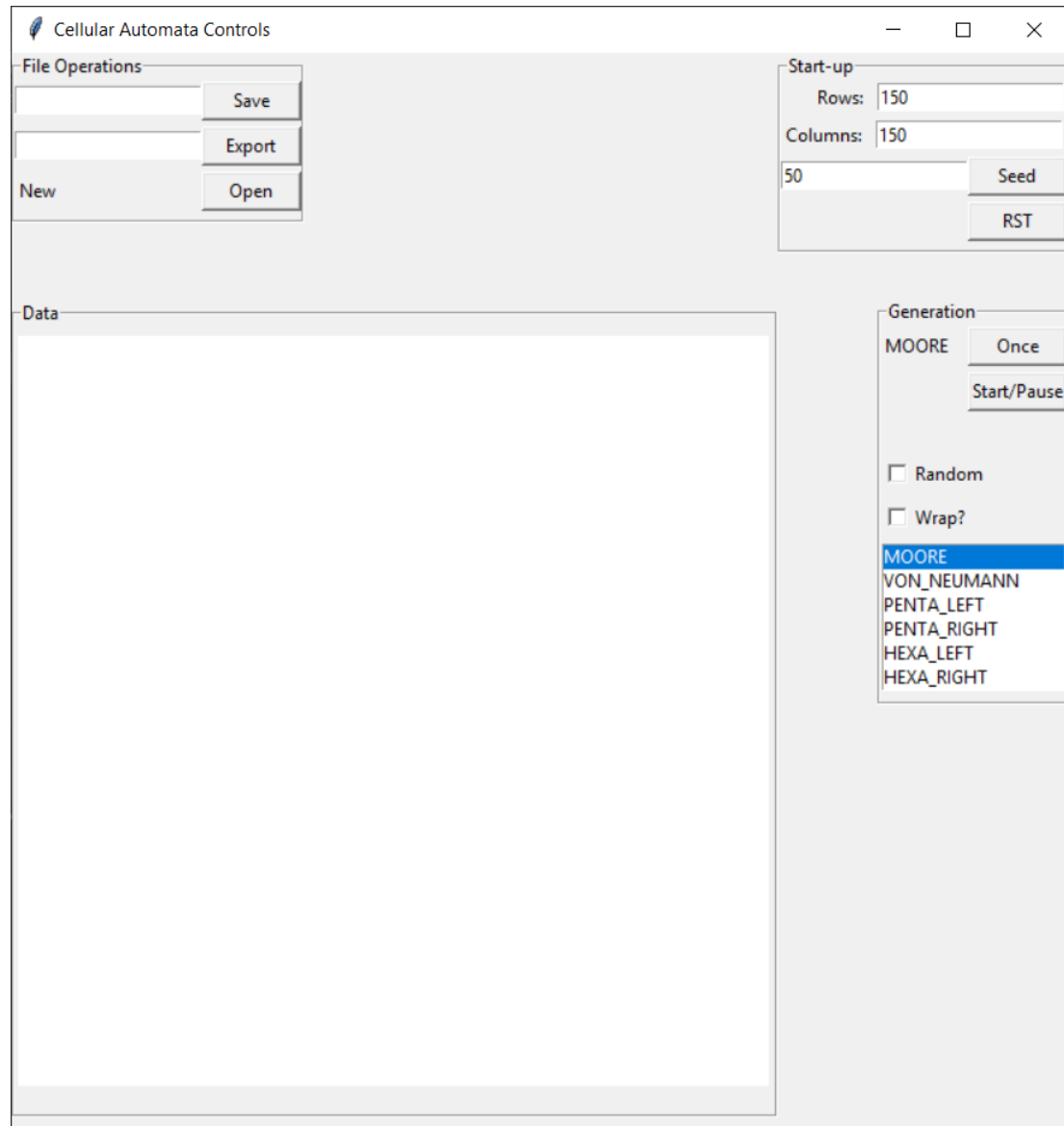
Implementation was done in **Python**. As the language is high-level and object-oriented there was a possibility to implement sophisticated algorithms relatively fast, what was crucial. Furthermore it supports number of libraries used for data structures manipulation and also computations of numerous types. Python offers an easiness of launching application on different systems without any additional tools.

As a version control system the Github is used, because of its reliability.

Link to Github: <https://github.com/SzymonIgor/MultiscaleModelling>

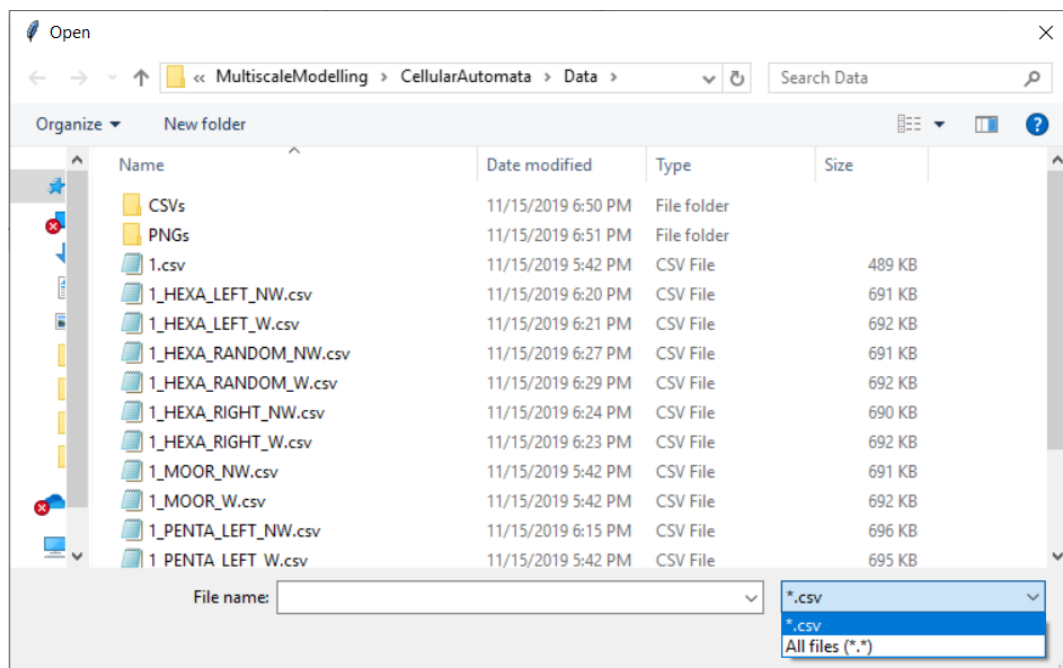
GUI

Graphical User Interface (shown below) was prepared in single-window, which parameters can be chosen in, simulation can be started, results can be exported in 3 types of files, also loaded to continue simulation that has not been ended.



Frames Description:

- File Operations – it is a place where data can be saved¹, exported² and imported(opened³)
 1. Save – allows to save current state of simulation in order to open it later on. The file format is - .csv. Default name is: CellularAutomata_YYYY-MM-DD_hhmmss (e.g. CellularAutomata_2019-11-15_200358).
 2. Export” button – creates two files. One of them is .csv file that contains 3 columns: [row, column, grainID or 0 (when empty)]. The second one is .png file that displays imaged version of data, where colour is based on grainID. There can be up to 300 different colours. Default name is: Export_YYYY-MM-DD_hhmmss (e.g.Export_2019-11-15_200358.csv).
 3. Open” button – allows to import data file to continue computation. After clicking the button the dialog box is opened and filter is applied (.csv files shown only).



- Data – Canvas where data is visualised. Initialized image has 500x500 pixels. There is a possibility to calculate through smaller not rectangular shapes, however bigger are not permitted for now.
- Start-up – this panel shall be used when new generation of seeds is needed, then these parameters are to be set.
 1. “Rows” entry – number of rows to be generated
 2. Columns:” entry – number of columns to be generated

3. "Seed" button – Generation of seeds that is given on the left side of the button, resetting of data is applied before generation
 4. "RST" button – reset of the data
- Generation – this panel is used to control the simulation
 - 1) "MOORE" label on the greyed background – current chosen mask that is used for simulating
 - 2) "Once" button – simulate one step
 - 3) "Start/Pause" button – Starting and Pausing the simulation steps
 - 4) "Random" checkbox – is considered when using masks: PENTA_LEFT, PENTA_RIGHT, HEXA_LEFT or HEXA_RIGHT. When is ticked left and right types are chosen randomly
 - 5) "Wrap?" checkbox – not ticked: zeros around the matrix. When ticked matrix is wrapped
 - 6) Listbox – list of masks available for usage

Results

Pairs of results of simulating grain growth using same template (500x500 matrix, no. of grains = 300, same initial grains positions). On the left sides are images of generation without checkbox “Wrap?” ticked, on the right with this option choosen.

- MOORE



- VON NEUMANN



- PENTA_LEFT



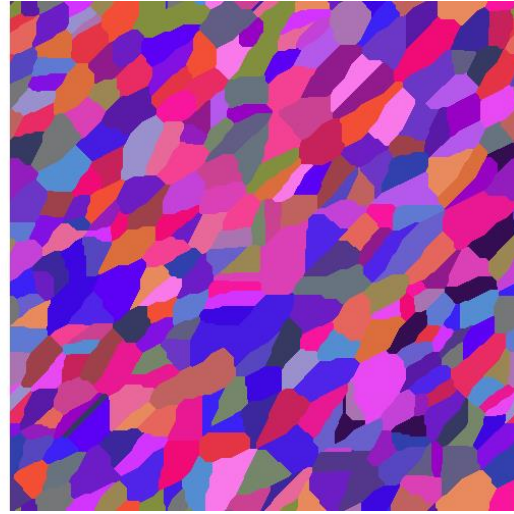
- PENTA_RIGHT



- PENTA_RANDOM



- HEXA_LEFT



- HEXA_RIGHT



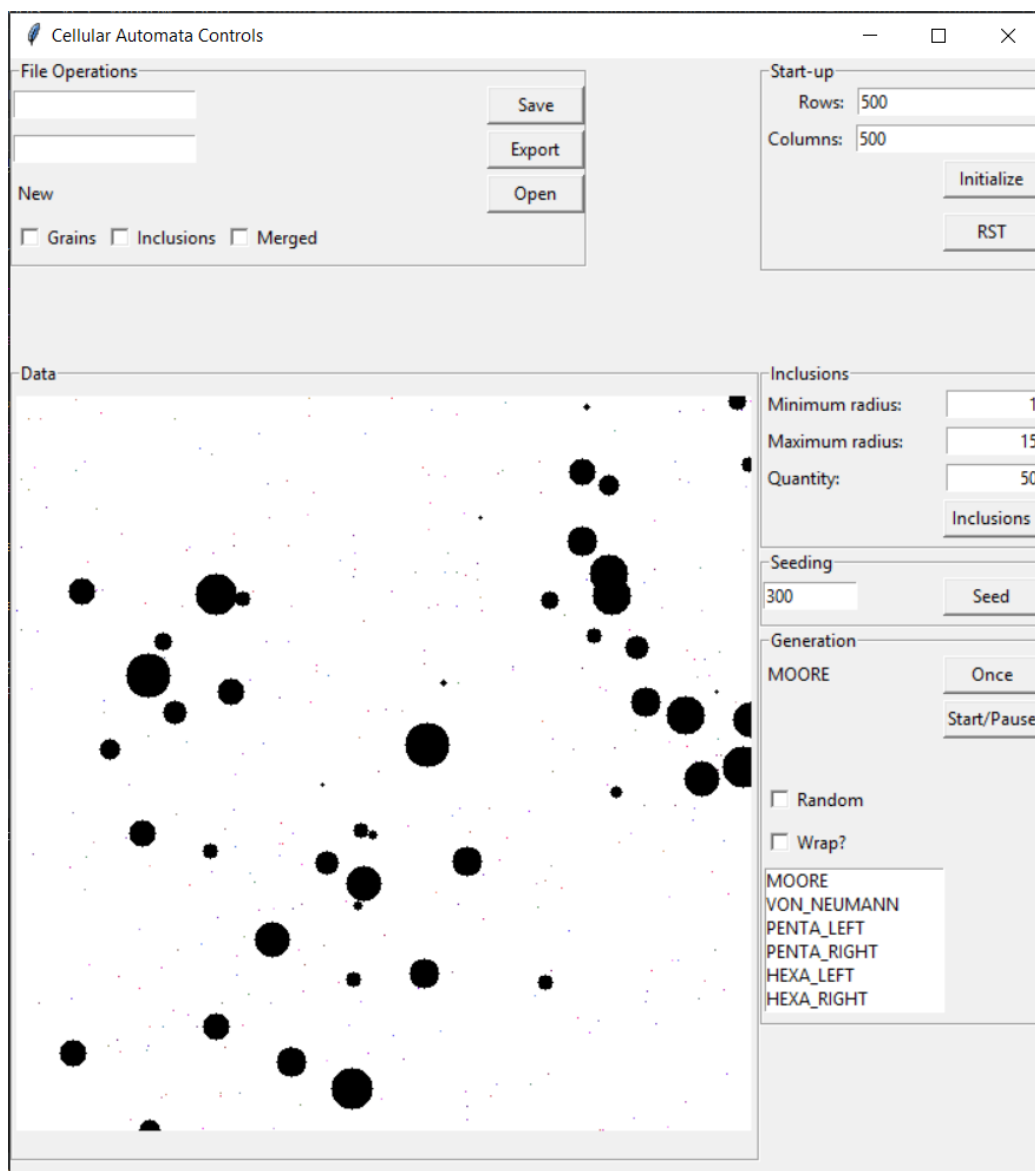
- HEXA_RANDOM



Inclusions

Requirements:

- User can specify no. of inclusions – DONE
- Inclusions should have round shape – DONE
- User can specify min and max radius – DONE
- Each inclusion should have random radius in range between selected min and max – DONE
- Add another internal variable “phase” to the model of the cell – the inclusions are another phase, include the new variable in the import/export functionality – DONE



“Start-up” frame has been adjusted to functionalities – Seeding is in another, new one label frame called “Seeding”.

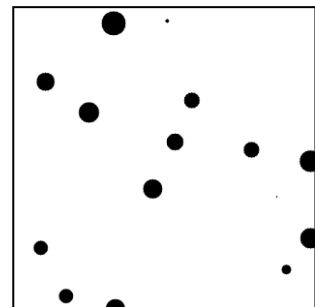
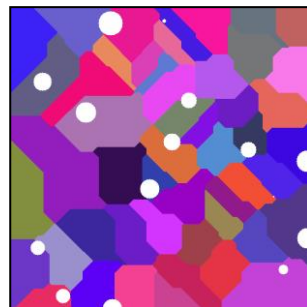
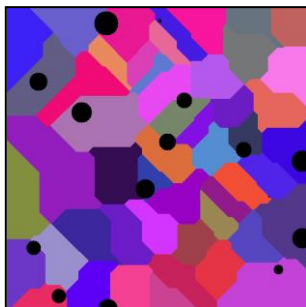
“Inclusions” label frame has been added. User can define minimal and maximal value that is going to be the range of randomly chosen radius of each and every inclusion. Number of inclusions also can be defined in this label frame.

“File Operations” label frame has been added three new checkboxes: *Grains*, *Inclusions* and *Merged*. User now can export/save data based on ones needs. Data are read the same way – one file at a time. Behaviour of opening can be changed - opening any number of files (one after another) and merging them - if there is a need and it would be useful – then, before opening, there is a required action from user – reset of the simulation (with the button). This approach is less “do-not-know-what-I-am-doing proof”. Should be discussed.

Below there are images of simulations of:

- Size: 500x500
- Grains: 50
- Inclusions: 15 in range from 1 to 20
- Kernel: MOORE
- Border conditions: 0s around

Images (starting from the left): merged, only grains and only inclusions.



Grain Boundary Curvature

Requirements:

- User can turn on / off the Grain Boundary Curvature (GBC) feature - DONE
- If GBC is turned on Boundary Condition selection component should be disabled with Moore option as pre-selected one – DONE
- User should be able to input threshold value for Rule no. 4 (X - probability of change) - DONE

The screenshot shows the 'Cellular Automata Controls' window. It features a 'File Operations' section with 'Save', 'Export', and 'Open' buttons. A 'Start-up' section includes 'Rows' and 'Columns' set to 150, with 'Initialize' and 'RST' buttons. The 'Data' section is a large empty area. On the right, the 'Inclusions' section has fields for 'Minimum radius' (1), 'Maximum radius' (10), and 'Quantity' (1), with an 'Inclusions' button. Below that, the 'Seeding' section has a 'Seed' button. The 'Generation' section shows 'MOORE' selected, with 'Once' and 'Start/Pause' buttons. At the bottom, there are checkboxes for 'GBC' (unchecked), 'Wrap?' (unchecked), and 'Random' (unchecked). A dropdown menu is open, showing 'MOORE' as the selected option, with other options including 'VON_NEUMANN', 'PENTA_LEFT', 'PENTA_RIGHT', 'HEXA_LEFT', and 'HEXA_RIGHT'. A 'Probability of change [%]' field is set to 50.

Cellular Automata Controls

File Operations

Save

Export

Open

New

☒ Grains ☒ Inclusions ☒ Merged

Start-up

Rows: 150

Columns: 150

Initialize

RST

Data

Inclusions

Minimum radius: 1

Maximum radius: 10

Quantity: 1

Inclusions

Seeding

50

Seed

Generation

MOORE

Once

Start/Pause

☐ GBC | Probability of change [%]: 50

☐ Wrap?

☐ Random

MOORE

VON_NEUMANN

PENTA_LEFT

PENTA_RIGHT

HEXA_LEFT

HEXA_RIGHT

Substructures and Dual-Phase

Requirements:

- User can delete selected grains after grain growth (by clicking on them ~~or by selecting from list~~) DONE
- User can perform second Grain Growth (Substructures feature) DONE
- User can perform second Grain Growth, now using another distinct phase (Dual-Phase feature) DONE

The screenshot shows the 'Cellular Automata Controls' window. It features a 'File Operations' panel on the top left with 'Save', 'Export', and 'Open' buttons, and a 'New' section with checkboxes for 'Grains', 'Inclusions', 'firstPhase', and 'Merged'. On the top right is a 'Start-up' panel with 'Rows' and 'Columns' set to 150, and 'Initialize' and 'RST' buttons. The main area is labeled 'Data'. On the right side, there are several configuration panels: 'Inclusions' with 'Minimum radius' (4), 'Maximum radius' (9), 'Quantity' (4), and an 'Inclusions' button; 'Seeding' with a value of 50 and a 'Seed' button; 'Generation' with 'MOORE' selected and buttons for 'Once' and 'Start/Pause'; a section with checkboxes for 'GBC', 'Wrap?', and 'Random', along with a 'Probability of change [%]' set to 50; and a 'Second Phase' panel with a 'Delete?' checkbox and buttons for 'Substructs' and 'Dual-phase'. A dropdown menu is open under 'MOORE', showing options: 'MOORE', 'VON_NEUMANN', 'PENTA_LEFT', 'PENTA_RIGHT', 'HEXA_LEFT', and 'HEXA_RIGHT'.

Usage of added options

- When user wants to delete specific grain, then one needs to select option: “Delete?” and just click the grain displayed in GUI.
- To Create substructures user needs to click button “Substructures”
- When user wants to create second phase one needs to click the button “Dual-phase”
- New checkbox “firstPhase” allows user to save/export results from only second phase
- In export file new column has been added – phase (it is 0 or 1) according to usage of option “Dual-Phase”

Examples

- Substructures
(Substructures_150x150_50_50_merged.png,
Substructures_150x150_50_50_merged.csv)



```
0;0;4;0  
0;1;4;0  
0;2;4;0  
0;3;4;0  
0;4;4;0  
0;5;4;0  
0;6;31;0
```

- Dual Phase
(Dual_Phase_150x150_gbc_50_50_merged.png,
Dual_Phase_150x150_gbc_50_50_firstPhase.png,
Dual_Phase_150x150_gbc_50_50_merged.csv,
Dual_Phase_150x150_gbc_50_50_firstPhase.csv)



```
0;5;5;1    0;3;5;1  
0;6;5;1    0;4;5;1  
0;7;5;1    0;5;5;1  
0;8;74;2   0;6;5;1  
0;9;74;2   0;7;5;1  
0;10;74;2  0;72;11;1  
0;11;74;2  0;73;11;1
```

Boundaries

Requirements:

- Check if grain is a boundary of the grain. DONE
- Calculate average size of the grain. DONE (**working correctly even if whole array is not calculated**)
- Calculate length of the boundary of each and every grain DONE

The screenshot shows the 'Cellular Automata Controls' window. It features a 'File Operations' section with 'Save', 'Export', and 'Open' buttons. A 'Start-up' section includes 'Rows' and 'Columns' set to 150, with 'Initialize' and 'Boundaries' buttons. A 'Data' section contains a large empty area. On the right, there are sections for 'Inclusions' (with radius and quantity settings), 'Seeding' (with a 'Seed' button), 'Generation' (with a dropdown menu showing 'MOORE', 'VON_NEUMANN', 'PENTA_LEFT', 'PENTA_RIGHT', 'HEXA_LEFT', and 'HEXA_RIGHT'), and 'Second Phase' (with 'Delete?', 'Substructs', and 'Dual-phase' options).

Cellular Automata Controls

File Operations

Save

Export

Open

New

☒ Grains ☒ Inclusions ☒ firstPhase ☒ Boundaries ☒ Merged

Start-up

Rows: 150

Columns: 150

Initialize

Boundaries

Data

Inclusions

Minimum radius: 4

Maximum radius: 9

Quantity: 4

Inclusions

Seeding

50

Seed

Generation

MOORE

Once

Start/Pause

☐ GBC | Probability of change [%]: 50

☐ Wrap?

☐ Random

MOORE

VON_NEUMANN

PENTA_LEFT

PENTA_RIGHT

HEXA_LEFT

HEXA_RIGHT

Second Phase

☐ Delete?

Substructs

Dual-phase

Usage of added options and changes

- “RST” button was replaced by button “Boundaries”, because (“RST”) was doing almost same thing as “Init” button (without checking the input of array – not really usable)
- “Boundaries” button can be clicked in every moment in simulation
- When export is being done – simulation behaves as if “Boundaries” button was clicked
- New column in export file is added – if cell is a boundary (True/False)
- Checkbox “boundaries” also has been added – to export only boundaries

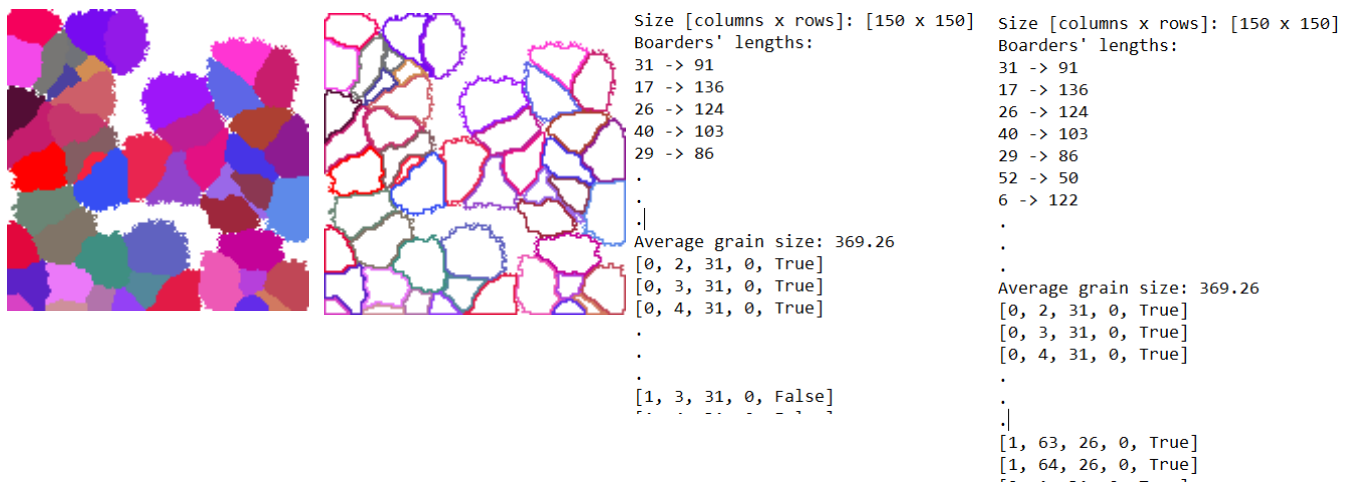
Examples

(Boundaries_150x150_gbc_50_merged.png,

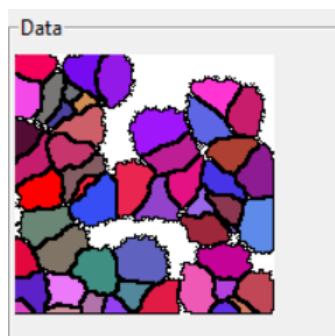
Boundaries_150x150_gbc_50_boundaries.png,

Boundaries_150x150_gbc_50_merged.csv [dots are only on screens for sake of readability],

Boundaries_150x150_gbc_50_boundaries.csv [dots are only on screens for sake of readability])



In the simulation after clicking “Boundaries” button the cells’ colours that are boundaries are changed to black.



Summary

The application is capable of simulating grain growth. Inclusion feature is also available. The Graphical User Interface is readable and user-friendly. Requirements are fulfilled. However, as time was crucial, there are a few possible improvements, such as: refactoring of the code, exception handling, GUI, optimization – multithreading / multiprocessing and probably some more – will be found during evolution of the program.

Inclusions option has been added.

Grain Boundary Curvature option has been added.

Deletion, Substructures and Dual-Phase options added.

Boundaries option added and separation into two threads (GUI + calculations)