Multiscale Modelling Report

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Github: https://github.com/gabrielg9/Multiscale-Modelling

General description

During “Multiscale Modelling” course we have learned all about grains and theirs growing. All different mesh of grains have another impact on microstructure. This methodology is based on the Cellular Automata technique which idea is to divide a specific part of the material into one-, two-, three-dimensional lattices of finite cells, where cells have clearly defined interaction rules between each other. In the app I created, there is two-dimensional lattices with Moore neighborhood (also available to implement: Von Neumann, Pentagonal random, Hexagonal random). Apart from the core of this course, I implemented some extra features which I will show in this report.

Project 1

For the first project I prepared defining the space size and the space, also number of new grains. In my app, new grains are located randomly on the mesh. In the next step I implemented Grain Growing with periodic and absorbing boundary conditions. In several iterations checking each CA cell in the space. Moreover, it’s possible to import generated microstructure to txt or bmp file, export from txt/bmp to app as well.

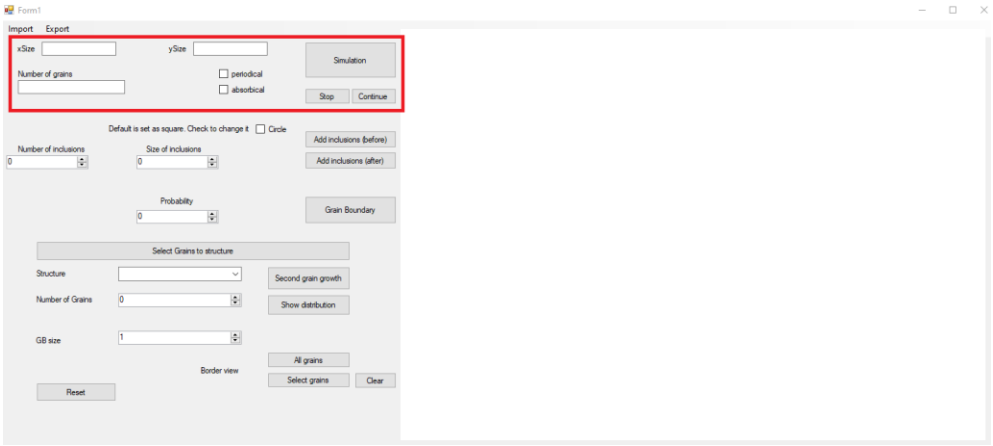

Image 1. GUI + space of generating mesh size and number of grains. Also here you can choose the type of boundary condition

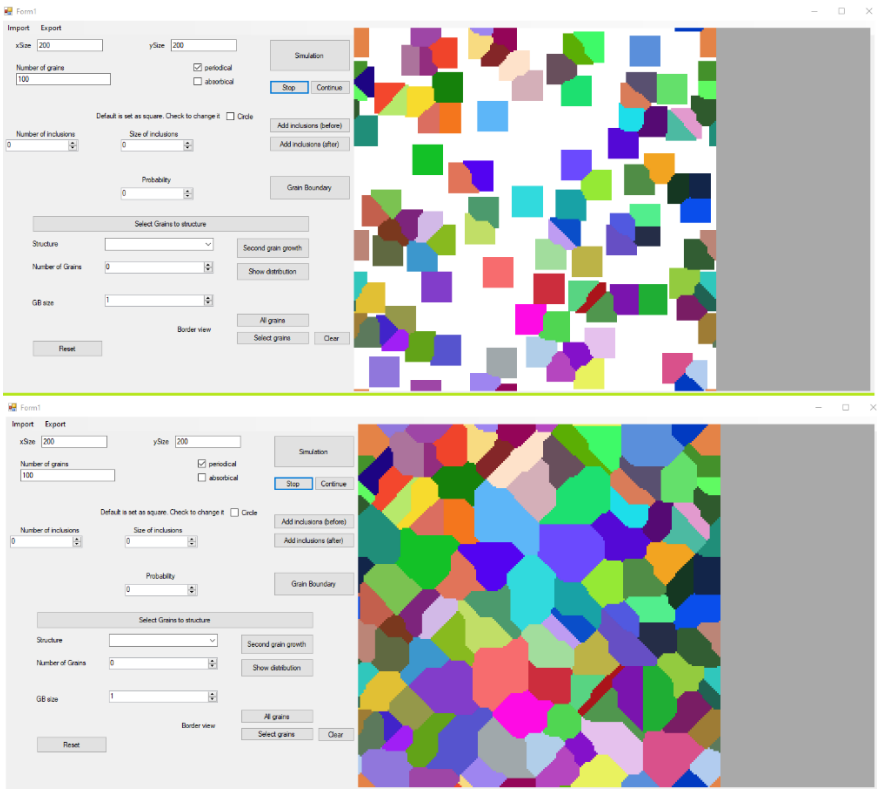

Image 2. View of grain growing for periodic boundary condition. Nucleations are generated randomly

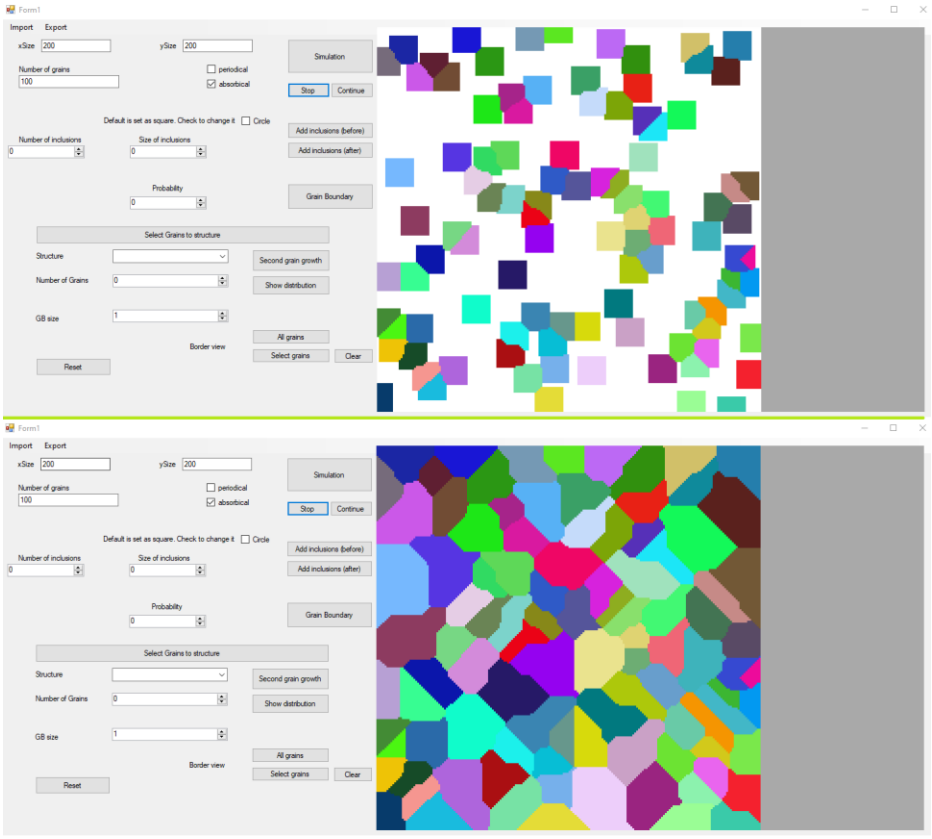

Image 3. View of grain growing for absorbic boundary conditions. Nucleations are generated randomly

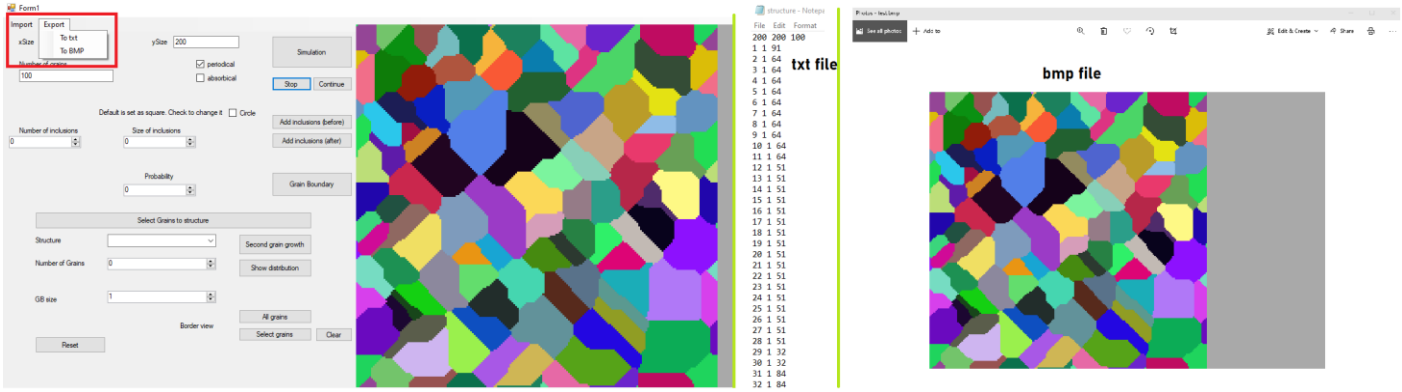

Image 4. Export microstructure to txt or bmp file. Txt file is showing in x, y, id format. It's also available to import data from file to app.

Project 2

At second project our target was create inclusions. There are two ways of generating it – before or after simulation. Also in both, user can choose type of inclusions – square or circle, in both set size of diagonal or radius. In before simulation once, user can choose where will be inclusions by pressing on the mesh. After that there will be generating grains and growing. In the second one, inclusions are generated after grain growing in place, where are borders of grains.

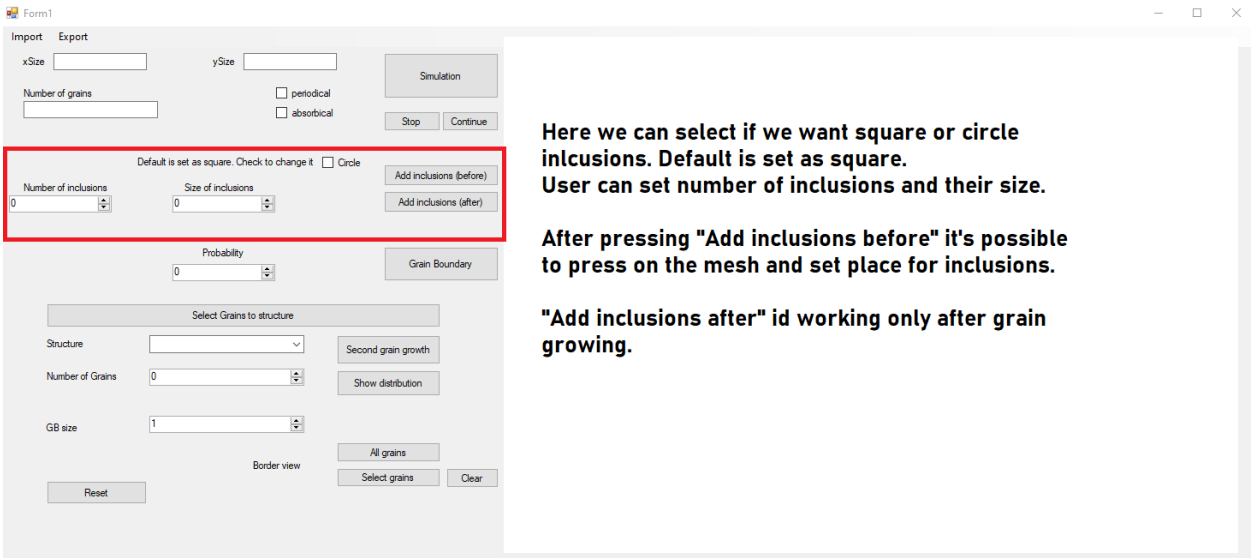

Image 5. GUI part of inclusions

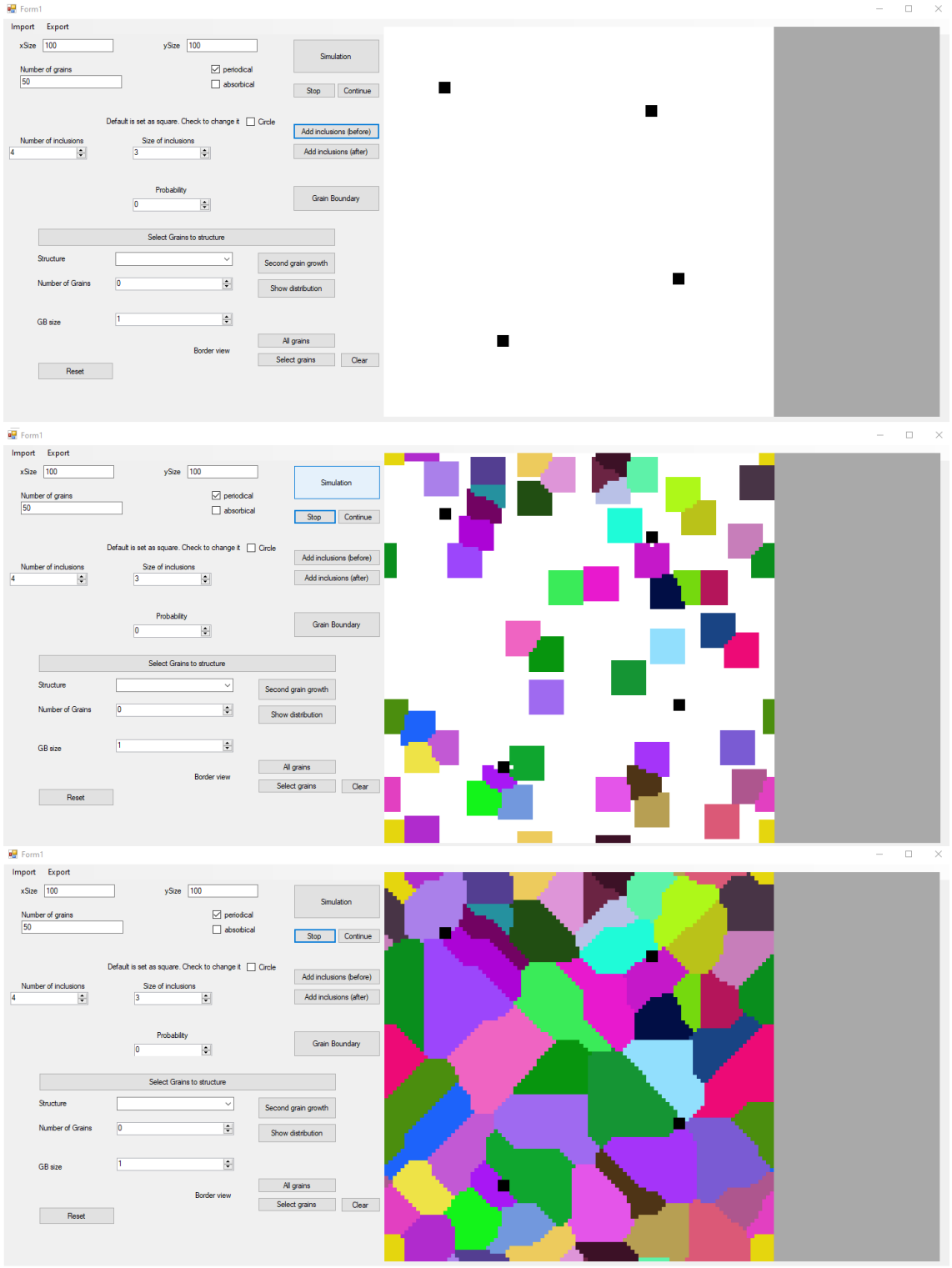

Image 6. Square inclusion before grain growing. Number of inclusions is 4, size is 3.

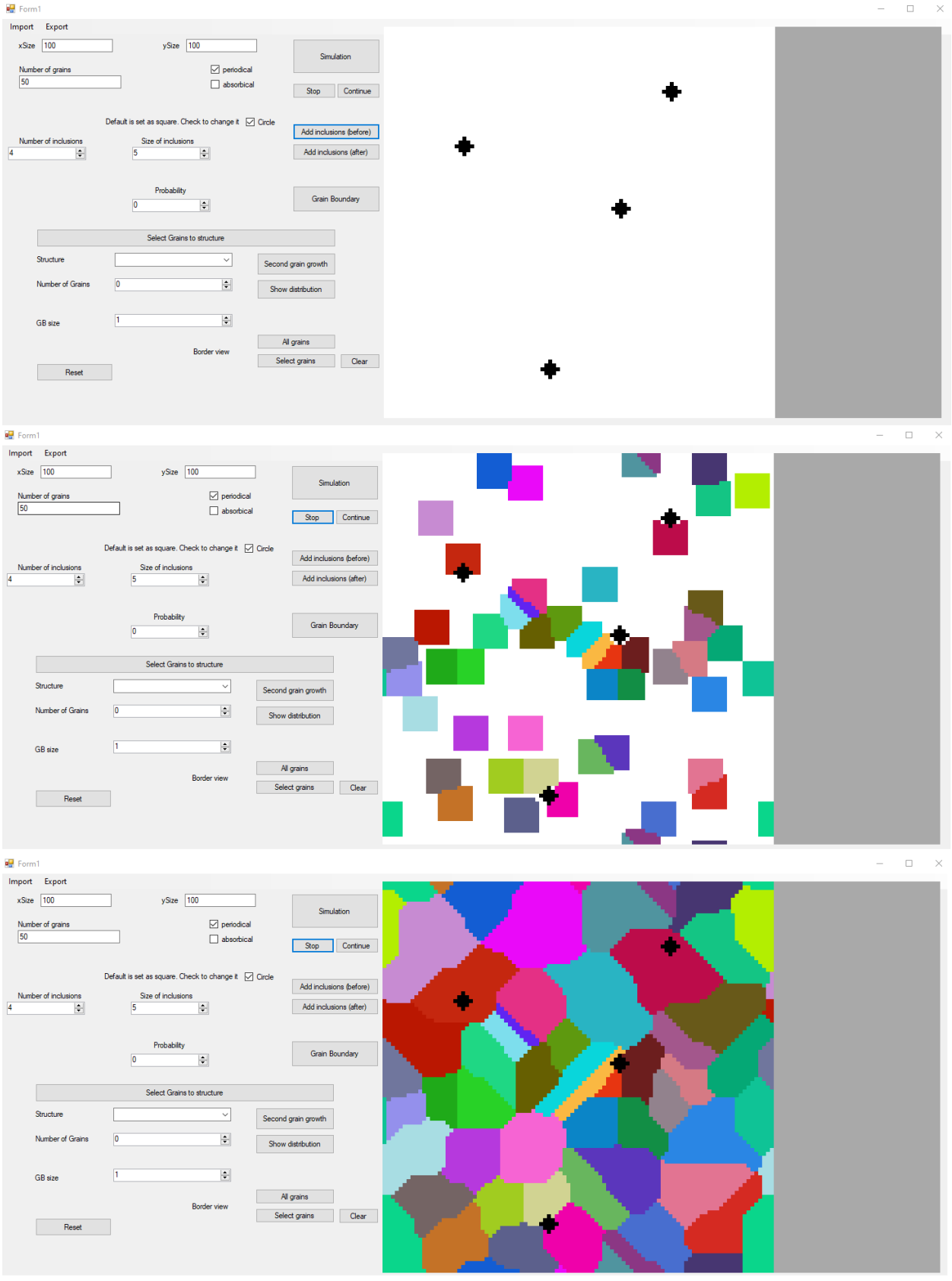

Image 7. Circle inclusions before grain growing. Number of inclusions is 4, size is 5.

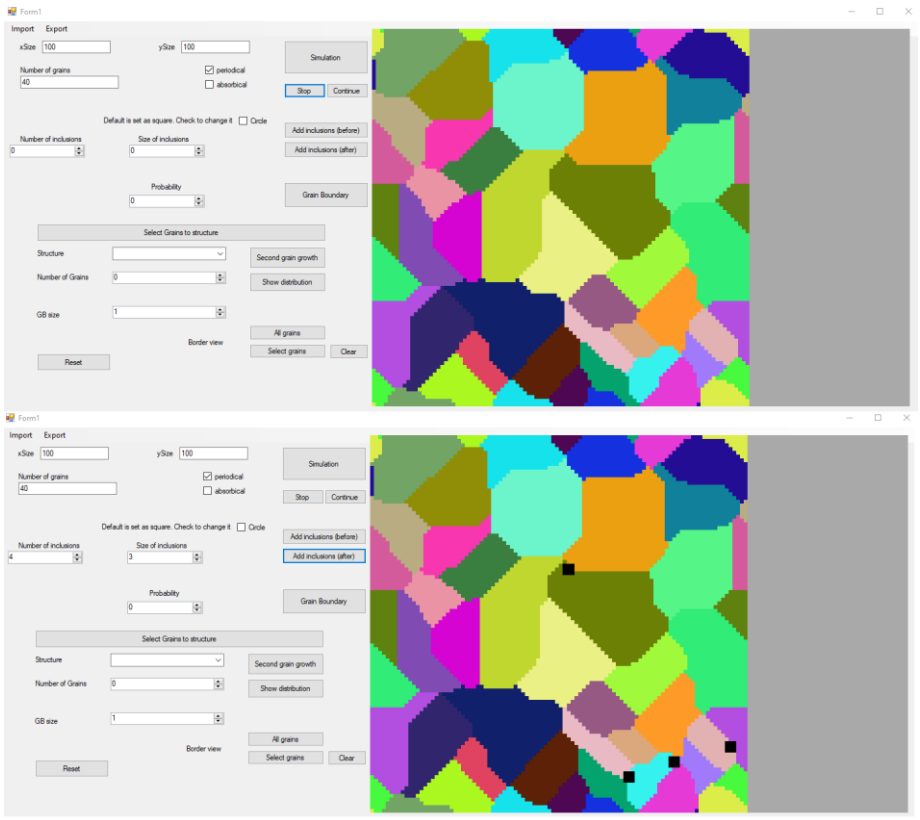

Image 8. View of 4 square inclusions inserted after simulation. There are located randomly from potentially place of grains borders.

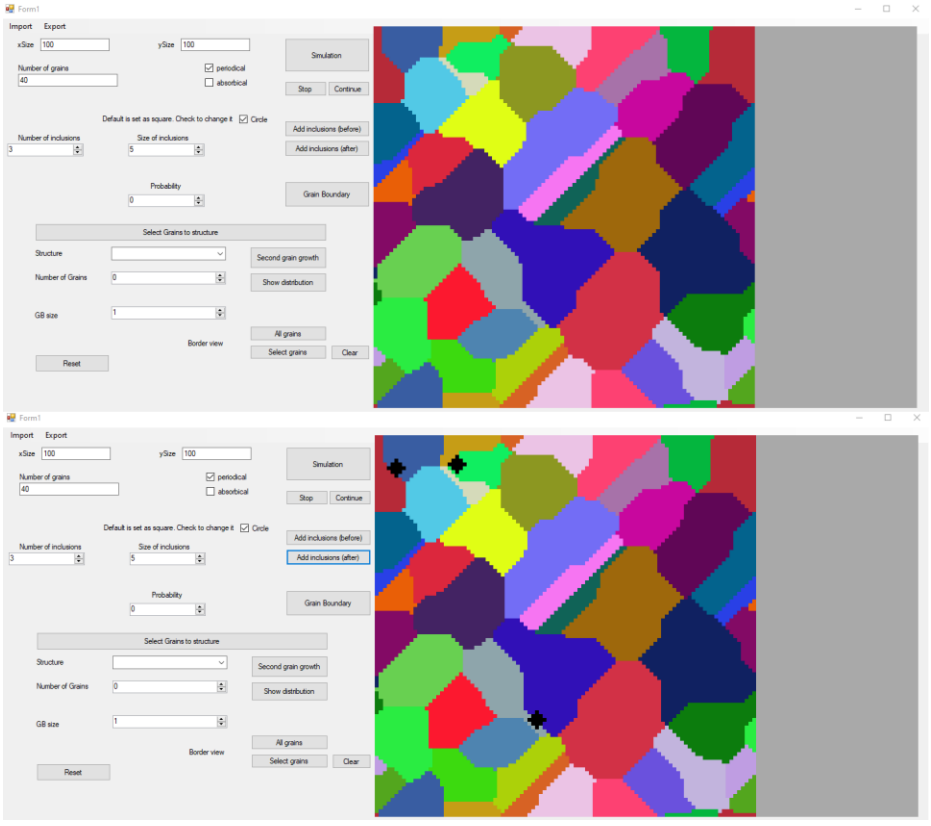

Image 9. View of 3 circle inclusions inserted after simulation. There are located randomly from potentially place of grains borders.

Project 3

In this part of app I implemented grain boundary shape control feature. It's a kind of grain growing but we can control the way of it providing the probability with which cells are changing theirs state. At first step we are checking how many neighbors have the same state from all eight available neighbors. If more or equal to five, we change the id of current cell to id neighbor cell. If not, we have to check how many the nearest neighbors have the same id. If more or equal to three, we change the id of current cell to id of neighbor cell. If not, in the next step we are checking how many further neighbors have the same state. If more or equal to three, we change the id of current cell to id of neighbor cell. But if not, in the last step we change the id of current cell to the most frequent id from all neighbors with provided % probability.

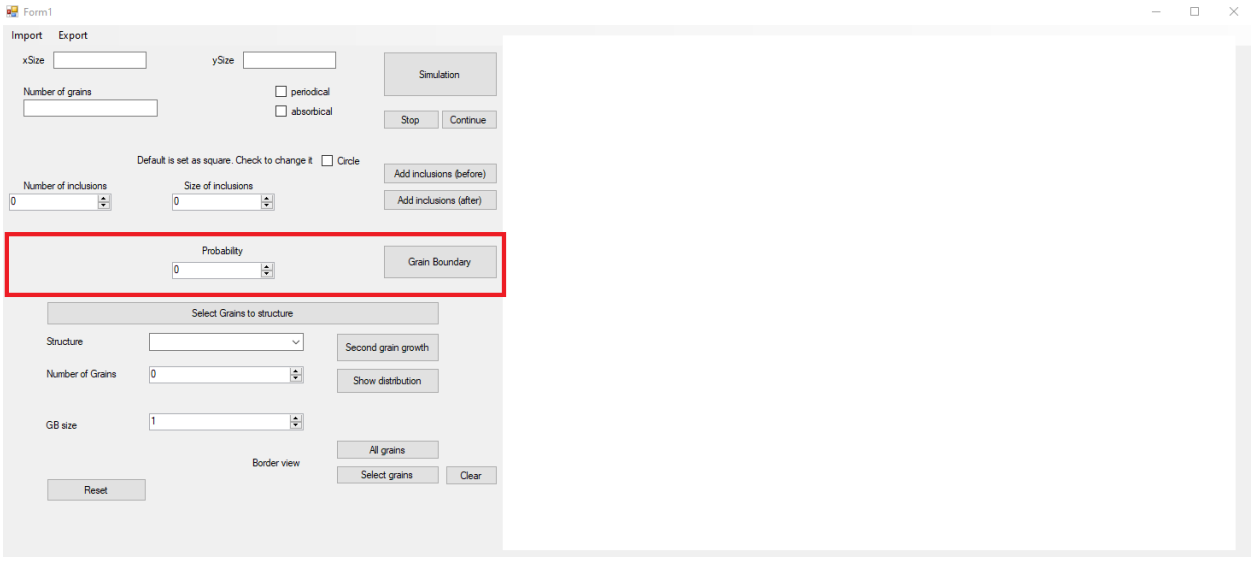

Image 10. GUI for Shape Control part. User can set probability for rule 4.

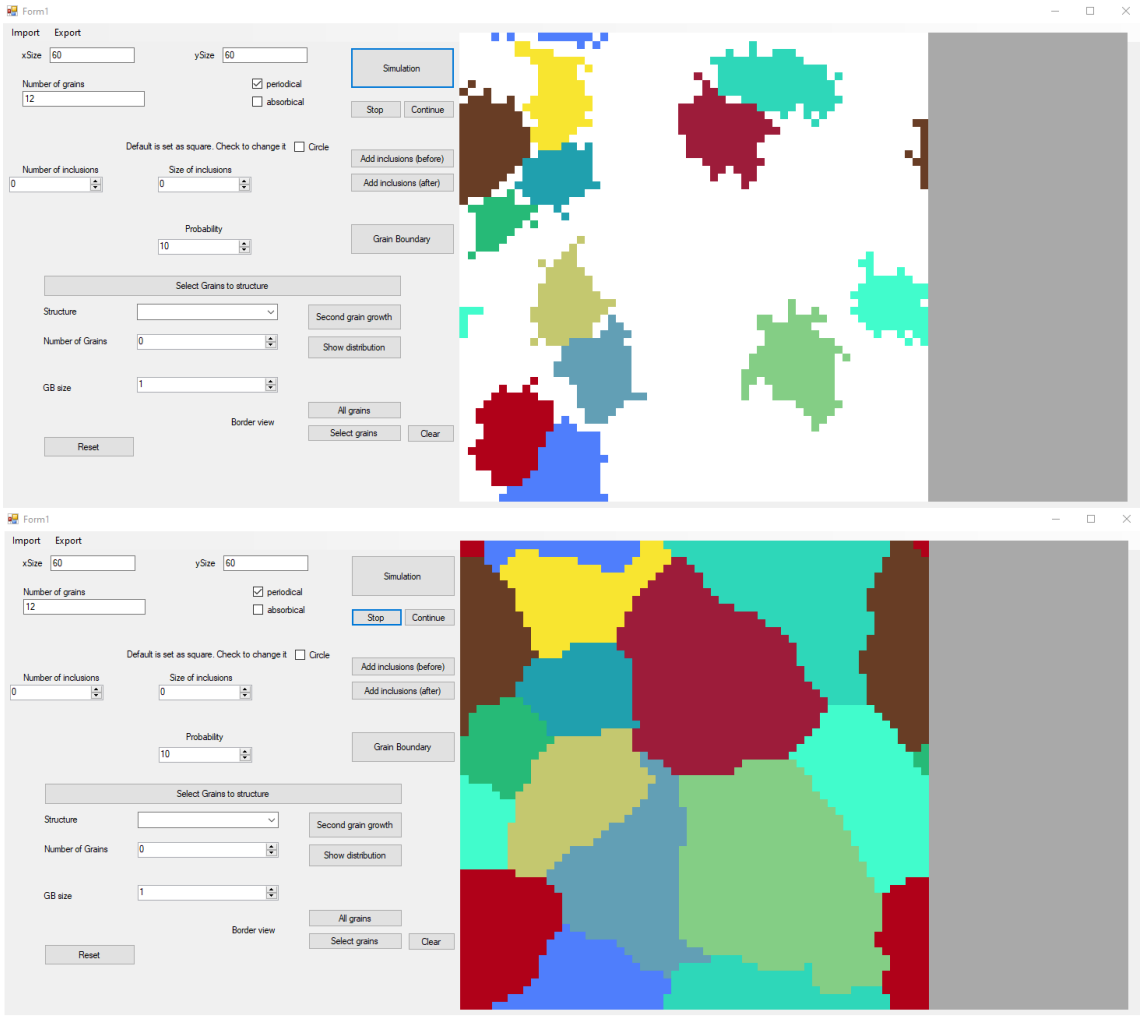

Image 11. Grain growth with 10% probability for rule 4

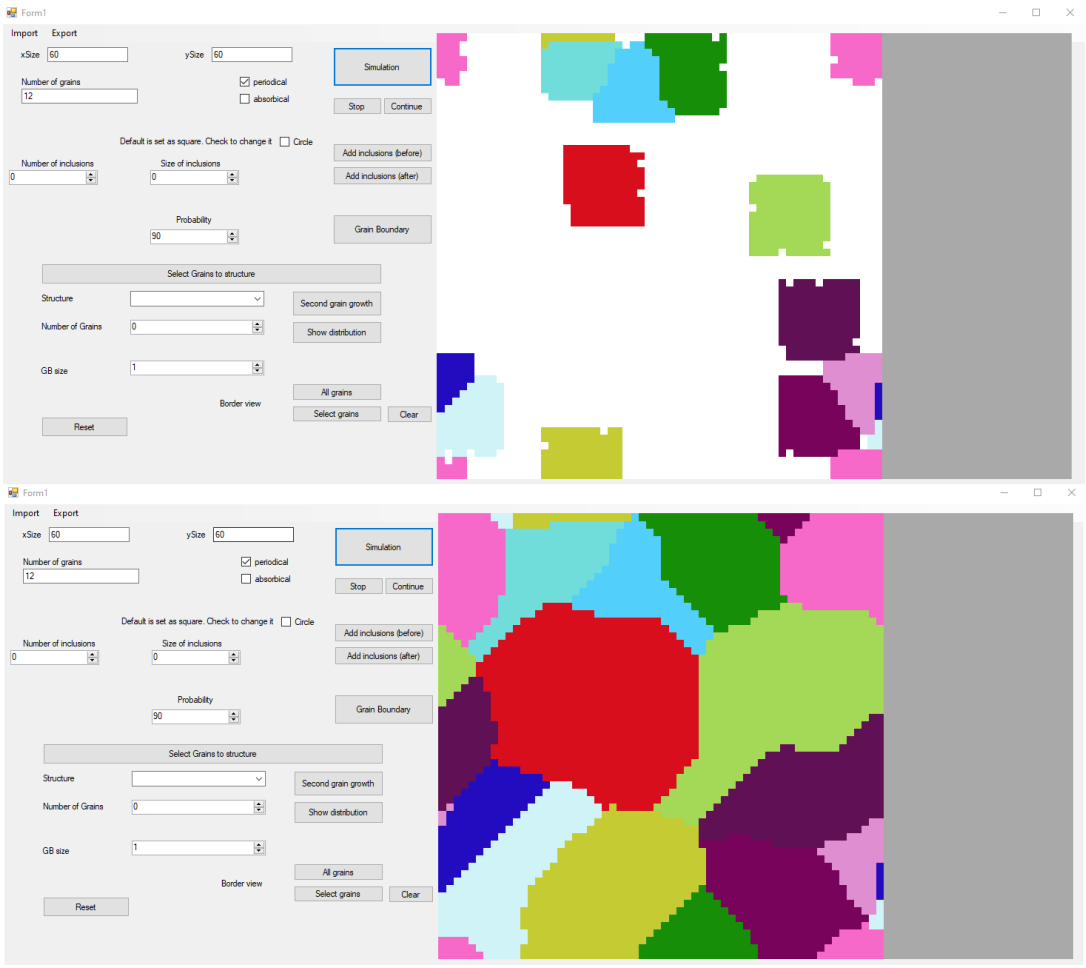

Image 12. Grain growth with 90% probability for rule 4.

Project 4

4th task required from us to implement second grain growth using CA methodology but in two ways – substructure and dual phase. In first one after grain growth simulation user can choose few grains which should stay on the mesh. The rest is disappearing and in their place (now blank) are generating new nucleations (user provide number of grains in second simulation). After that is growing of new grains. In "dual phase" type the difference is in one thing. Selected grains which should stay on the mesh, receive id of first selected grain.

After both types of second growing, it's possible to generate txt file pressing "Show distribution" button. In this file is list of id, number how many cells have this id and % contribution of each id in comparison to all cells.

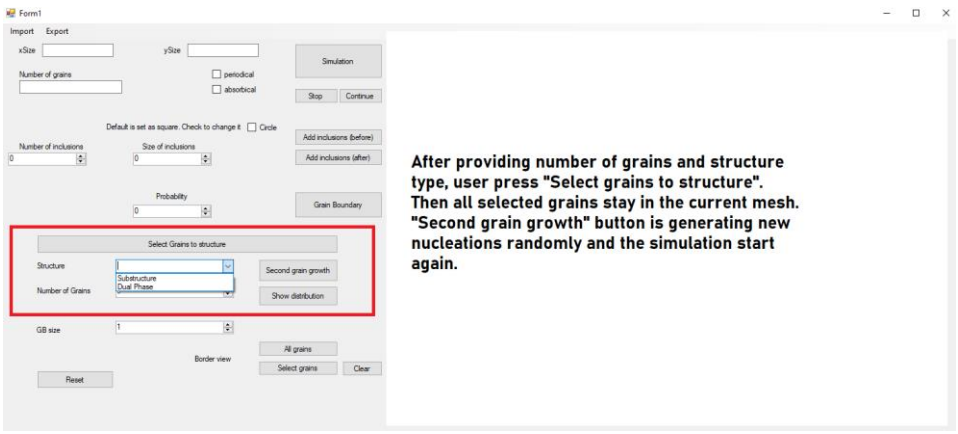

Image 13. GUI for Second grain growth of selected type of structure.

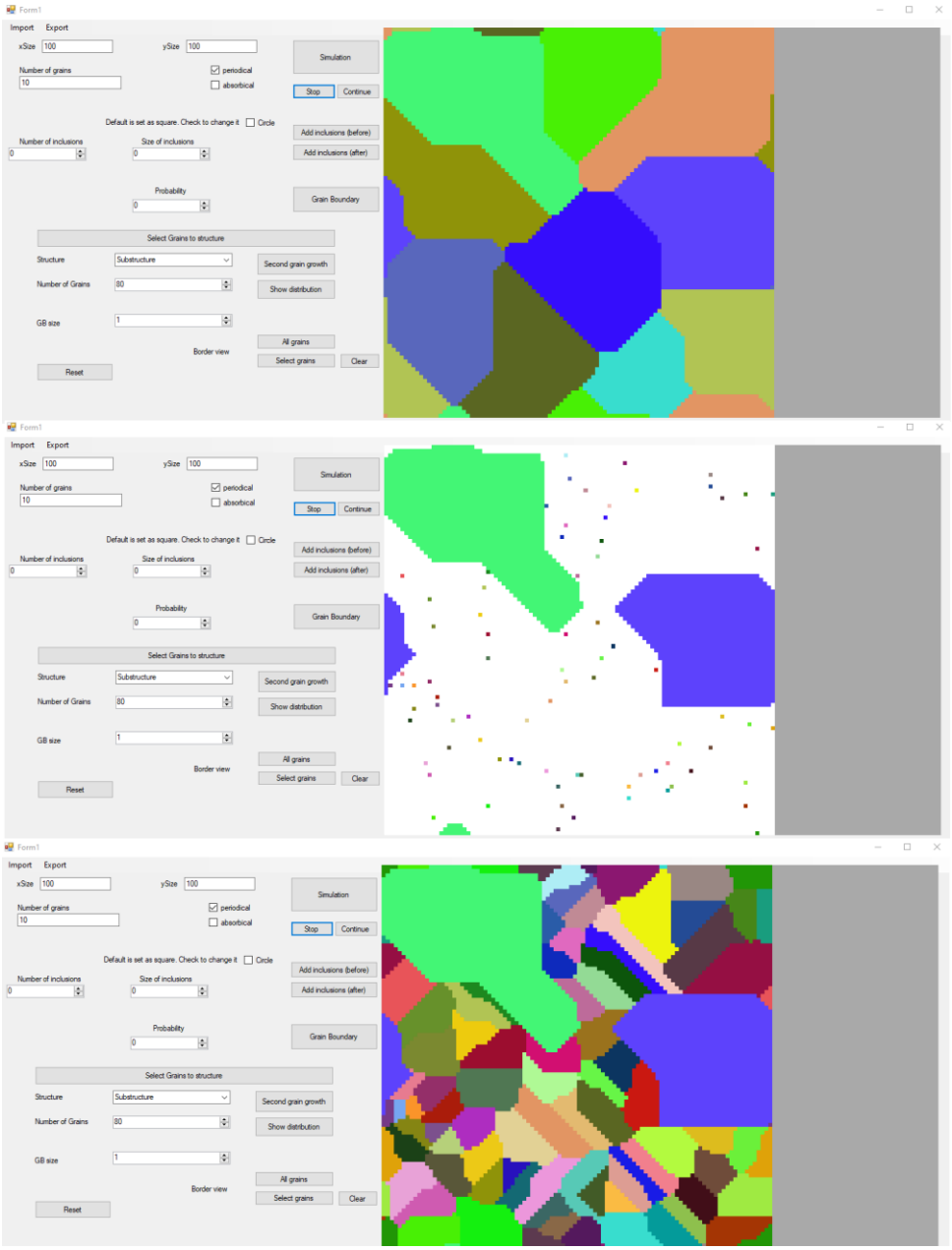

Image 14. Second grain growth for 80 new nucleations – substructure. Selected only 2 grains from first simulation

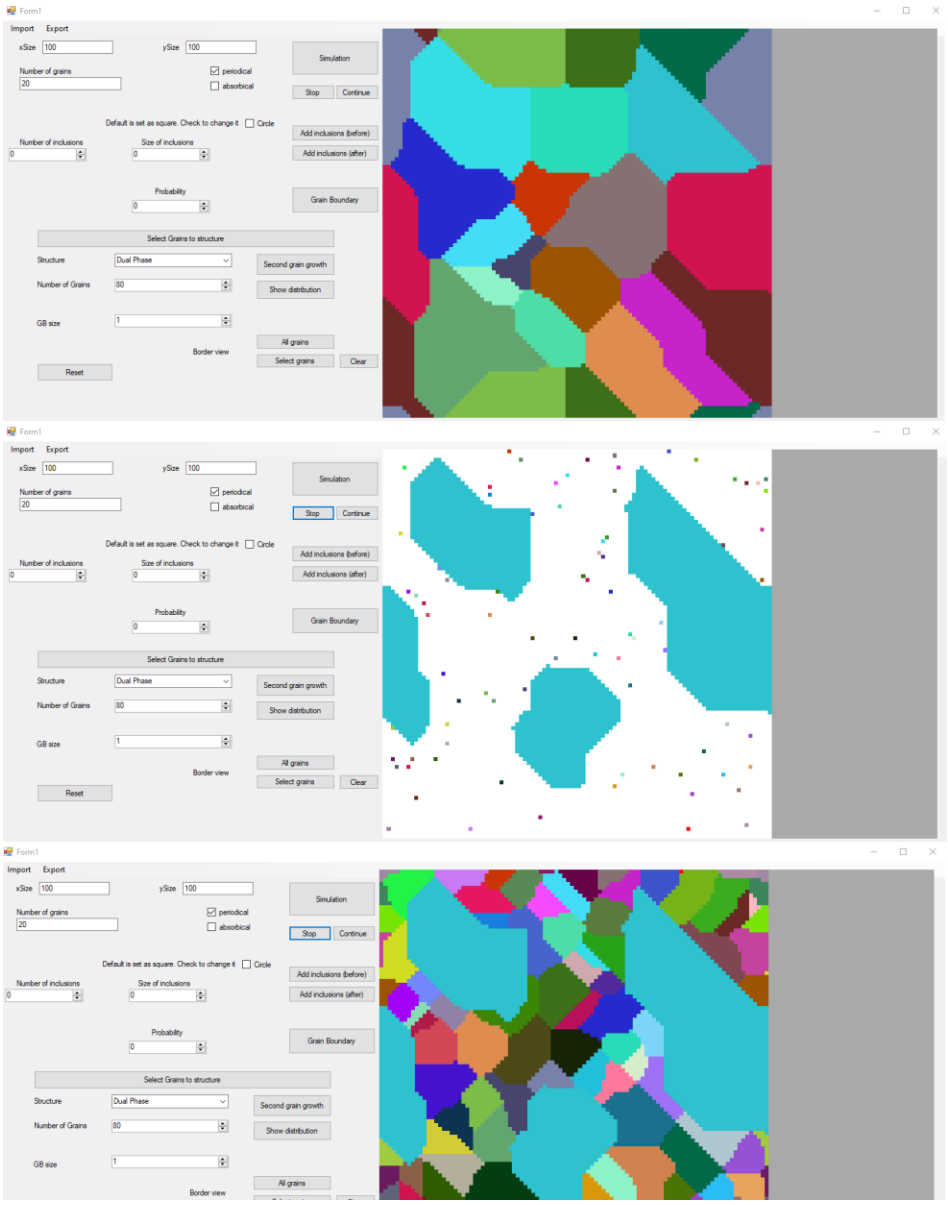

Image 15. Second grain growth for 80 new nucleations – dual phase. Selected 5 grains from first simulation.

distribution - Notepad

File Edit Format View Help

```
id size %
0 0 0
1 3061 30.61
2 57 0.57
3 144 1.44
4 86 0.86
5 63 0.63
6 113 1.13
7 55 0.55
8 89 0.89
9 68 0.68
10 102 1.02
11 118 1.18
12 154 1.54
13 89 0.89
14 142 1.42
15 76 0.76
16 23 0.23
17 47 0.47
18 70 0.7
19 25 0.25
20 125 1.25
```

Image 16. Distribution file. It's showing all available id, count how many cells have this id and % contribution in all mesh.

Project 5

The last part of app is related to borders of grains. The most important is provide size of borders in “GB size” text box. After grain growth user can generate borders of all or only selected grains. To do this, “All grains” button will show borders of all grains with GB size. But when user press “Select grains”, he can choose which grains should show theirs borders. “Clear” button will show us borders of selected grains.

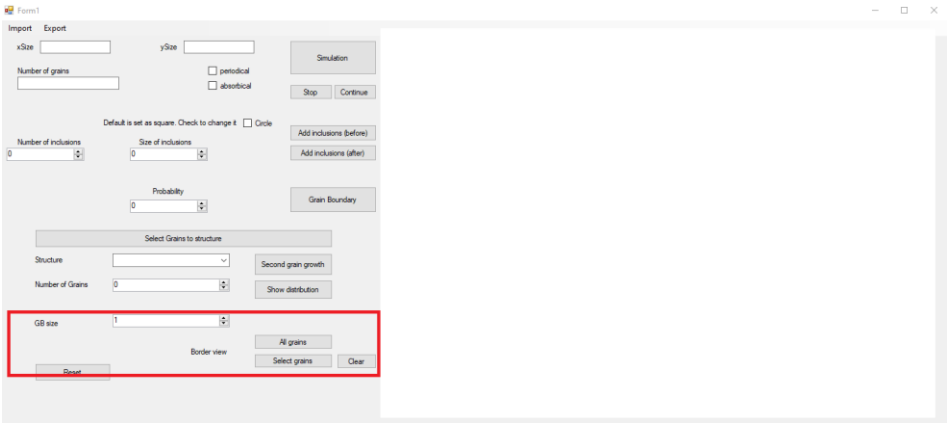

Image 17. GUI for grain borders part.

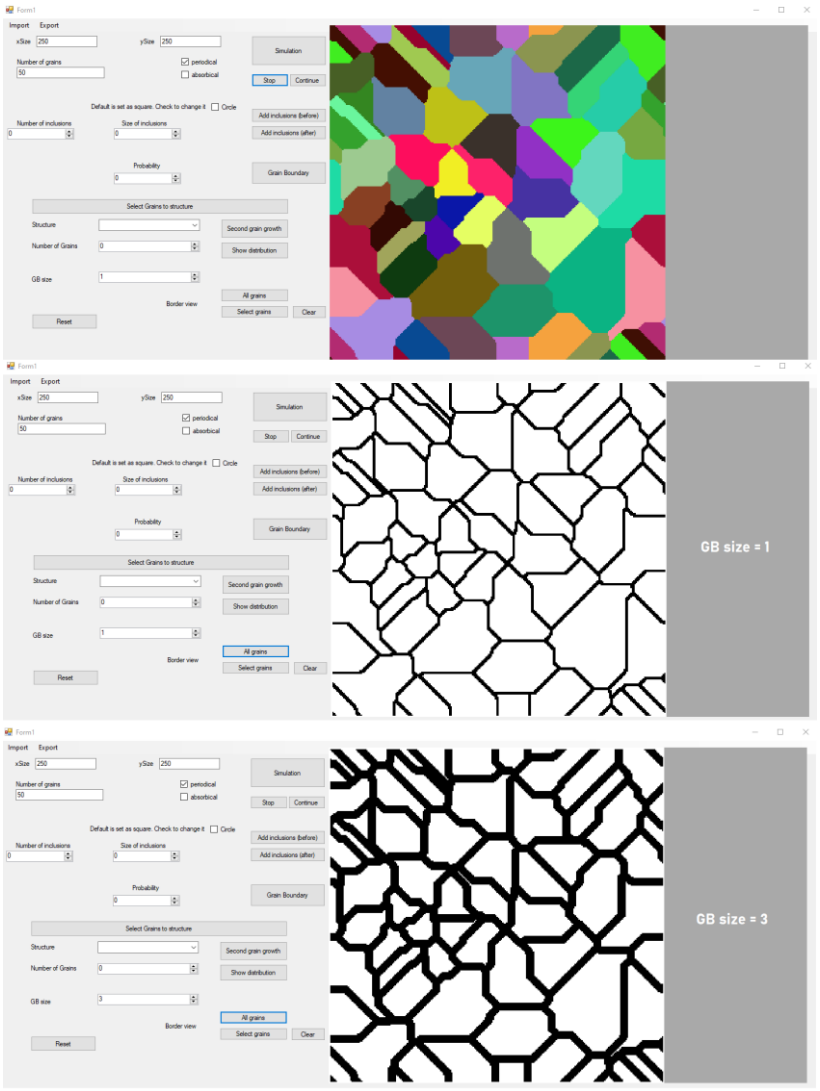

Image 18. Borders of all grains with 1 and 3 border size.

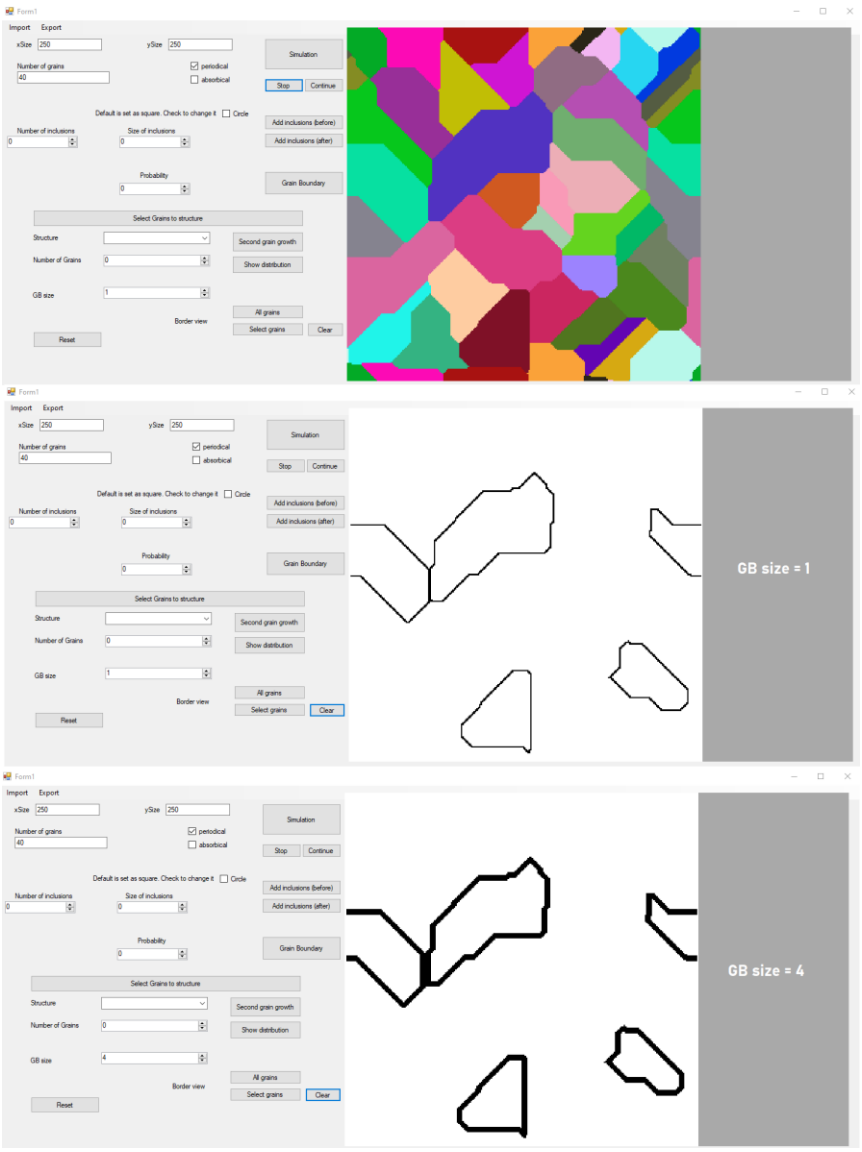

Image 19. Borders of selected grains with 1 and 4 border size.

Summarize

Created app has many features. I successfully implemented the most important – grain growth with Moore neighborhood. Apart from that I have showed inclusions (before and after grain growing), Shape Control CA, second grain growth in two types (substructure and dual phase) and grain borders with setting of border size. These features presents that it's possible to develop this app further. Implementing more and more functionalities can simulate many extra variants of microstructure.