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Grain growth - report

Multiscale Modelling

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1. GUI description

1.1. Main menu - *Ref. 1*

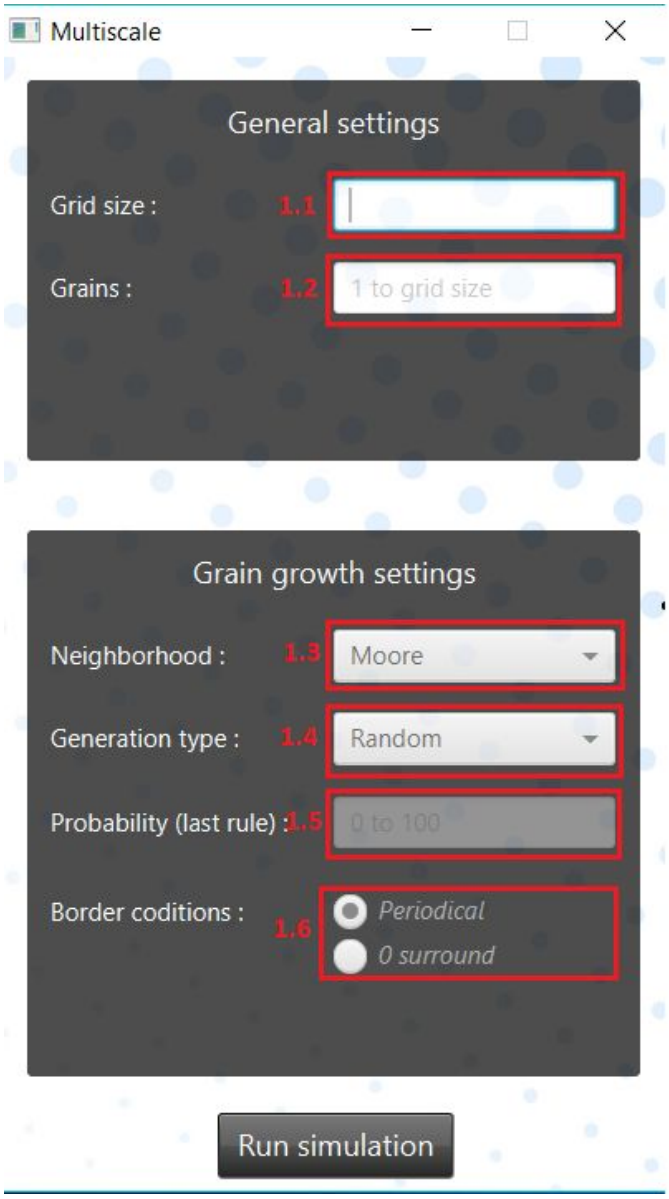
It contains all necessary settings for simulation:

- *Grid size:* ***(1.1)***,
    - Range: 10 - 1920
- *Grains:* ***(1.2)***,
    - Range: 1 - *Grid size*

like also more advanced information:

- *Neighborhood:* ***(1.3)***
    - *Moore*
    - *Advanced - Moore* with specific probability for last rule
- *Generation type:* ***(1.4)***
    - *Random*
    - *Manual selection*
- *Probability (last rule):* ***(1.5)*** - available only in *Neighborhood - Advanced*
    - Range: 0 - 100 *(in percent)*
- *Border conditions:* ***(1.6)***
    - *Periodical*
    - *0 surround*

To start simulation press button: *Run simulation*.



Ref. 1 Main menu

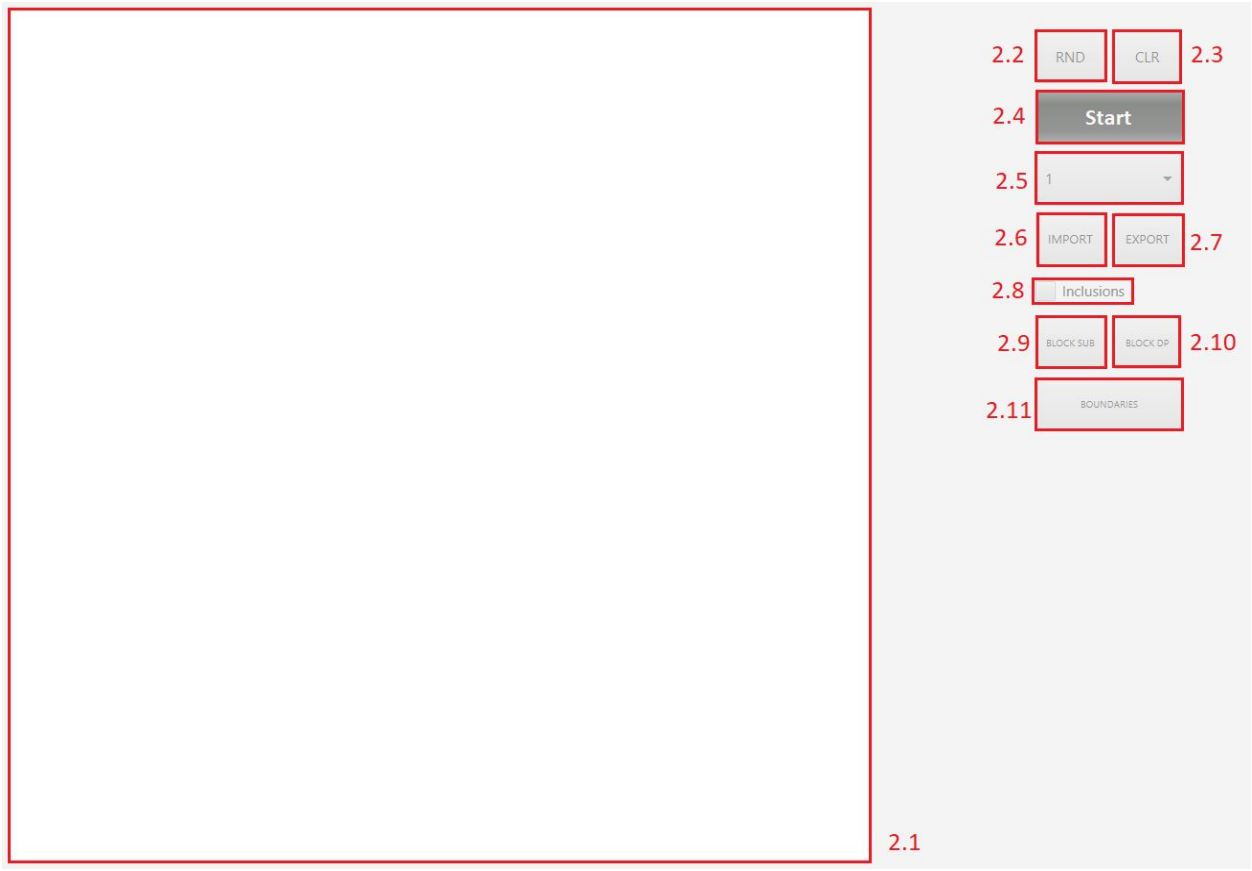
1.2. Simulation window - *Ref. 2*

After click *Run simulation* button in *Main menu, Simulation window* will shown in fullscreen.

Window contains:

- *Simulation canvas:* ***(2.1)***
    - Show current state of simulation.
- *Randomize grains button:* ***(2.2)***
    - Create random grains on *Simulation canvas* ***(2.1)*** - depends of the number of *Grains* ***(1.2)*** from *Main menu.* Can be used multiple times.
- *Clear canvas button:* ***(2.3)***
    - Clear everything that was shown in *Simulation canvas*
- *Start/Stop simulation button:* ***(2.4)***
    - Start/stop simulation
    - Number of iterations depends of ***(2.5)***
- *Number of iterations dropdown:* ***(2.5)***
    - Set number of iterations
    - Available: 1, 10, 50, 100, 500, 2000, Continuous
- *Import button:* ***(2.6)***
    - Import external file which will be shown in *Simulation canvas* ***(2.1)***
    - Available formats: .txt, .csv, .bmp, .gif, .png
- *Export button:* ***(2.7)***
    - Export current state of *Simulation canvas* ***(2.1)***
    - Available formats: .txt, .csv, .bmp, .gif, .png
- *Inclusions checkbox:* ***(2.8)***
    - Set inclusions to be used in simulation
    - More at: **chapter 1.3**, **2.3**
- *Block substructure button:* ***(2.9)***
    - Set selected grain(s) in *Simulation canvas* ***(2.1)*** to be blocked as substructure
    - More at: **chapter 2.5**

- *Block dualphase button:* ***(2.10)***
    - Set selected grain(s) in *Simulation canvas* ***(2.1)*** to be blocked as dualphase
    - More at: **chapter 2.5**
- *Boundaries button:* ***(2.11)***
    - Show boundaries of grains with chosen width
    - More at: **chapter 2.6**



Ref. 2 Simulation window

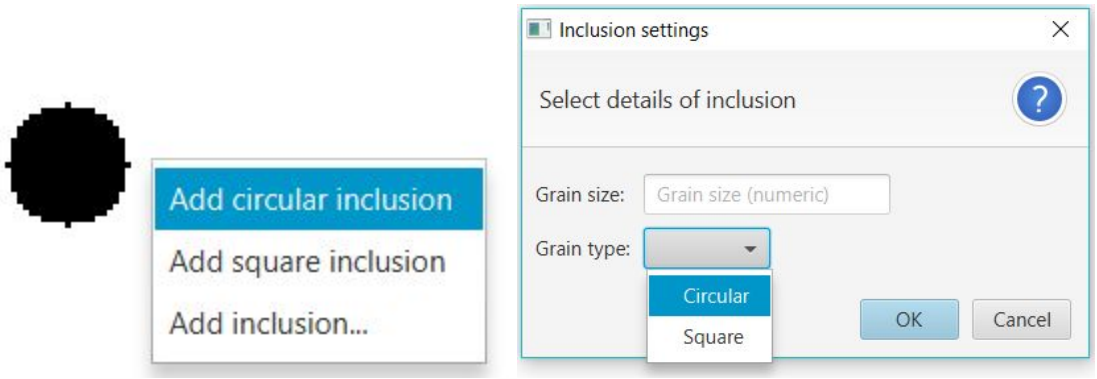
1.3. Inclusions - *Ref. 3*

If checkbox ***(2.8)*** is checked and *Simulation canvas* ***(2.1)*** is empty, after you click *Randomize grains button* ***(2.2)***, random grains and random inclusions will be generated (circular or square).

If simulation is completed checkbox ***(2.8)*** and click on ***(2.2)*** will generate random inclusions on grains boundaries (circular or square).

If *Generation type:* ***(1.4)*** is selected as *Manual selection*, you are be able to use *Inclusions context menu*, when you use *Right Mouse Button.* In which position you click on *Simulation canvas* ***(2.1)***, there inclusion will appear.

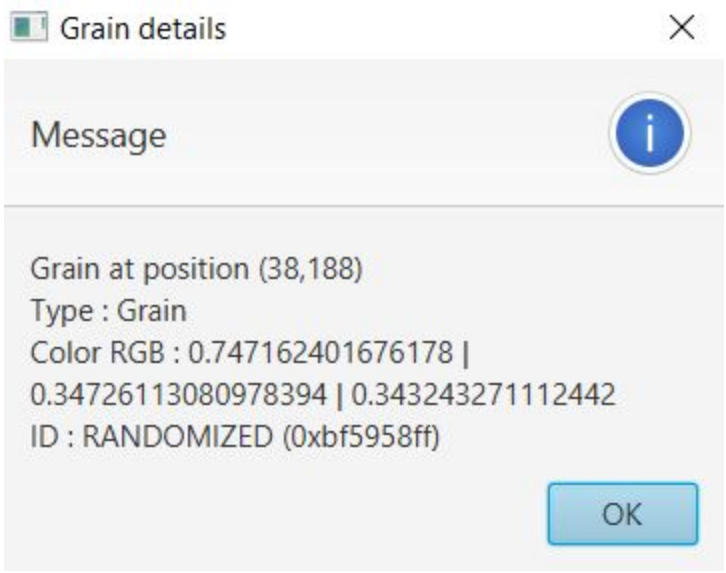
- *Inclusions context menu* ***(3.1)*** contains:
    - *Add circular inclusion* - predefined default circular inclusion
    - *Add square inclusion* - predefined default square inclusion
    - *Add inclusion…* - create custom inclusion
        - *Grain size* - size of inclusion, for circle is radius, for square is width
        - *Grain type* - type of inclusion
            - Available: *Circular, Square*



Ref. 3 Inclusion context menu and Inclusion settings

1.4. Grain details - *Ref. 4*

If *Simulation canvas* ***(2.1)*** contains some results, you are able to click on any grain using shortcut *Ctrl + LMB*. After this popup window with information about this grain will be shown



Ref. 4 Grain details popup window

2. Tips and results

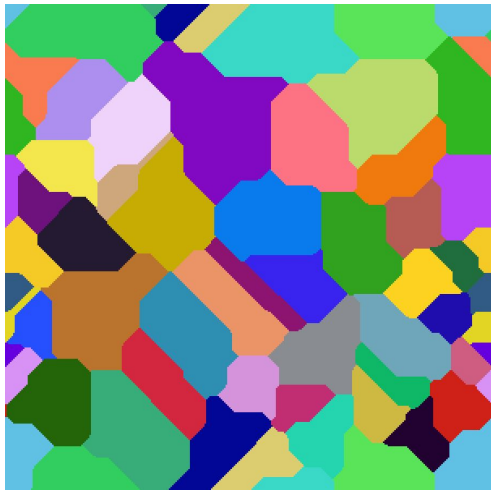
*Every result is by using Grid size **(1.1)** = 300, Grains **(1.2)** = 50 and if it used Probability (last rule): **(1.5)** = 50*

2.1. Simple grain growth

To run simple grain growth:

- Step 1. Set valid values for *Grid size **(1.1)*** and *Grains **(1.2)***
- Step 2. Set *Neighborhood **(1.3)*** to *Moore*
- Step 3. Set *Generation type **(1.4)*** depends of your preferences.
- Step 4. Run simulation
- Step 5. After this *Simulation window **(Ref. 2)*** will be shown
- Step 6. Click *RND button **(2.2)*** to generate random grains OR Select grains manually on *Simulation canvas **(2.1)***
- Step 7. Set value for *Number of iterations dropdown **(2.5)***
- Step 8. Click *Start/Stop simulation button **(2.4)***
- Step 9. You can pause simulation whenever you want by Click *Start/Stop simulation button **(2.4)*** again.

Results:



Ref. 5 Simple grain growth with Moore neighborhood

2.2. Import and Export

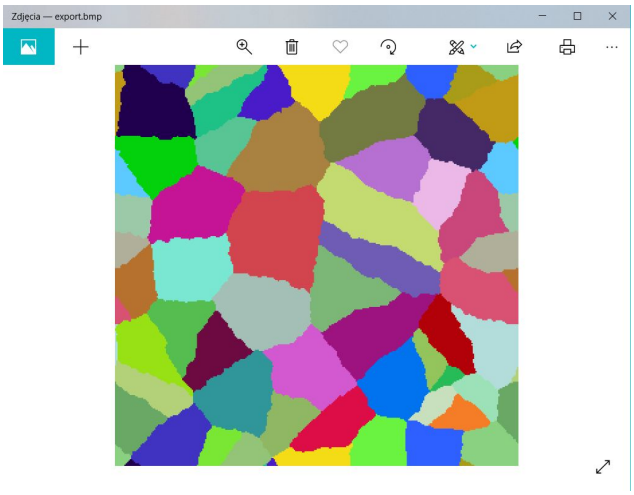
To import external simulation results:

- Step 1. Proceed Stap 1 - 4 from **chapter 2.2**
- Step 2. Click *Import button* ***(2.6)***
- Step 3. Choose your valid file
- Step 4. After few seconds your file should be available for further changes on *Simulation canvas* ***(2.1)***
- **WARNING!** If you want to import file in format .txt or .csv you need to use pattern from ***Ref. 7*** (for .txt) or ***Ref. 8*** (for .csv)

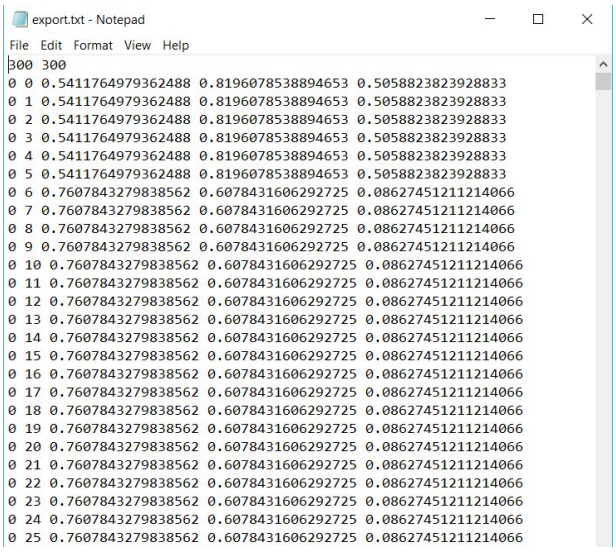
To export current state of *Simulation canvas* ***(2.1)***:

- Step 1. Finish simulation or pause it in some stage by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Click *Export button* ***(2.7)***
- Step 3. Choose extension of file and location to save
- Step 4. After few seconds your file should be saved in chosen location.

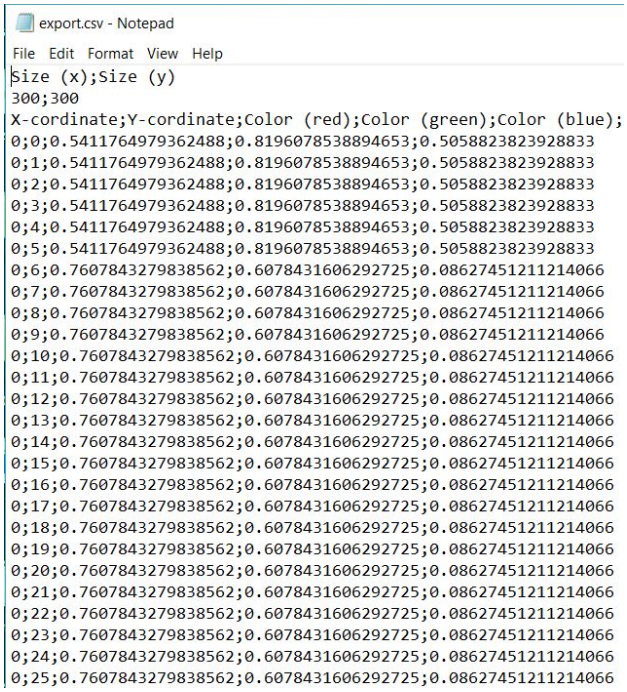
Results:



Ref. 6 Export as .png file



Ref. 7 Export as .txt file



Ref. 8 Export as .csv file

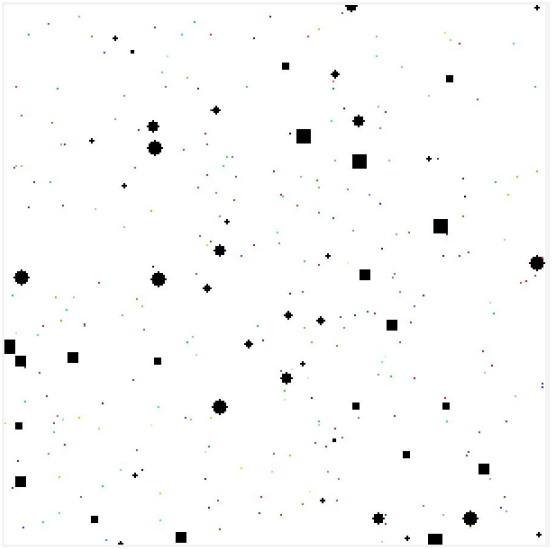
2.3. Inclusions

To include inclusions in simulation you can do it to two different ways:

2.3.1. Add inclusions before simulation

- Step 1. Run simulation
- Step 2. Check *Inclusions checkbox:* ***(2.8)***
- Step 3. Click *RND button* ***(2.2)***
- **INFO:** If you choose *Generation type:* ***(1.4)*** to *Manual selection* you can also use *Inclusions context menu* ***(3.1)*** from **chapter 1.3**
- Step 4. Set value for *Number of iterations dropdown* ***(2.5)***
- Step 5. Click *Start/Stop simulation button* ***(2.4)*** to proceed

Results:

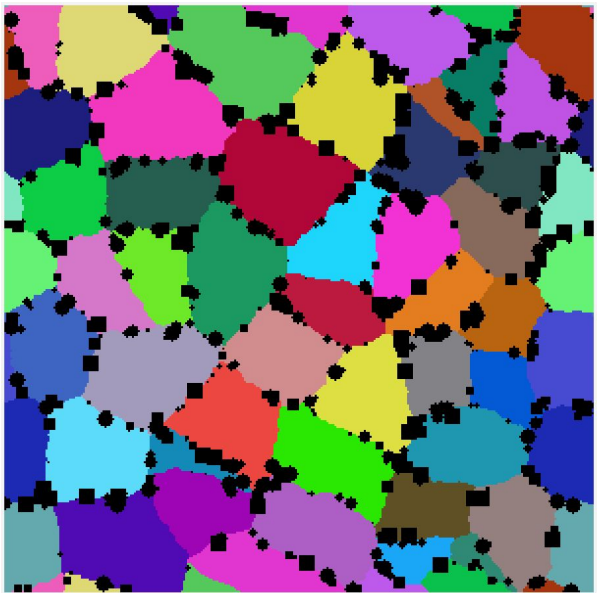


Ref. 9 Generated inclusions before simulation

2.3.2. Add inclusions after simulation on grains boundaries

- Step 1. Finish simulation by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Check *Inclusions checkbox:* ***(2.8)***
- Step 3. Click *RND button* ***(2.2)***
- Step 4. Inclusions will be shown on grains boundaries

Results:



Ref. 10 Inclusions on grains boundaries

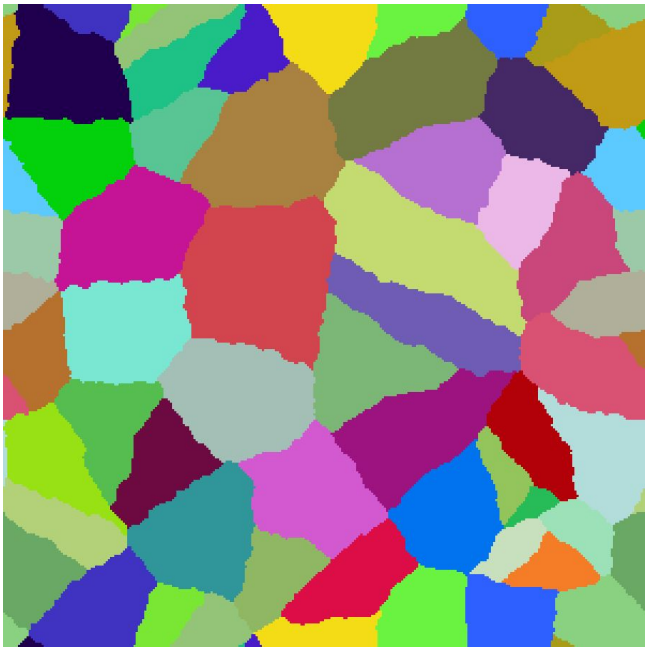
2.4. Advanced Moore

To run simulation using probability for last rule:

- Step 1. Proceed Step 1- 3 from **chapter 2.1**
- Step 2. Select *Advanced* from *Neighborhood* ***(1.3)***
- Step 3. Enter custom *Probability (last rule):* ***(1.5)***
- Step 4. Run Simulation
- Step 5. Proceed Step 5 - 9 from **chapter 2.1**

INFO: Instructions from **chapter 2.2** and **2.3** also work in this type of simulation

Results:



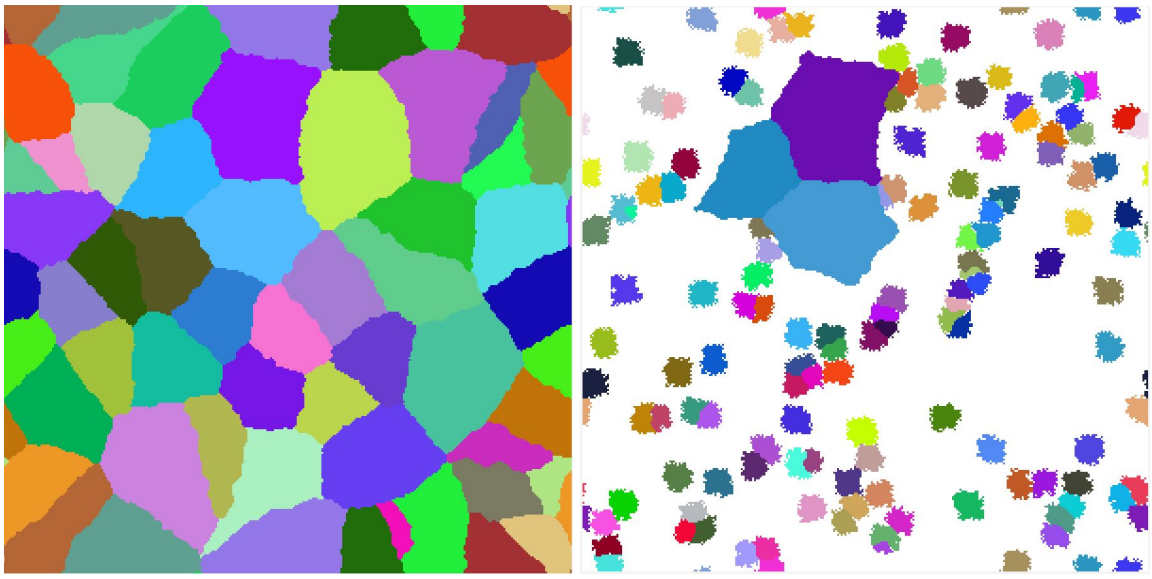
Ref. 11 Simulation with probability set to 50

2.5. Substructure and dualphase

To use substructure:

- Step 1. Finish simulation by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Click grains on *Simulation canvas* ***(2.1)*** that you what to add to substructure
- Step 3. Click *Block substructure button:* ***(2.9)***
- Step 4. Click *RND button* ***(2.2)***
- Step 5. Set value for *Number of iterations dropdown* ***(2.5)***
- Step 6. Click *Start/Stop simulation button* ***(2.4)***
- Step 7. Simulation with blocked grains will run

Results:

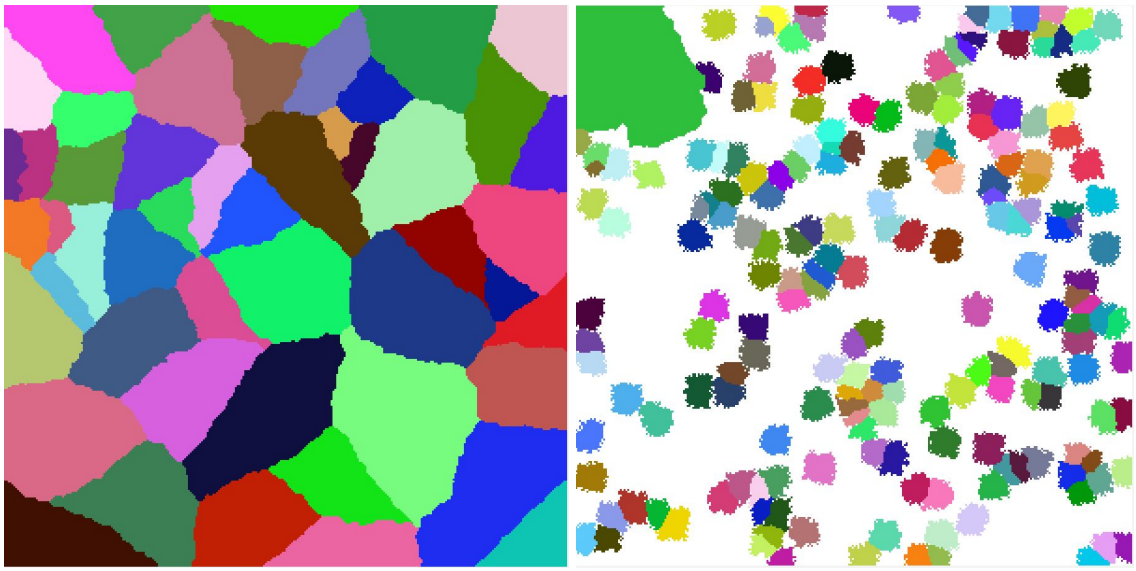


Ref. 12 Before and after block grains for substructure

To use dualphase:

- Step 1. Finish simulation by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Click grains on *Simulation canvas* ***(2.1)*** that you what to add to substructure
- Step 3. Click *Block dualphase button:* ***(2.10)***
- Step 4. Click *RND button* ***(2.2)***
- Step 5. Set value for *Number of iterations dropdown* ***(2.5)***
- Step 6. Click *Start/Stop simulation button* ***(2.4)***
- Step 7. Simulation with blocked grains will run

Results:



Ref. 13 Before and after block grains for dualphase

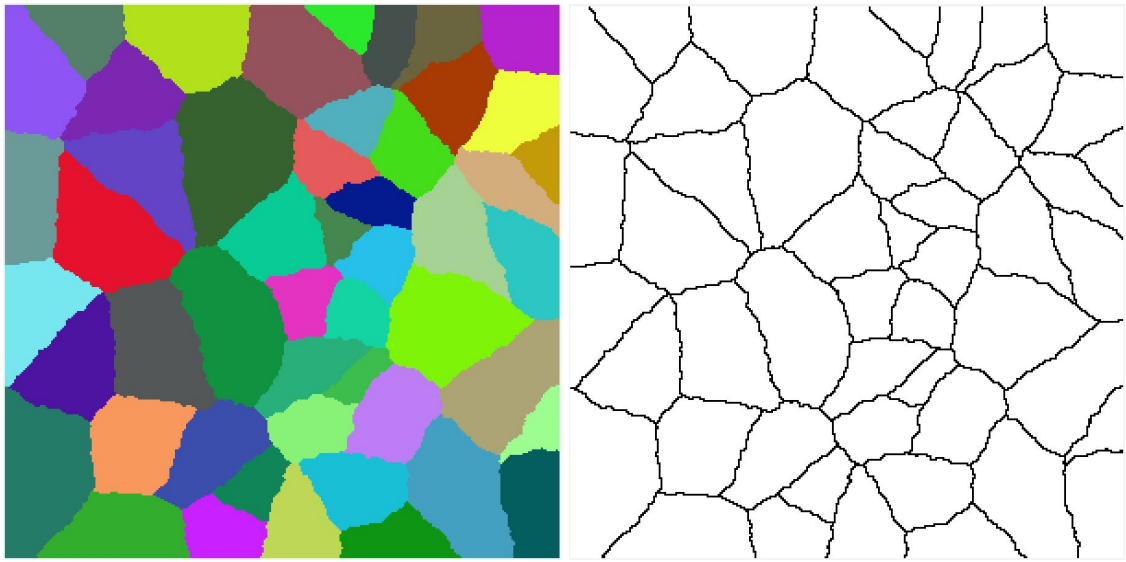
2.6. Grains boundaries

To display boundaries in simulation you can do it to two different ways:

2.6.1. Overall boundaries

- Step 1. Finish simulation by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Click on *Boundaries button* ***(2.11)***
- Step 3. Popup window will be shown ***Ref. 16***, enter your border width
- Step 4. Click *OK*

Results:

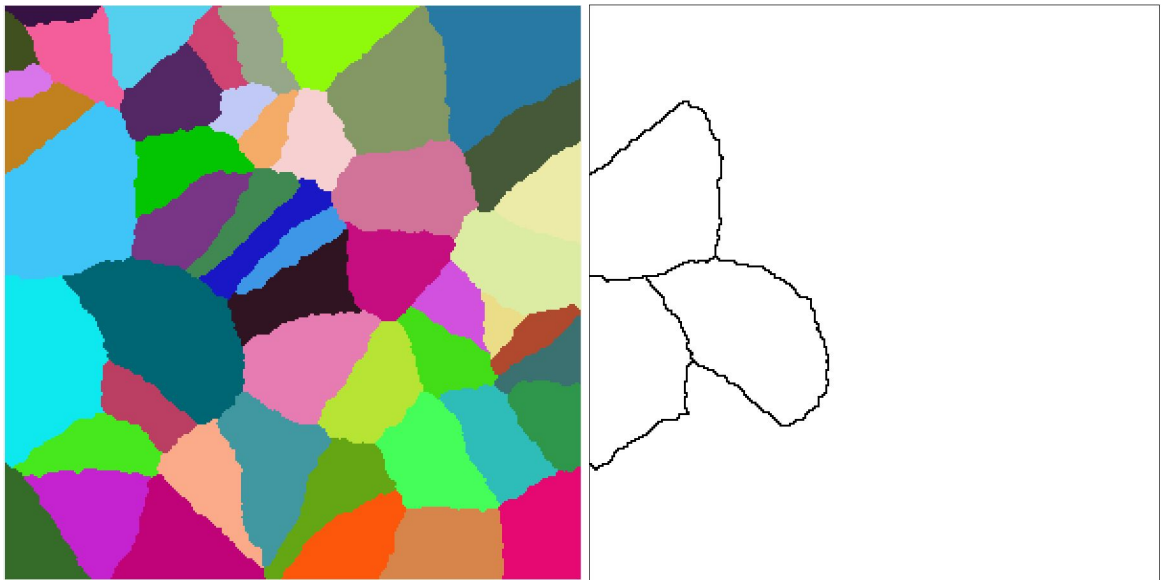


Ref. 14 Overall grains boundaries

2.6.2. Boundaries for selected grains

- Step 1. Finish simulation by clicking *Start/Stop simulation button* ***(2.4)***
- Step 2. Click grain(s) on *Simulation canvas* ***(2.1)*** that you what to show boundaries
- Step 3. Click on *Boundaries button* ***(2.11)***
- Step 4. Popup window will be shown ***Ref. 16***, enter your border width
- Step 5. Click *OK*

Results:



Ref. 15 Boundaries for selected grains

3. Summary and conclusions

Described project is fully complete and ready to use. All application tests, which was done, finished successfully. Requirements that was given on classes are done in at least minimum state or higher. Also was added some new extra features like *Grain details* **chapter 1.4** and import/export files in different formats (.csv, .png, .gif).

There is a lot of features which can be used to improve this project. New neighborhoods, different types of simulation, even add *Monte Carlo* method are couple of many possibilities to make this application better and more usable for different issues.