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MULTISCALE MODELLING

Grain growth project report, part I

Application for simple grains growth simulation (Fig. 1)

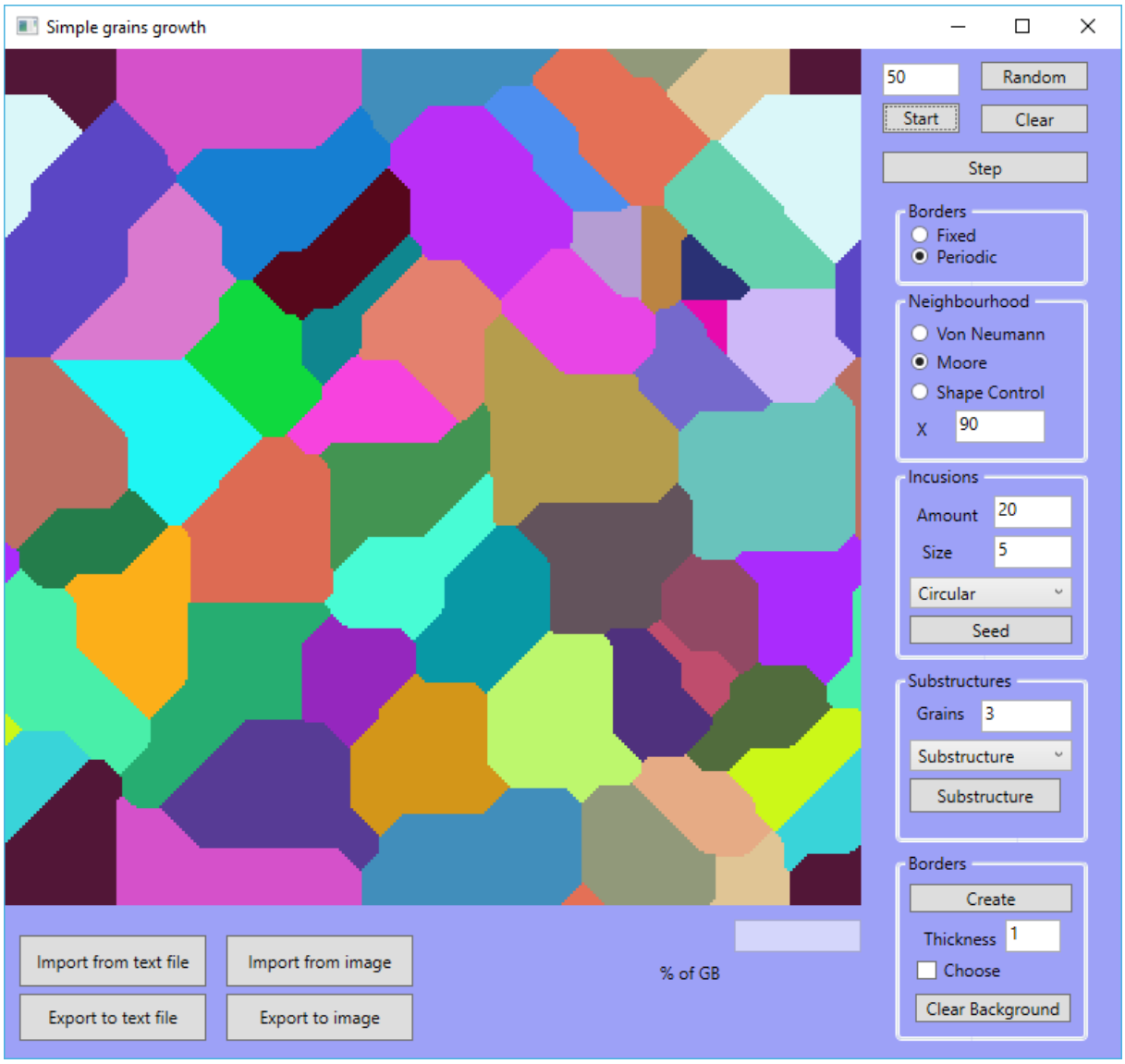

Figure 1. Grains growth application interface

Technologies used:

- .NET 4.7 - is a software framework developed by Microsoft that runs primarily on Microsoft Windows. It includes a large class library named Framework Class Library (FCL) and provides language interoperability (each language can use code written in other languages) across several programming languages.
- WPF - is a graphical subsystem by Microsoft for rendering user interfaces in Windows-based applications.

- C# - is a general-purpose, multi-paradigm programming language encompassing strong typing, imperative, declarative, functional, generic, object-oriented (class-based), and component-oriented programming disciplines.

The reason, why .NET technologies were used for this project, is ther simplicity, quick set-up and transparent API for high-level programming. WPF allows rapid development of desktop applications, and is supported with rich documentation.

Code available at: https://github.com/TMaj/MultiScaleGrainsGrowth

This program is intended to be used for simulating simple grains growth algorithm. It is based on cellular automata, and provides user with possibilities of adjusting simulation parameters such as boundaries, neighbourhood or inclusions. All features are listed below:

Application features

1. Random nucleons seeding (Fig. 2)

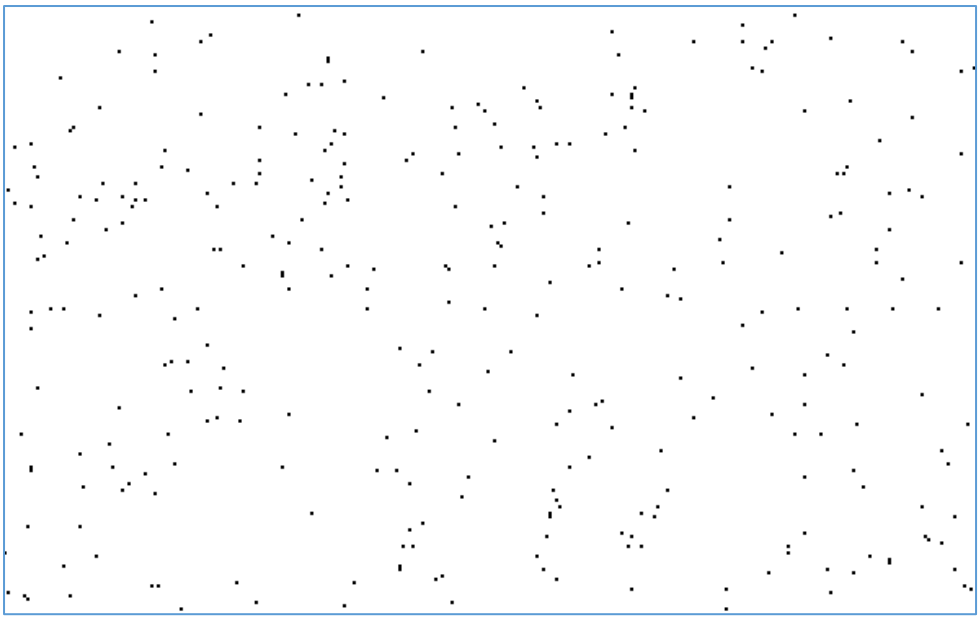

Figure 2. Randomly generated nucleons

2. Border style choice

- *Fixed borders (Fig. 3)*

Figure 3. Non-periodic borders in simulation. As highlighted, grains do not overflow simlation area.

- *Periodic borders (Fig. 4)*

Figure 4. Example of periodic borders in simulation. Highlighted area shows grains overflowing simulation area.

3. Simulation neighbourhood

- *Von Neumann (Fig. 5)*

Figure 5. Von Neumann neighbourhood.

- *Moore (Fig. 5)*

Figure 6. Moore neighbourhood.

- *Extended Moore (Shape control)*
  - *X factor at 90% (Fig. 7)*

Figure 7. Extended Moore simulation with 90% X.

- *X factor at 50% (Fig. 8)*

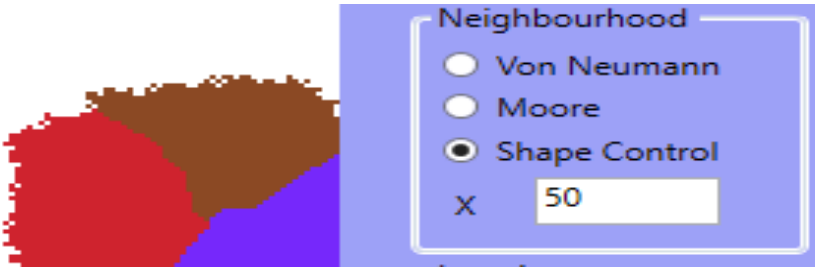

Figure 8. Extended Moore simulation with 50%.

- *X factor at 20% (Fig. 9)*

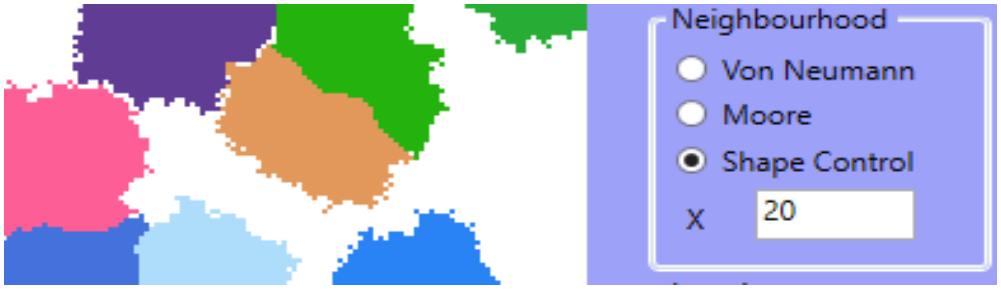

Figure 9. Extended Moore simulation with 20% X.

4. Inclusions

Inclusions are always rendered at grains borders. If no borders are present in simulation, they are rendered randomly on matrix. User has possibility to choose size, type and number of inclusions.

- *Square inclusions (Fig. 10)*

Figure 10. Square inclusions example.

- *Circular inclusions (Fig. 11)*

Figure 11. Circular inclusions example.

5. Substructures

Substructures are generated by preserving specified number of random grains on simulation area.

- *Substructure (Fig. 12)*

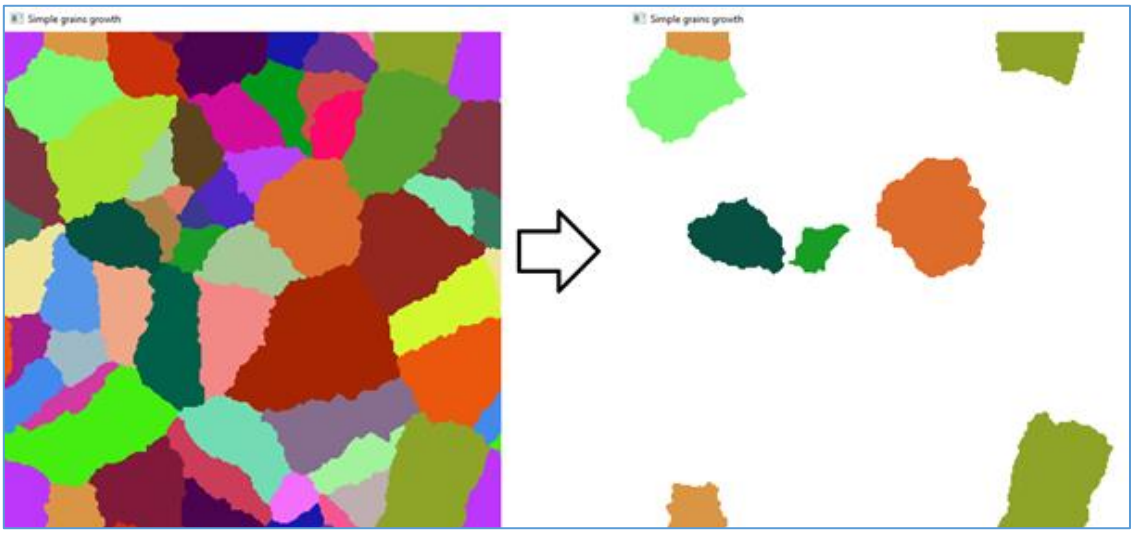

Figure 12. Generating substructure.

- *Dual phase (Fig. 13)*

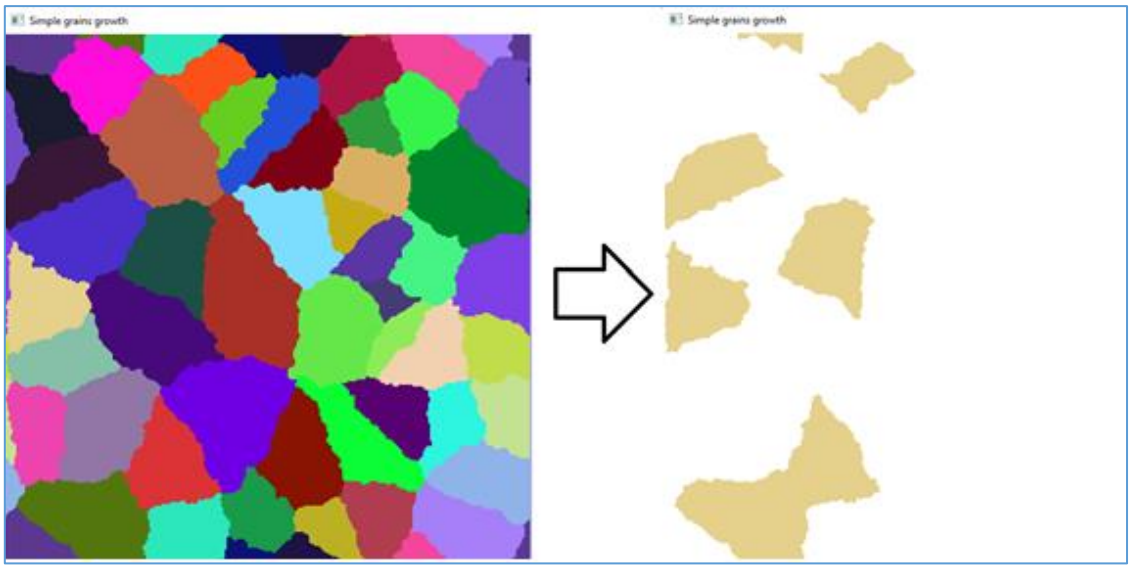

Figure 13. Generating dual phase substructure.

6. Borders

User is able to generate borders between grains, and specify their thickness. (Fig. 14, 15, 16, 17)

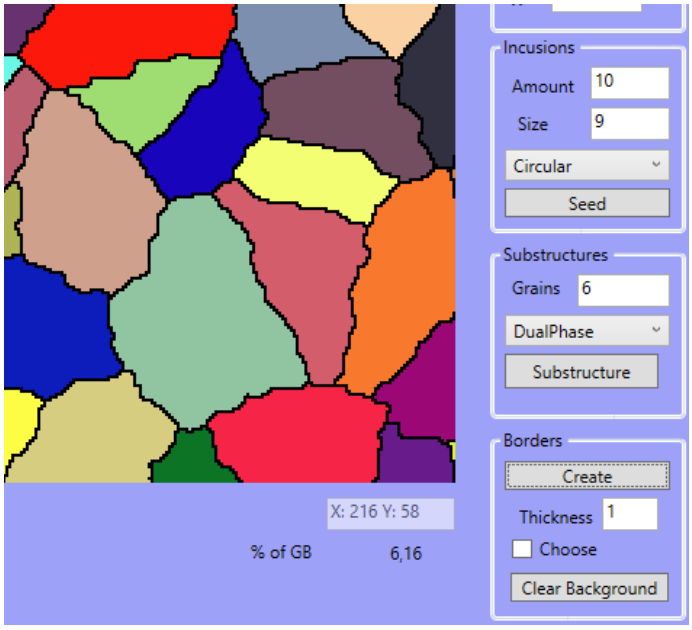

Figure 14. Thickness =1, whole area

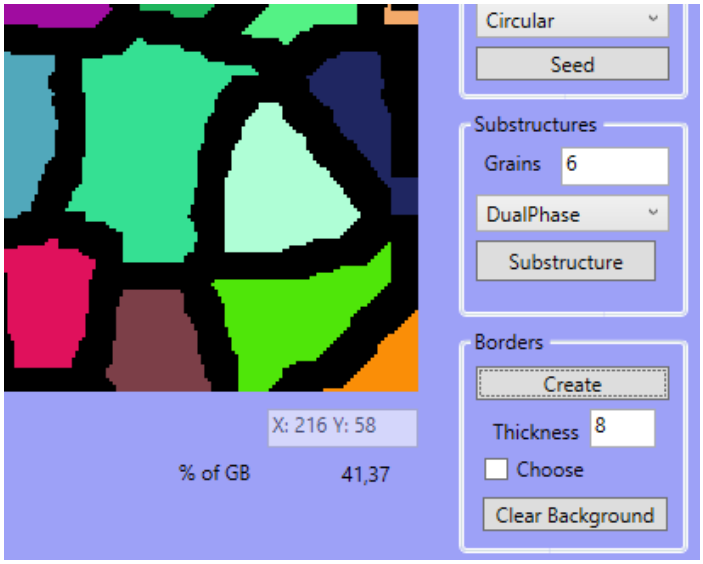

Figure 15. Thickness =8, whole area.

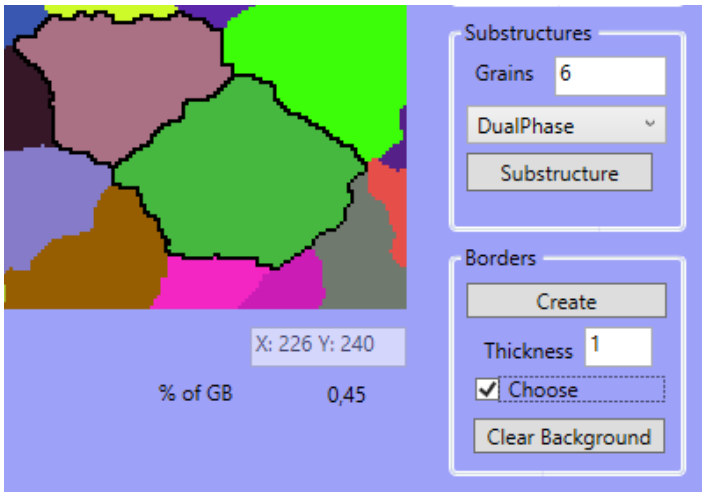

Figure 16. Thickness =1, chosen grains only.

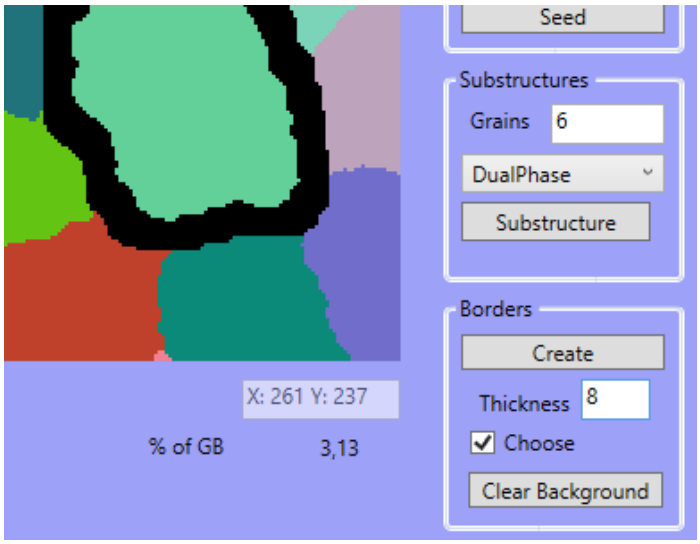

Figure 17. Thickness=8, chosen grains only

After each boundaries creation user is informed about percentage of grains boundaries in entire simulation area (Fig. 18):

Figure 18. Percentage of grain boundaries on simulation area.

When boudaries are drawn, user can erase grains, preserve boundaries and conduct next simulation (Fig. 19)

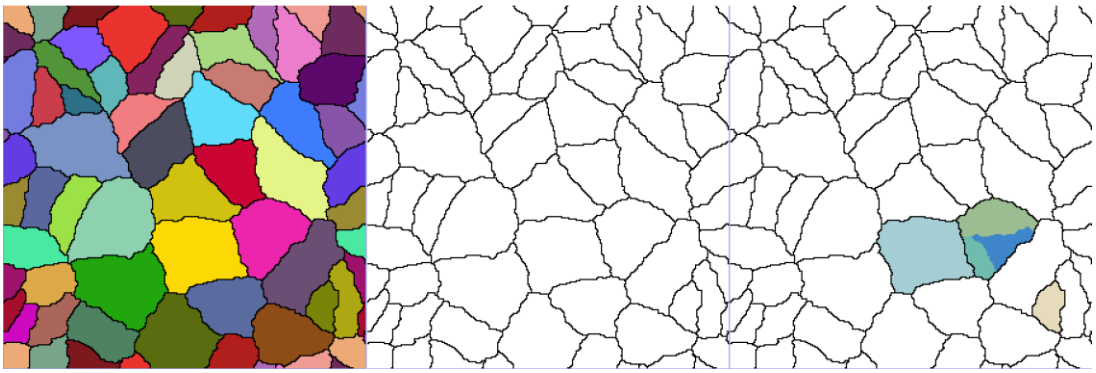

Figure 19. New simulation after preserving grains boundaries

7. Simulation results import and export

- *To text file (Fig.20)*

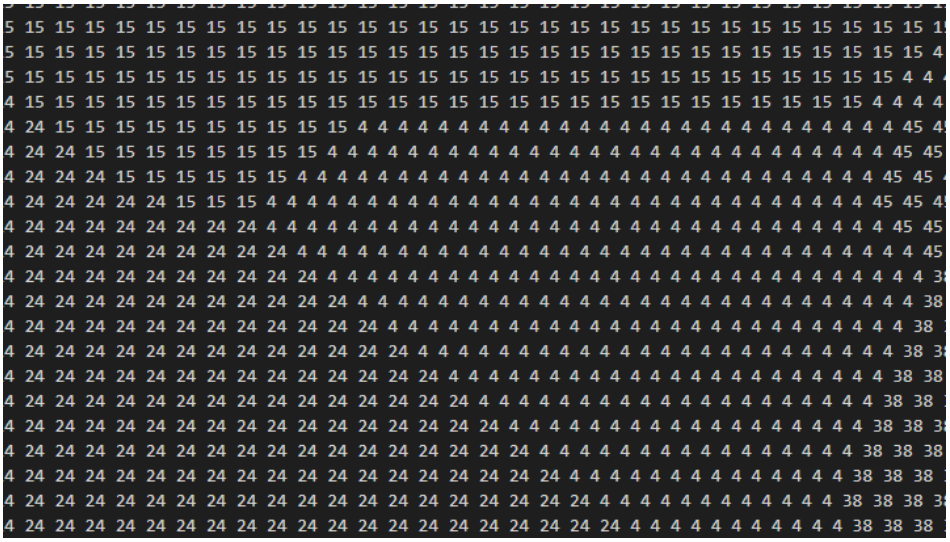

Figure 20. Text file output

- *To png image (Fig. 21)*

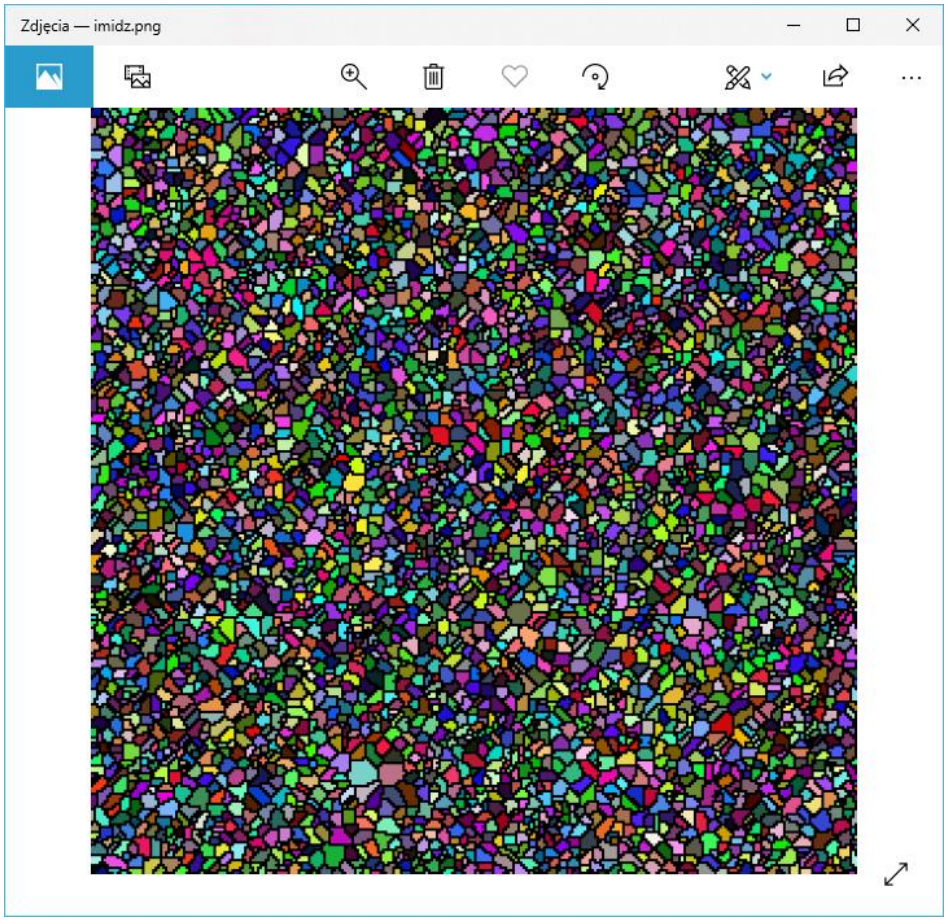

Figure 21. Image output result.

User Interface manual

User interface is presented on Figure 22.

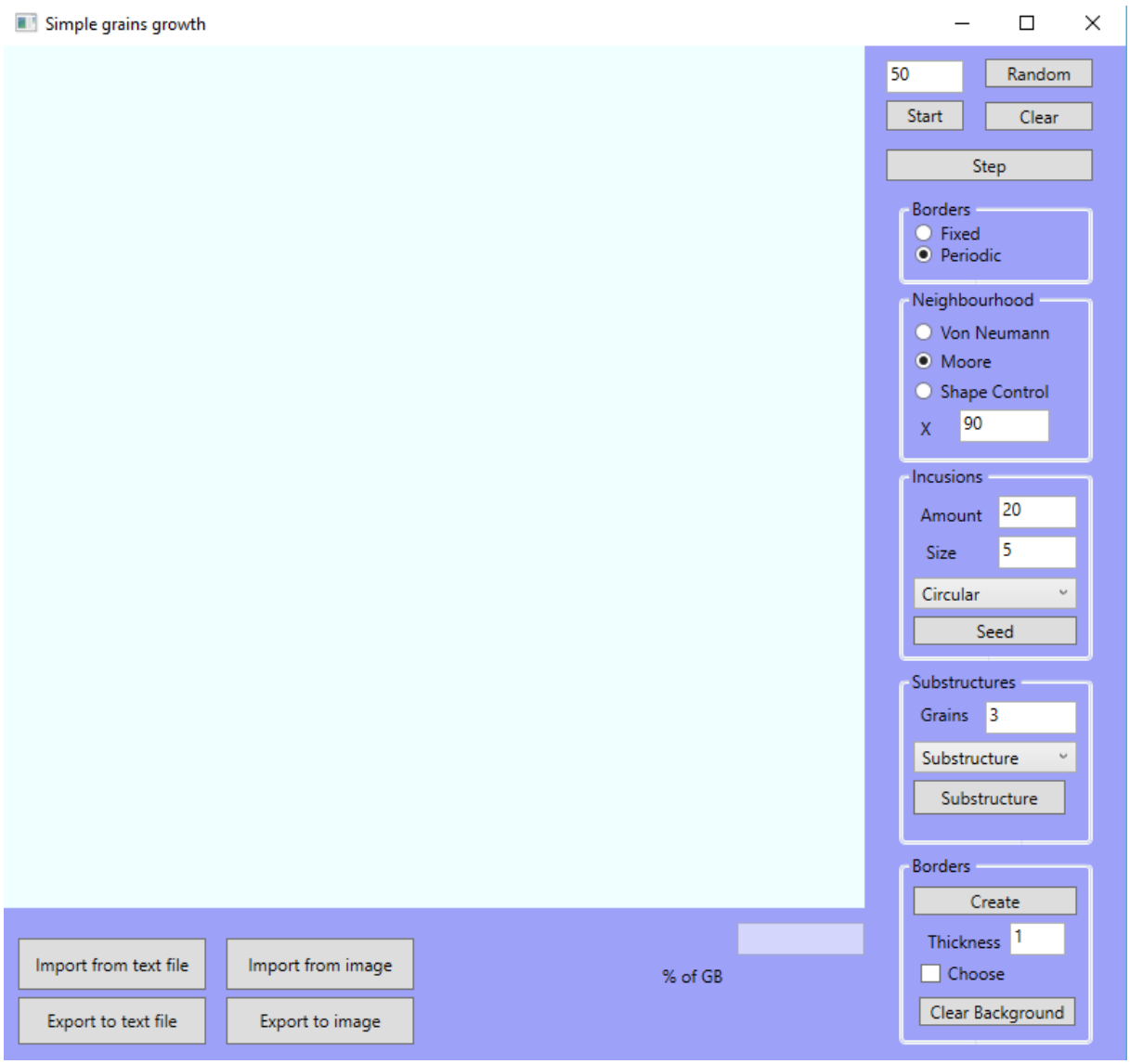

Figure 22. User interface.

Random button renders a specified number of nucleons in random order on simulation area.

Start button starts simulation. When simulation is running, clicking on it will stop simulation.

Clear button clears entire simulation area.

Step button performs single step of simulation.

Borders group box allows to choose between ***Fixed*** or ***Periodic*** borders of simulation area.

Neighbourhood group box allows to choose beetween neighbourhoods in grains growth algorithm: ***Von Neumann***, ***Moore*** or ***Shape Control*** (Extended Moore). ***Shape control*** has text box specifying possibility parameter ***X*** used in last step of extended Moore Neighbourhood algorithm.

Inclusions group box determines number, size and type of inclusions. ***Seed*** button renders inclusions on simulation area.

Substructures group box specifies how many grains should be used to create substructure or dual phase (this is determined by combo box). Button ***Substructure*** generates substructure.

Borders group box contains text field for specifying border ***thickness***. Button ***Create*** generates borders between all grains present in simulation. Ticking ***Choose*** checkbox allows user to click on desired grains in order to surround them with borders. ***Clear background*** button clears all grains and preserves their boundaries.

Textbox below simulation canvas displays coordinates of clicked grain. Label which is placed below indicates percentage of borders on simulation area.

Buttons for importing and exporting simulation to text/image display prompt user for selecting desired source or destination of smulaiton file.

Comparison of simulation results and real material

The purpose of grains growth simulation is to predict phenomenons occuring in real materials. After proper adjustment of simulation parameters, it is possible to generate structure which is quite similar to real material, for example dual-phase steel.

First attempt of re-creating real substance was aimed at dual phase steel - Fe-0.15C-1.5Mn-1.5Si (wt%) (Fig. 23). This material consists of ferrite (white area) and martensite mixed with retained austenite (dark area with white spots).

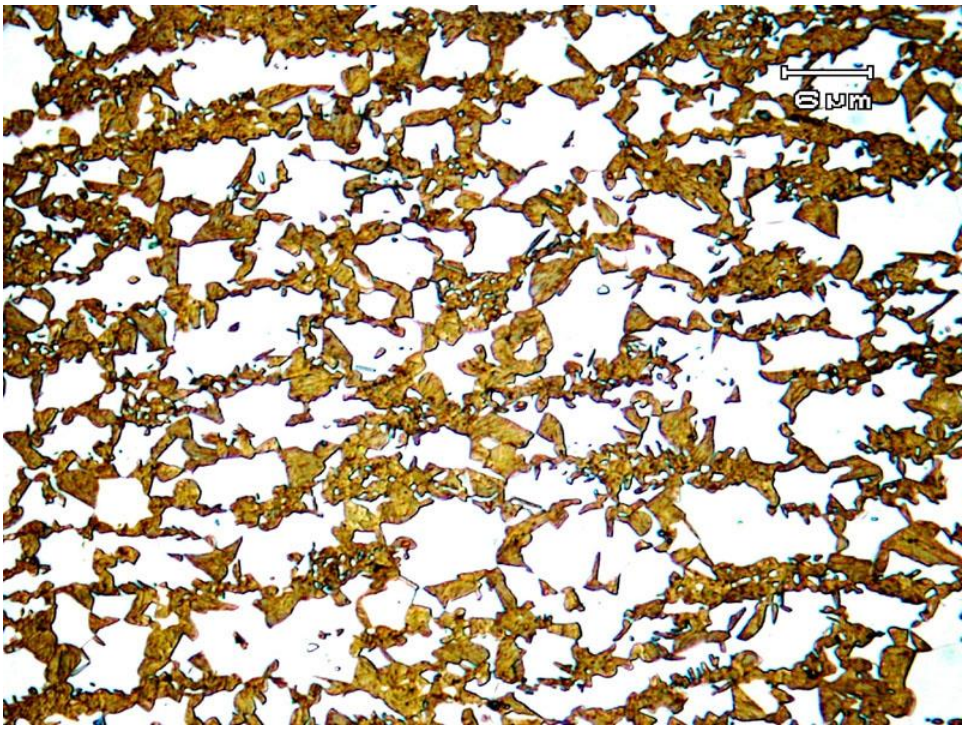

Figure 23. Dual phase steel - composition of the steels is Fe-0.15C-1.5Mn-1.5Si wt%

After several different setups, the best result was achieved after using 2000 random nucleons, extended Moore neighbourhood with parameter X at 60% value, and dual-phase substructure with 750 grains specified (Fig. 24).

This configuration managed to achieve similar grains shape and size. However, it did not manage to render small spots of retained austenite inside bigger martensite grains. Overall, the created image seems to be quite accurate attempt of simulating this kind of material.

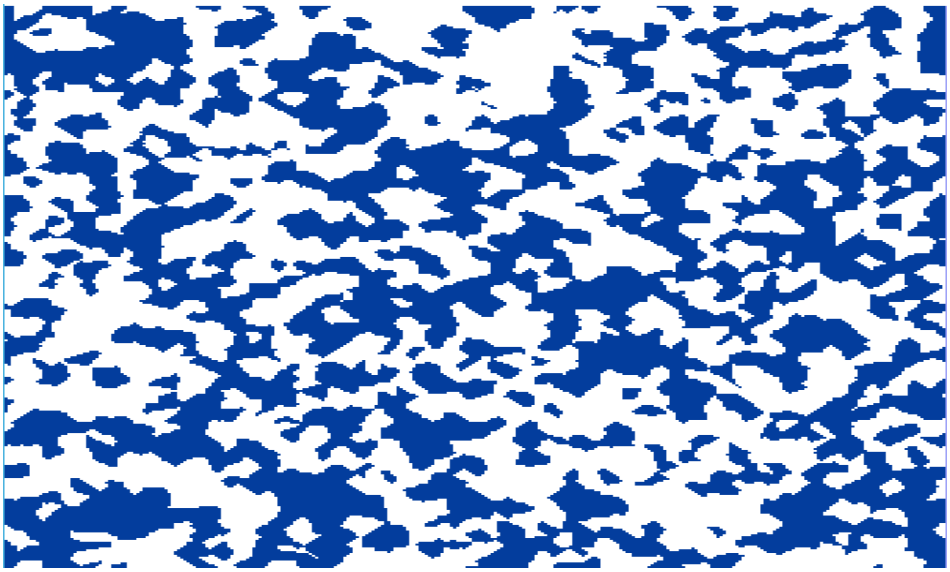

Figure 24. Simulation result - 2000 grain nucleons, dual-phase with 750 grains parameter.

Second material, which recreation was attempted, was solid solution of carbon (perlite) and iron (ferrite) Fe, C 0.2 (wt%) (Fig. 25) (it forms at high temperatures).

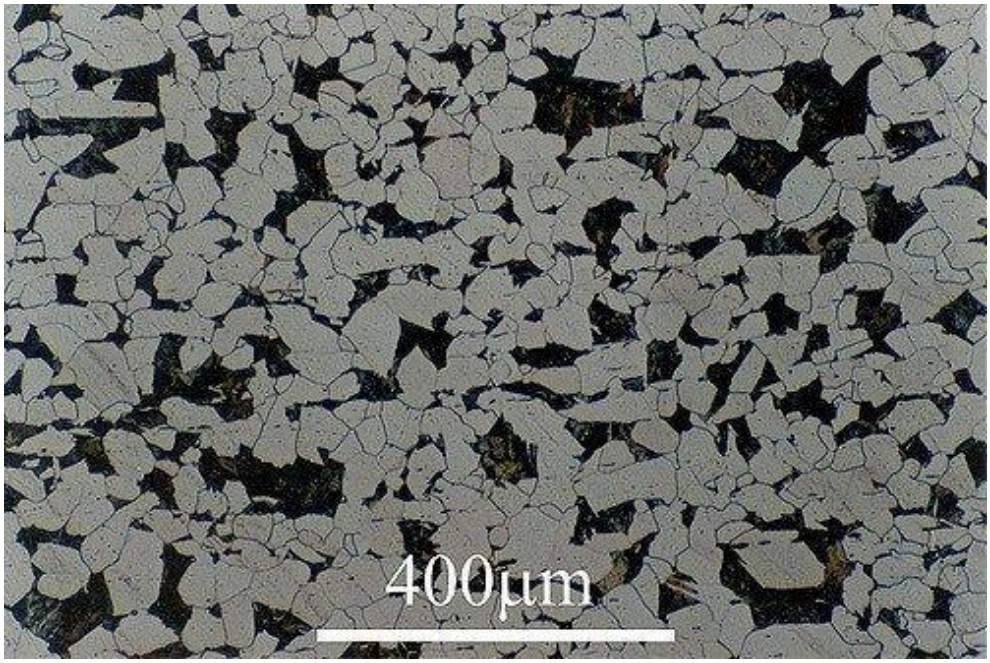

Figure 25. Ferrite with the darker pearlite regions around the ferrite grains

To create this material by simulation, several steps were made. Firstly, 600 nucleons were chosen and grown (extended Moore neighbourhood, X = 40%). Then, borders were addded and dual-phase microstructure with 400 grains was made (Fig. 26).

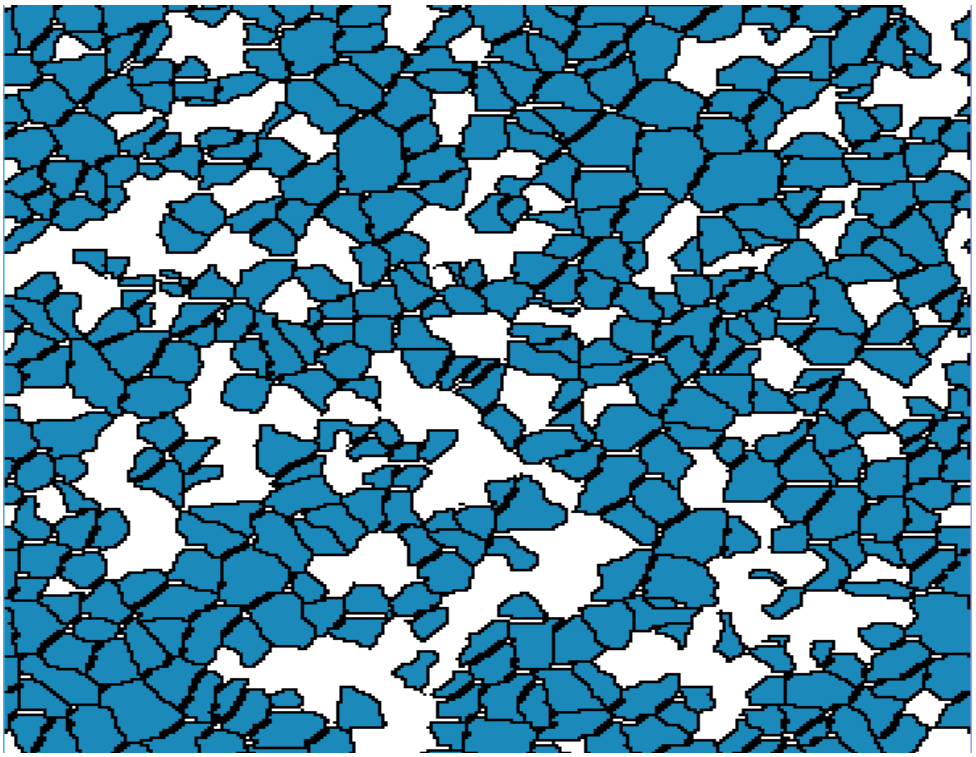

Figure 26. Second simulation result.

As viewer may notice, colors on simulation are inverted, but the result seems to imitate real structure quite accurately. Grains of ferrite have appropriate shape and size.

The last re-created material was Arcelor's Mittal Dual Phase 600 steel – C0.14Mn2.1Si0.4. (Fig. 27)

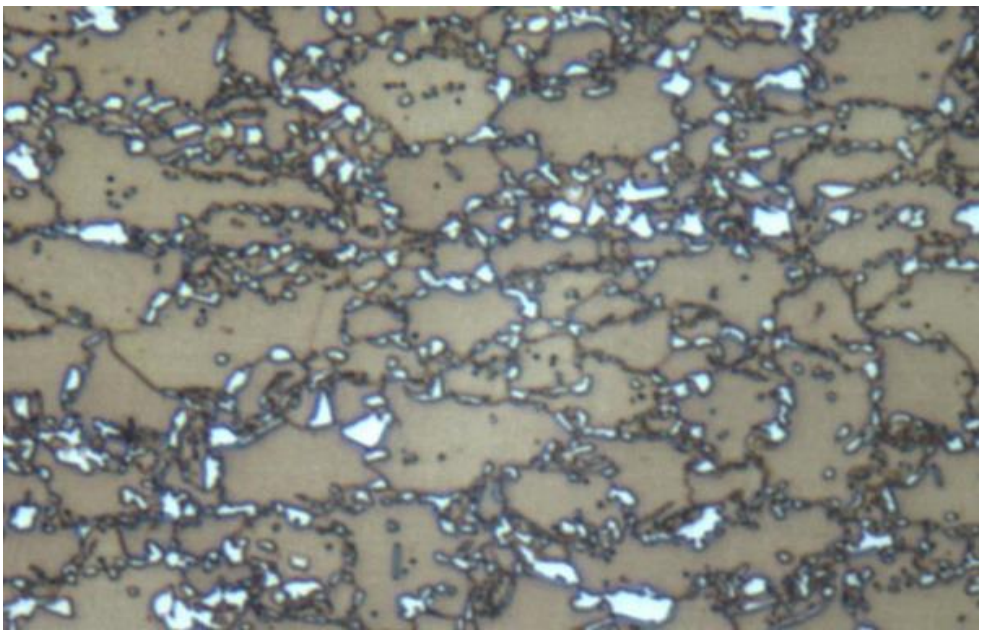

Figure 27. DP 600.

This microstrucure was difficult to imitate, because it contains very small and detailed inclusions. Simulation was conducted with growing 300 nucleons (extended Moore neighbourhood, X = 10%), creating dual phase substructure with 150 grains, adding borders, and then growing 300 additional nucleons (Fig. 28).

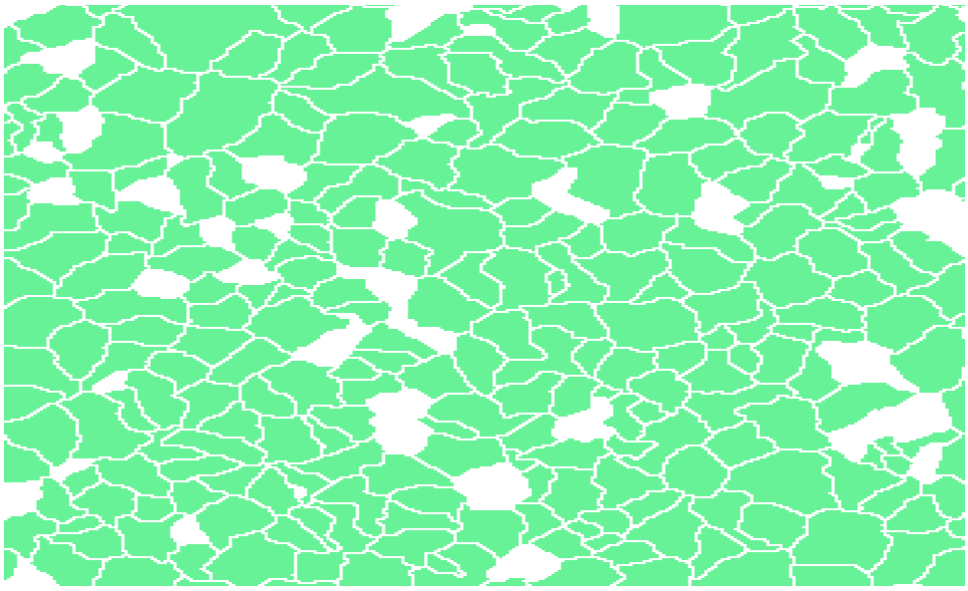

Figure 28. Third simulation result.

This attempt failed to imitate small structures of this dual phase steel. Bigger grains resembles real steel elements, but smaller grains are not small and complicated enough.

Sources:

First dual phase steel:

http://www.phase-trans.msm.cam.ac.uk/2008/dual.html

Solution of iron and carbon:

http://www.flickriver.com/photos/core-materials/3838605259/

Second dual phase steel (DP 600):

https://automotive.arcelormittal.com/europe/products/AHSS/DP/EN