Akademia Górniczo-Hutnicza
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Multiscale Modeling

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First project report

Introduction

Application’s purpose is to simulate grain growth using cellular automata method.

The application is written in Python, using **pygame** framework to visualize the process and **PyQt5** for creating GUI.

Project source codes are hosted on GitHub: https://github.com/umatbro/msm-1/
There is also online version of this document (with direct references to code): https://umatbro.github.io/msm-1/

Project Implementation

GUI

Main application window is presented on **Image 1**.

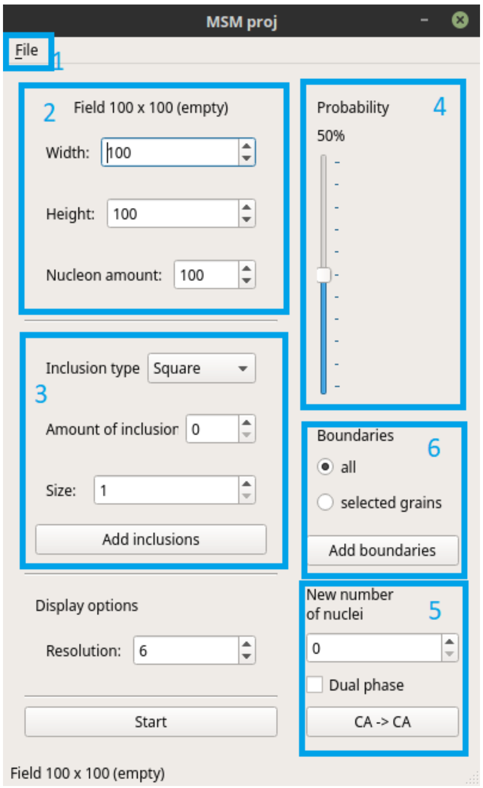

Image 1: Main application window

Highlighted GUI elements serve different purposes:

1. Import/export functionality
2. Grain growth
3. Inclusions
4. Boundary shape control
5. Substructures (different microstructure type)
6. Adding grain boundaries

Import and export functionality

Results obtained during simulation can be exported to either text file or image. Exported files can be imported and simulation may be continued.

Export to text

Text files are formatted in such way:

- first line contains field dimensions (width, height)
- following lines contain **(x, y)** coordinates and **ids** assigned to them

Text file being result of exporting field after simulation.

```
200 200
0 0 42
0 1 42
0 2 42
0 3 42
0 4 42
0 5 42
0 6 42
0 7 42
0 8 42
0 9 42
0 10 42
0 11 42
0 12 42
0 13 42
0 14 42
0 15 42
0 16 42
0 17 42
0 18 42
(...)
```

Export to image

Image export is pretty straightforward - what you see on the screen gets imported to **.png** file.

Saved images can also be imported.

Image file after exporting from application is presented on **Image 2**.

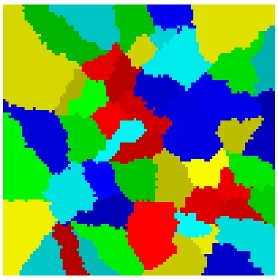

Image 2: image of 100x100 field that will be saved on hard drive

Grain growth

This section allows user to select initial grain field size (width and height).

Additionally number of grains to be added in random positions can be set.

After pressing `Start` button, visualisation will start running. Results can be seen on Image 3.

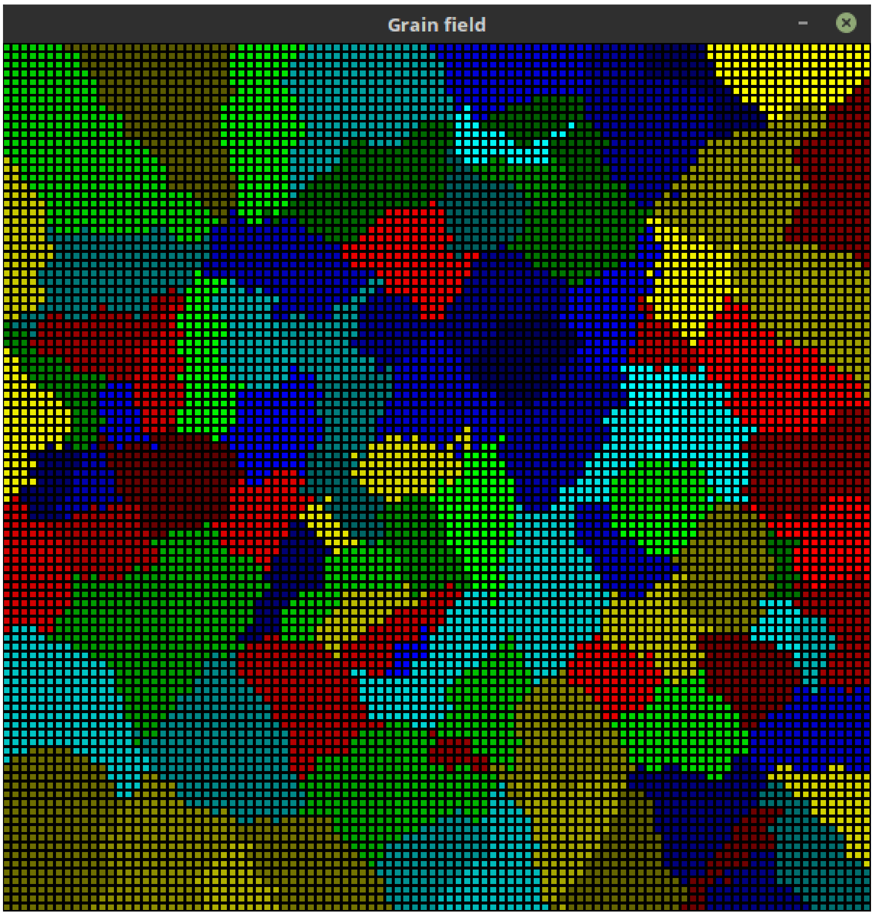

Image 3: Result of grain growth simulation (100x100 field)

Inclusions

Inclusions functionality involves:

- adding inclusions:
    - before starting simulation
    - after simulation, when the field is filled with grains. Inclusions are added on grain boundaries in this case.
- different shapes of inclusions
    - square
    - circle

Cells which represent inclusion do not affect neighbour cells. This means that if we add inclusion it will not grow and will not be modified throughout simulation.

Image 4 (below) presents few circle and square inclusions added *after* filling grain field (after simulation).

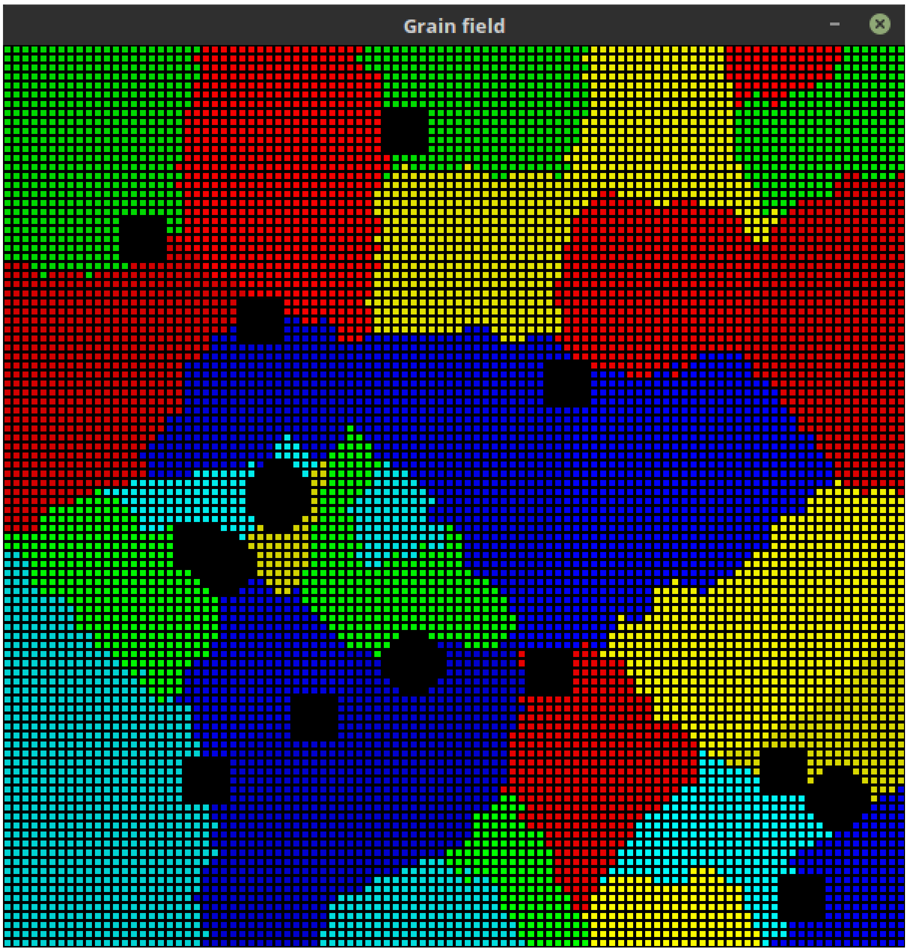

Image 4: Field visualization after adding inclusions

Boundary shape control

Probability slider lets user to control the shape of grain boundaries in some way.

Comparison between simulation results for **probability** values set to **99%** (left) and **1%** (right) (**Image 5**).

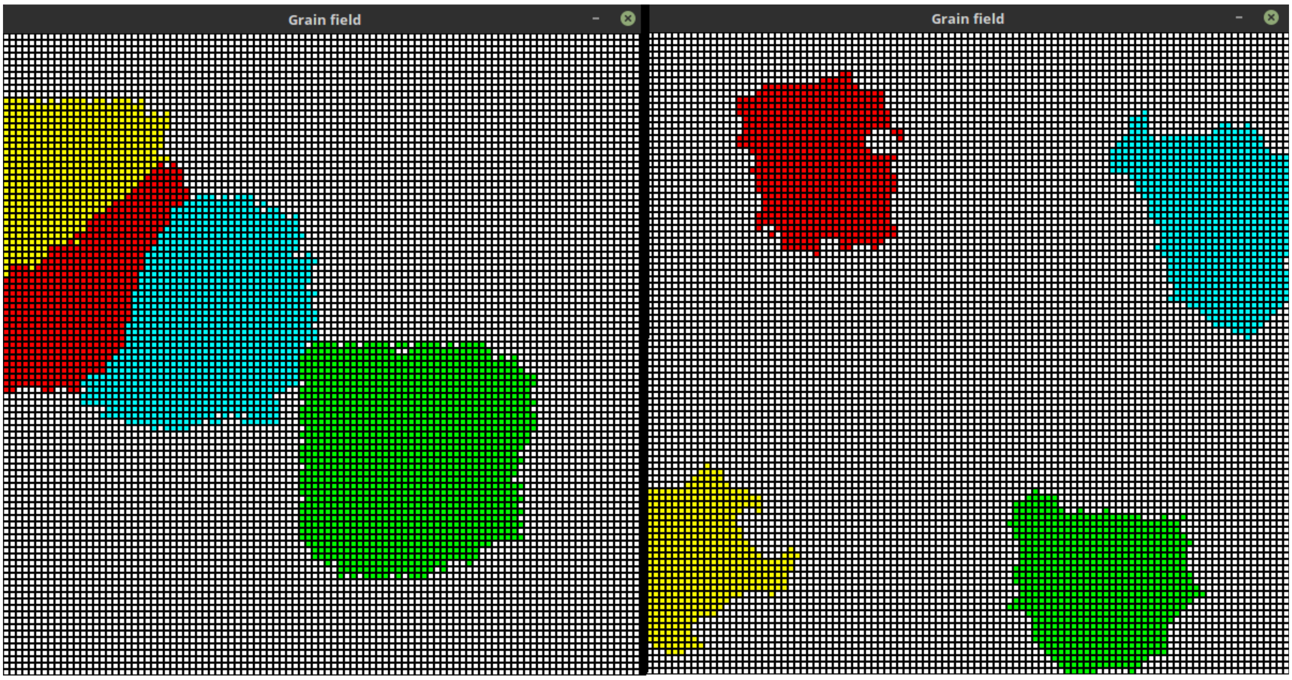

Image 5: difference between different probability settings

Algorithm

Future state of an empty cell is determined by checking 4 rules:

1. 5 or more cells from **Moore** neighbourhood
2. 3 or more cells from **nearest** Moore neighbourhood
3. 3 or more cells from **further** Moore neighbourhood
4. any cell from neighbourhood if probability test is positive

Substructure

During visualisation user can select grains by mouse clicks.

Selected grains are highlighted in light pink color (**Image 6**).

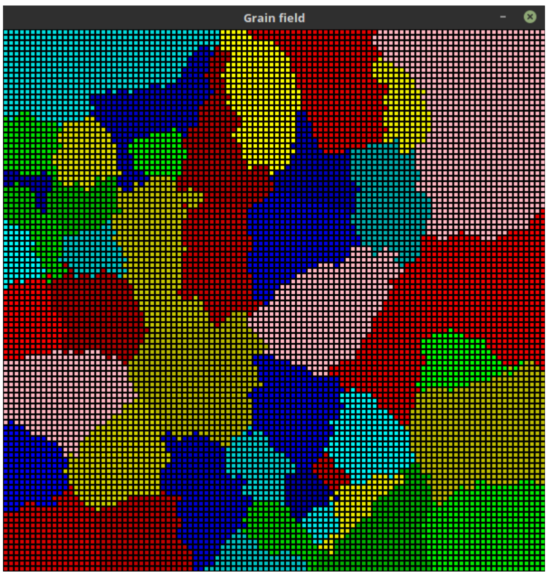

Image 6: selecting grains (ligt pink color)

After grains have been selected, whole field can be cleared leaving selected grain untouched.

Clicking `CA -> CA` button will perform different actions depending of the state of `Dual phase` checkbox.

- Unchecked

  Selected grains will maintain their state but after clearing field they won't increase in size (**Image 7**).

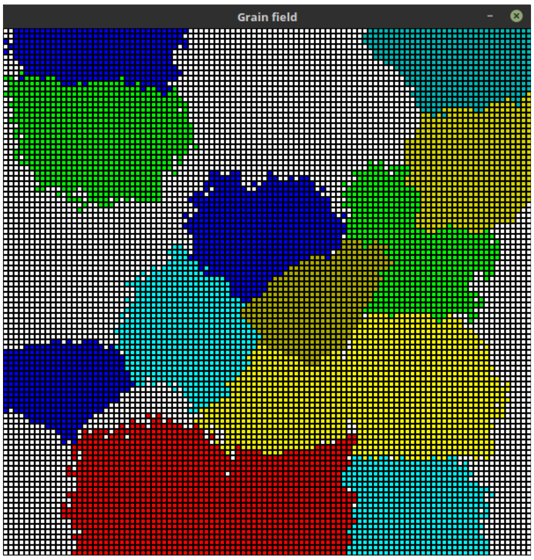

Image 7: cleared field with locked grains

- Checked

  All selected grains get the same color and also do not grow (**Image 8**).

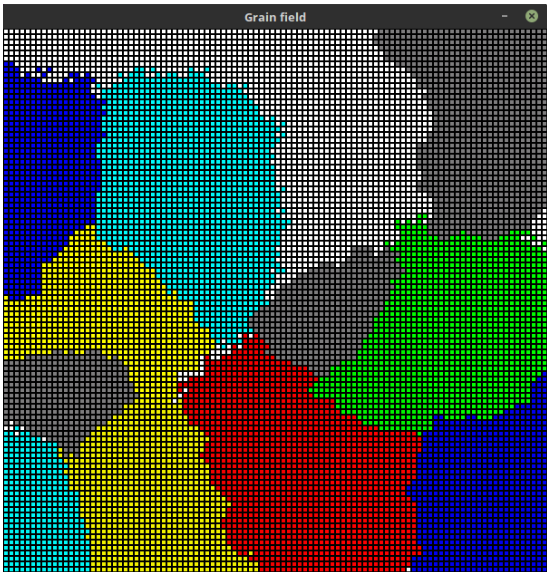

Image 8: cleared field with dual-phase.

Grain boundaries

User can add boundaries to the field after simulation. He can decide whether he wants to add boundaries to all grains or only to the selected ones. The process of selecting grains is the same as in previous section (**Substructure**).

- boundaries for all grains

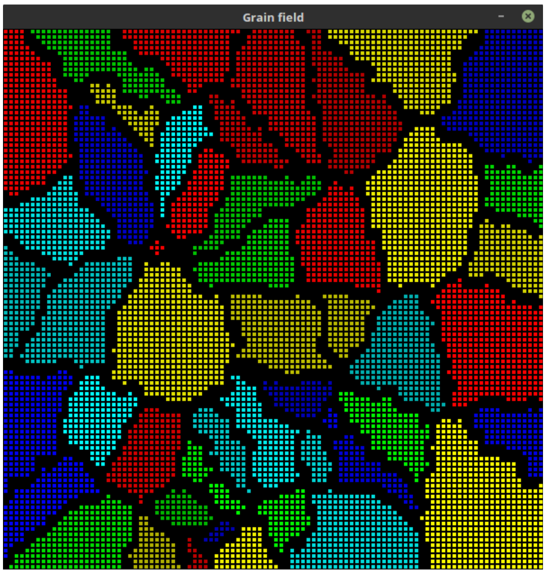

Image 9: Boundaries for all grains

- boundaries for selected grains

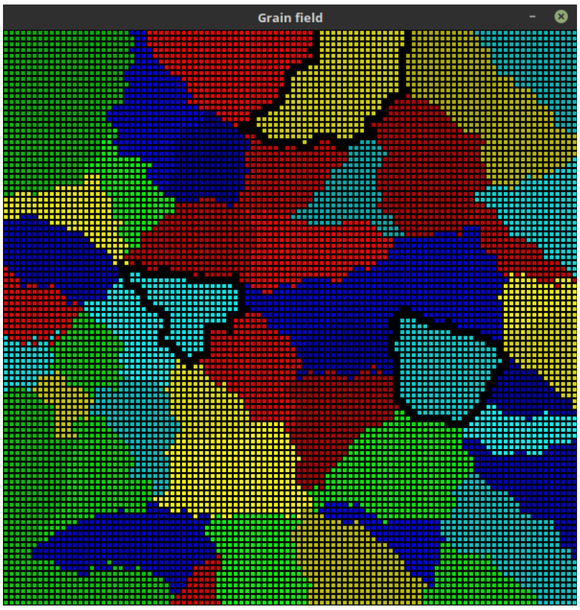

Image 10: boundaries for selected grains

After boundaries have been added, the percentage of the surface that they occupy is calculated. The result is displayed in the left bottom corner of application window.

Clear space

Again, using `CA -> CA` button we can clear all grains, leaving boundaries untouched. Additionally we can run simulation with new grains (**Image 11**).

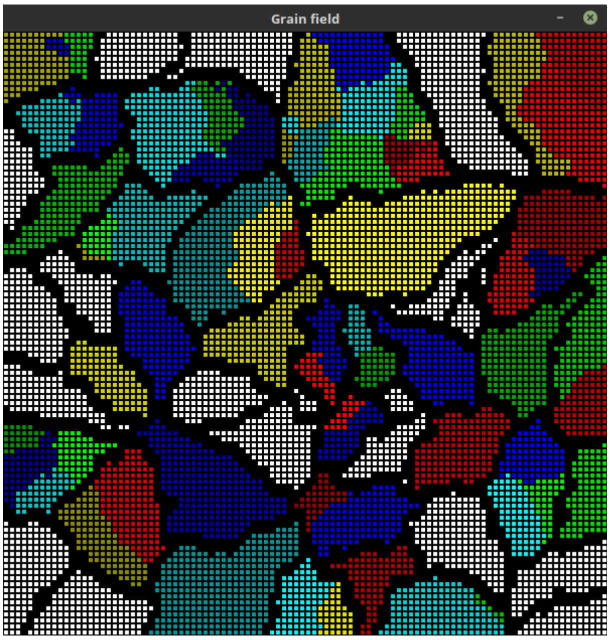

Image 11: Field after running simulation again with boundaries

Summary

Cellular automata method used to simulate grain growth which is important problem in metallurgy. It gives possibility to simulate with good accuracy the basic grain growth in DP steel. Von Neumann`s and Moore`s growth algorithm gives very accurate results.

Grain growth is an important matter in metallurgy, microstructure of the material is important to control mechanical and physical properties.

Cellular automata method chosen for project can give precise results but the process can be time-consuming dependin on the field size.