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Multiscale modeling – Project report

1. General project description

In this project we are preparing kind of Cellular automation that will be simulate process of grain growth. In first approach our application has implemented some particular functionalities that will be describe below.

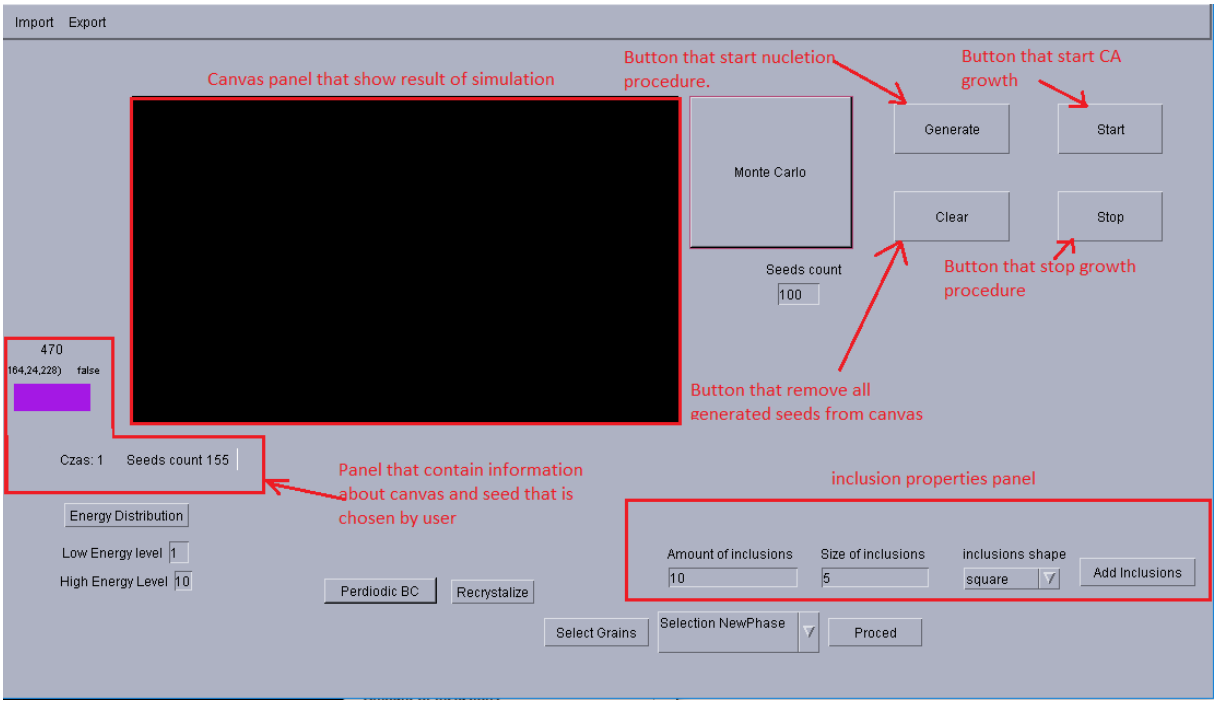


Fig 1. General interface view.

Simple Grain growth

This functionality allows to simulate process of grain growth. Whole procedure is divided in two steps, nucleation and growth. For CA method we are using Moore type of Neighborhood.

From the interface point of view, user have to first of all generate new seeds. That happens after click in to “Generate button” and then “Start” (Fig 1). Seeds are generated with random position, but there is also possibility to set seed in place specified by user. It is done by clicking in particular place on the canvas. Result of procedure is shown on Fig 2.

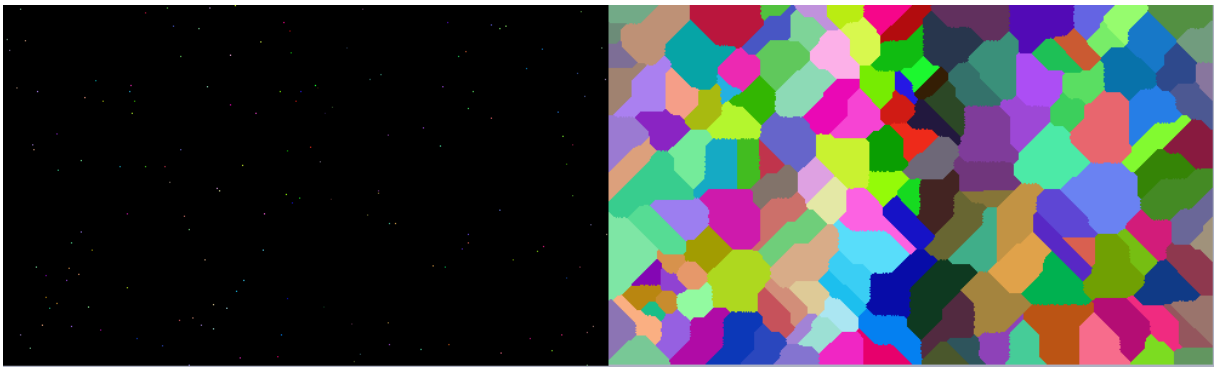


Fig 2. Canvas after nucleation and growth procedure

Import/export microstructure from/to .txt or .bmp file

User can save generated microstructure to file and then for example share his work or load it later. To do that user have to chose Import/Export option from general menu (Fig 3).

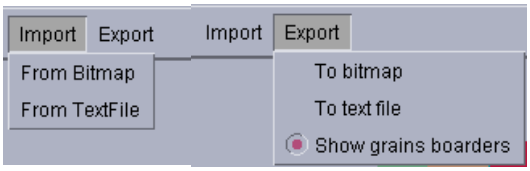


Fig 3. Import Export on menu.

8,0,0,140,116,180 8,1,0,140,116,180 8,2,0,140,116,180 8,3,0,140,116,180 8,4,0,140,116,180 8,5,0,140,116,180 8,6,0,140,116,180 8,7,0,140,116,180 8,8,0,140,116,180 8,9,0,140,116,180 8,10,0,140,116,180 8,11,0,140,116,180 8,12,0,140,116,180 8,13,0,140,116,180 8,14,0,140,116,180 8,15,0,140,116,180 8,16,0,140,116,180 8,17,0,140,116,180 8,18,0,140,116,180 8,19,0,140,116,180 8,20,0,140,116,180 8,21,0,140,116,180 ……..	

Table 1. Example of structures imported to text file and bitmap.

Inclusions addition functionality

User can add inclusions to structure with two different shapes square and circular, moreover user can determine size and amount of inclusion. Points could be added on two different steps, after nucleation and after growth (Fig. 4).

All specified properties are defined in the inclusion panel (Fig. 1)

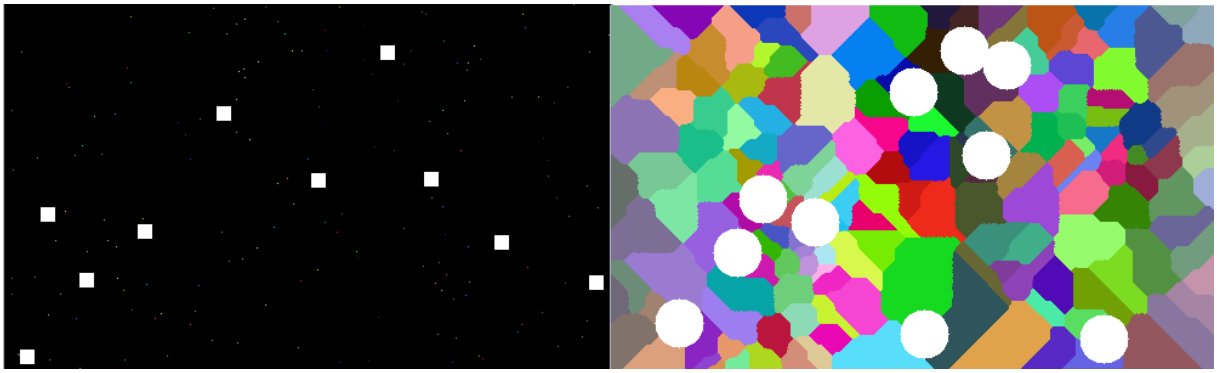


Fig. 5 Example of inclusions addition to microstructure

Extended Moore neighborhood.

Additional neighborhood that use different rules of grain growth is available on the combobox by selection “Extended Moore” (Fig. 6), then user can define Probability of growth in the final rule.

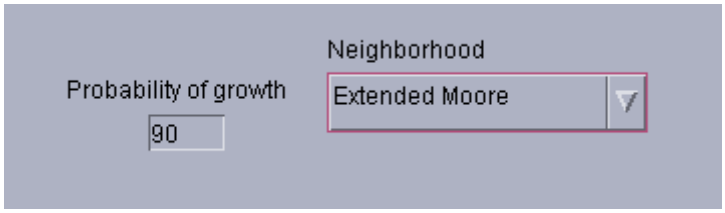


Fig.6 Example of extended Moore neighborhood chose

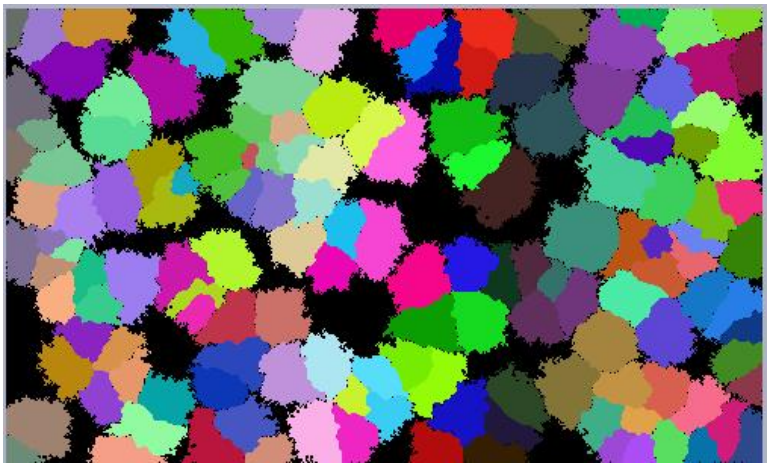


Fig.7 Example of Extended Moore

Different microstructure type: – substructure – dual phase (CA -> CA).

Functionality allow user to choose some grains from generated microstructure and remove others, then user have possibility to start nucleation process one more time and growth new generated seed but earlier chosen grains will still have same size and shape. Chosen grains could be treated as grains with different cellular ids (Dual Phase selection), or selected Grains could have same new selected id (New phase selection). User is choosing grains by clicking on the canvas. (Fig. 8)

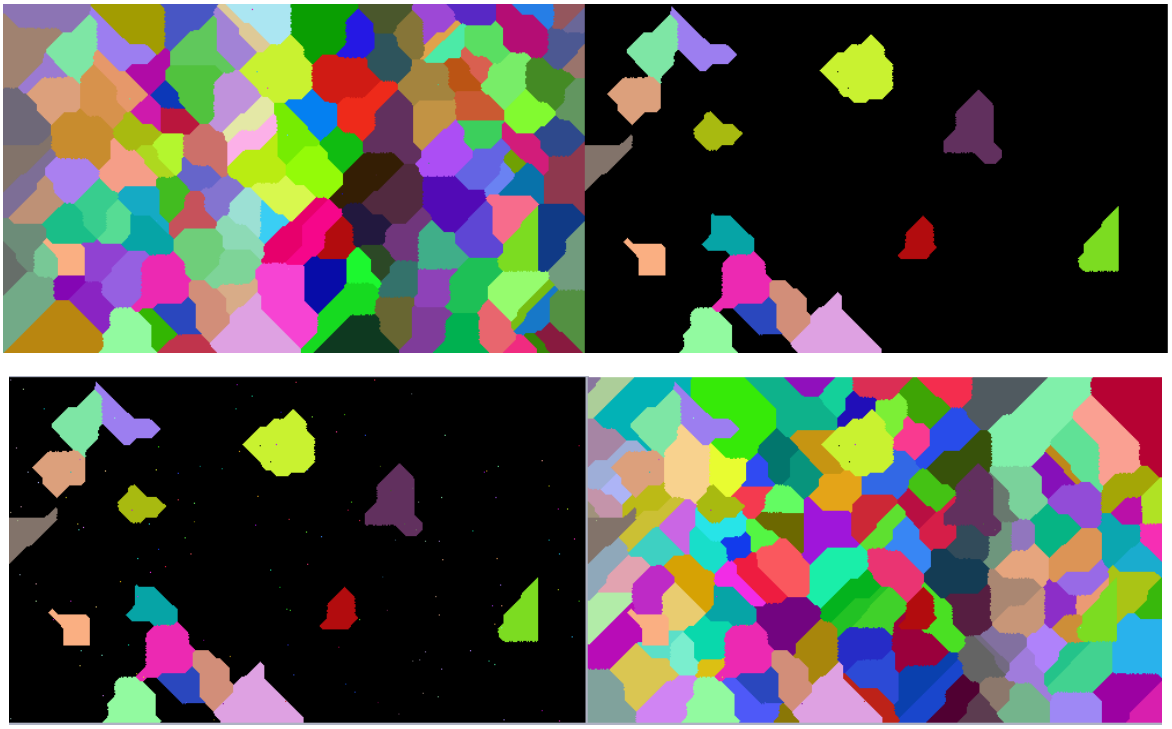
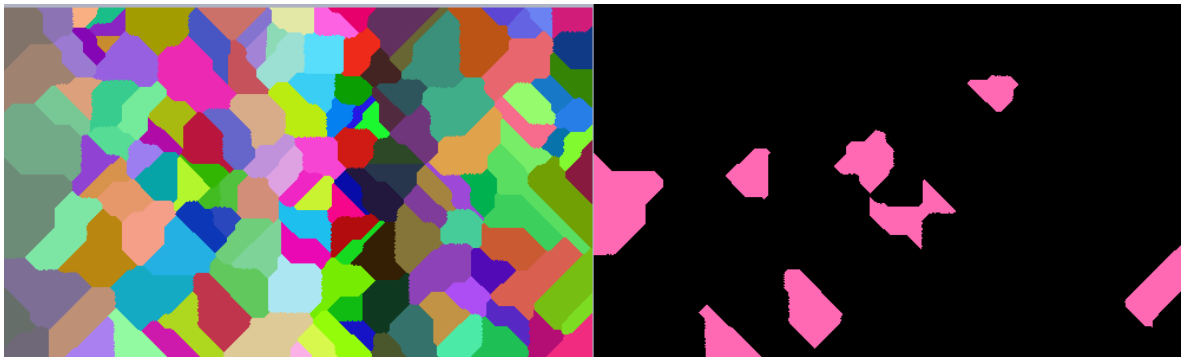
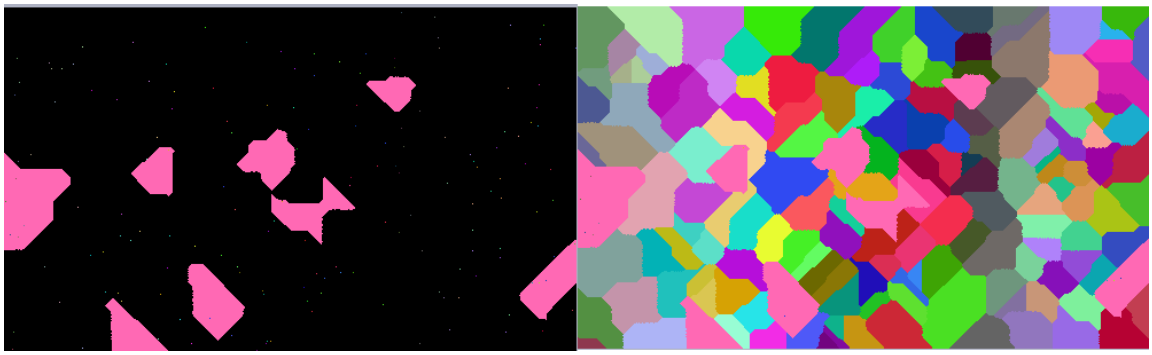


Fig 8. Selection of new Dual phase section, nucleation and growth





Grain boundaries selection (GB size, selection of grains).

This app functionality allow user to choose specified grains (by clicking on the canvas) and add boundaries of each grains. User can growth boundaries by clicking proceed button more than one time. To add boundaries user has to select “Get boundaries” from the combobox. Result are presented on Fig. 9.

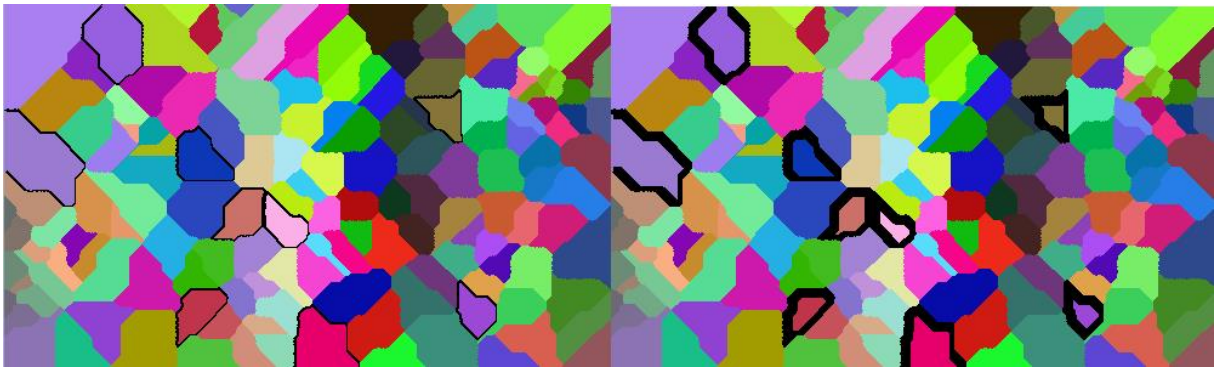


Fig. 9 Grain boundaries selection example

2. Technology used in project.

Project is written in Java. Only requirement to run program is Java Runtime Environment. To develop new functionalities Java SDK minimum version 8 is required. Project is cross platform software could be run on Windows OS and Linux as well. To make front end interface I used NetBeans which give easy and effective plugin to create Swing GUI.

3. Comparison with real microstructure photo

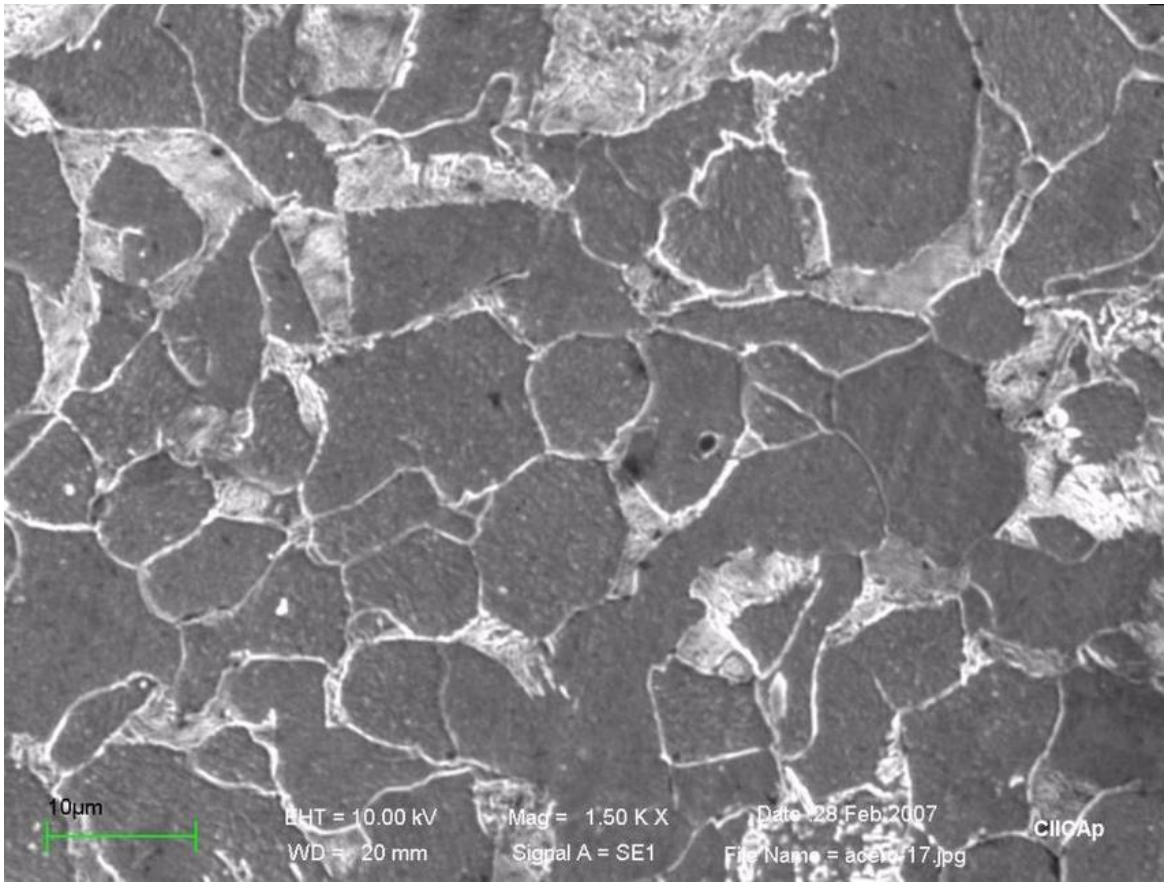
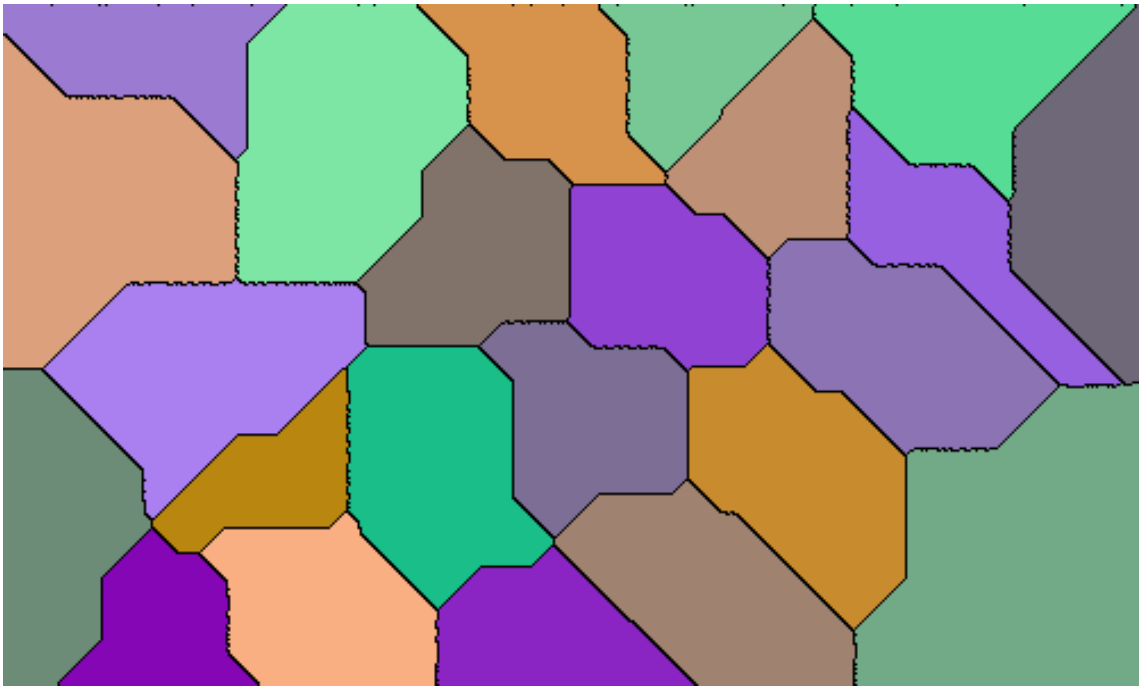


Fig. 10 Optical images of the microstructure of carbon steel. https://www.researchgate.net/figure/Optical-images-of-the-microstructure-of-carbon-steel_fig1_266258854



As we can see our application allow us to generate microstructure that looks really similar to real photo. Additionality we can add some of inclusion and make further actions to make microstructure more reliable.

Such simulation could be very useful for person who works with metallurgy problems. Instead making a lot of photos, he can make one photo of steal determine properties of steal (grains number, inclusions shape and size) and simulate lot of combinations. That is less time absorbing and more effective.