AGH

UNIVERSITY OF SCIENCE AND TECHNOLOGY CRACOW

Metals Engineering and Industrial Computer Science

Multiscale Modelling 2nd Report:

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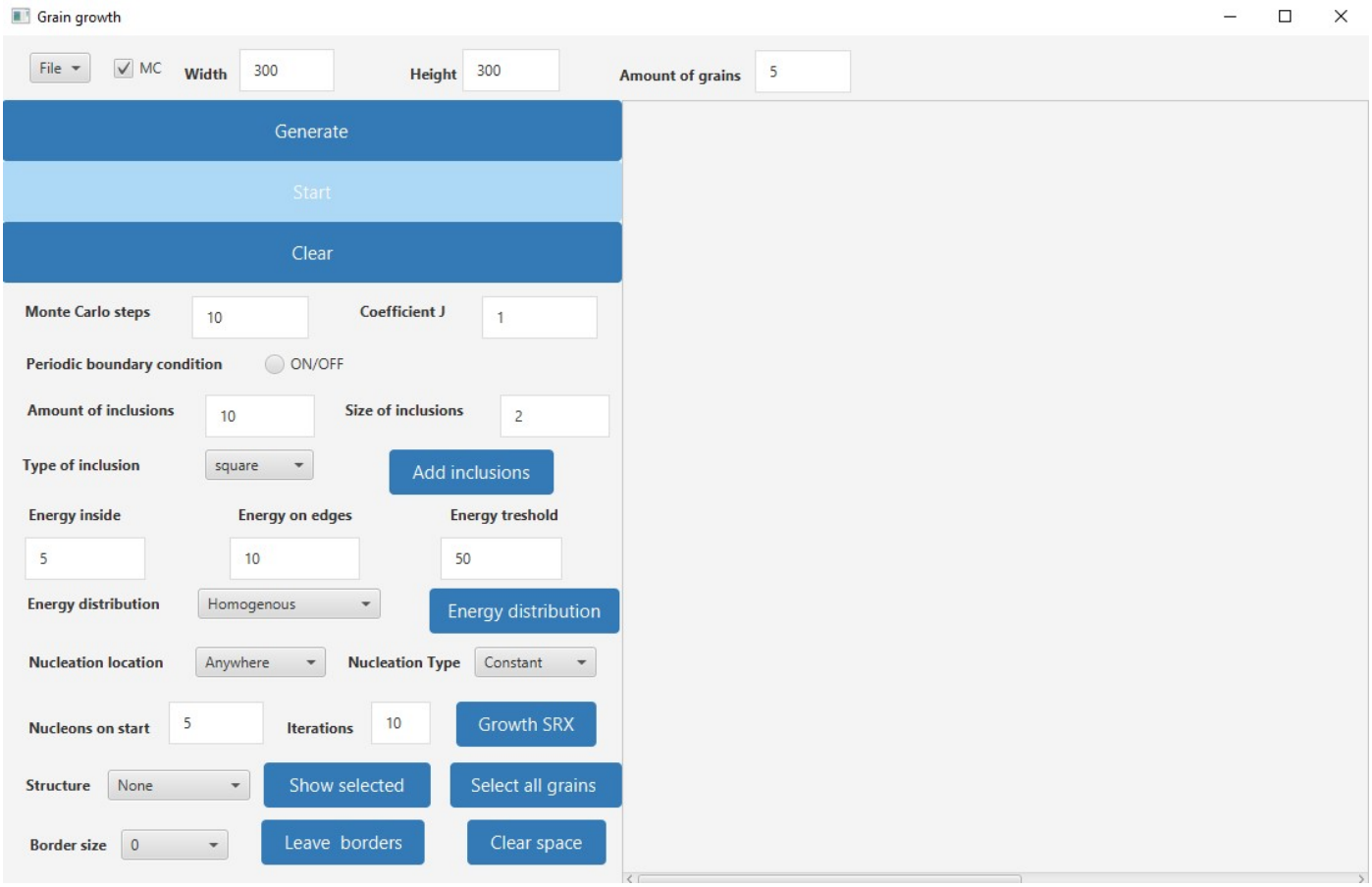
Repository:	**https://github.com/FabiolaDabros/MultiscaleModeling**
Course:	**Multiscale Modelling**

1. Technology

The application was created by extending the application which was presented in the previous report. Just like before I have used Java, which is a high-level programming language, to create the application. The Graphical User Interface was implemented with the JavaFX library, which is a very powerful tool to make GUI based java applications.

2. Graphical User Interface

The picture 1 presents the main window of the application.

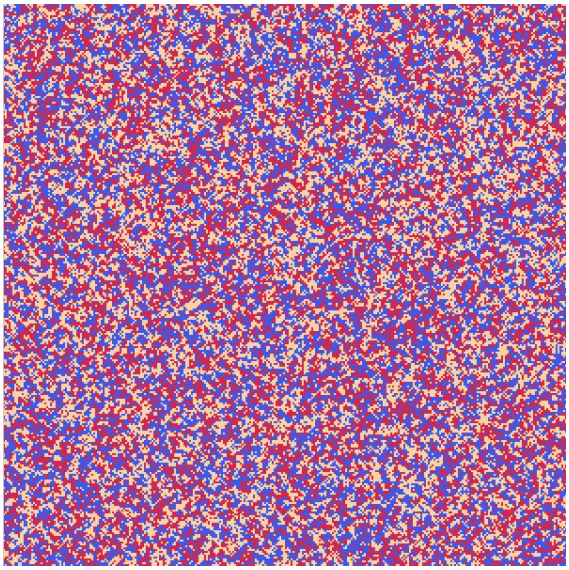


Picture 1. Graphical User Interface - main application window.

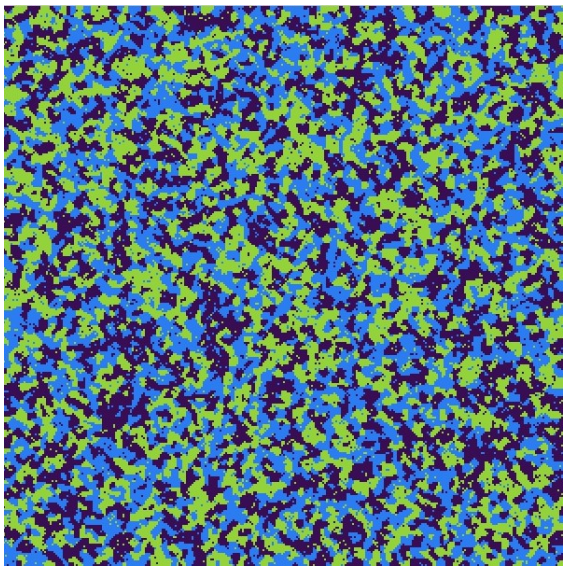
The main window of the application allows the user to make a lot of actions, which are described in second section. On the empty space appears generated image of the microstructure. The user can switch between ‘CA’ and ‘MC’ options.

2.1 Simple grain growth Monte Carlo

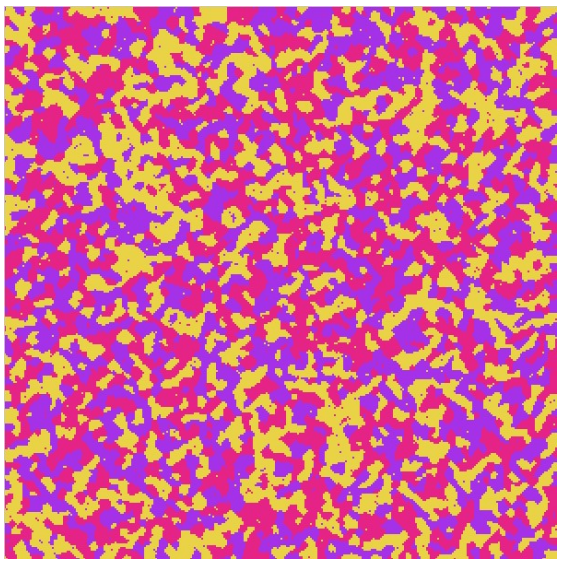
To make simple grain growth using Monte Carlo method the user has to check the ‘MC’ checkbox, which is placed at the top of the application. This option exposes all elements related to Monte Carlo. First of all, the user has to set the dimension of the grid by entering width and height data. The minimum size is 300x300 but the user can also define rectangular grid. Another component is a textfield that allows to insert different number of nucleons. The user can also check the periodic boundary conditions. But the new aspect is textfield where the user has to input the number of Monte Carlo steps and another textfield that allows to insert the value of J coefficient. After setting all of the options the user has to press “Generate” button to start the process of growth. During that process, the most important thing is to calculate the energy of lattice site surrounding concerned element which is selected randomly. Then the investigated cell changes the state to one of the available states. Next step is to calculate the energy of that element caused by orientation changes. And the orientation state is accepted with the defined probability. Pictures 2, 3, 4 and 5 show results of these actions with Moore neighborhood and three numbers of grains, but with different number of Monte Carlo steps.



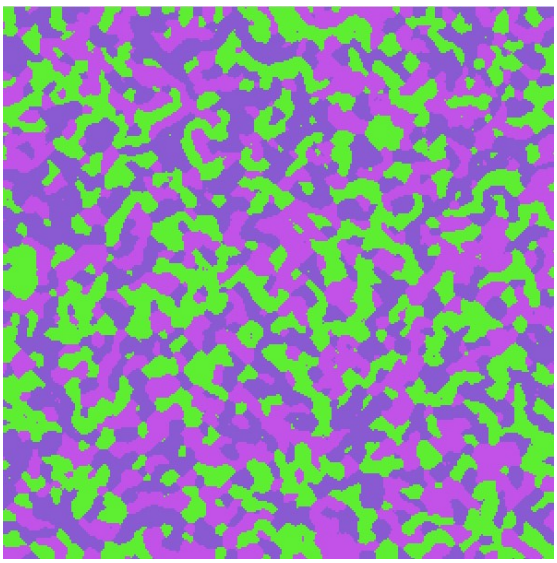
Picture 2. Microstructure generated with 1 Monte Carlo steps.



Picture 3. Microstructure generated with 5 Monte Carlo steps.



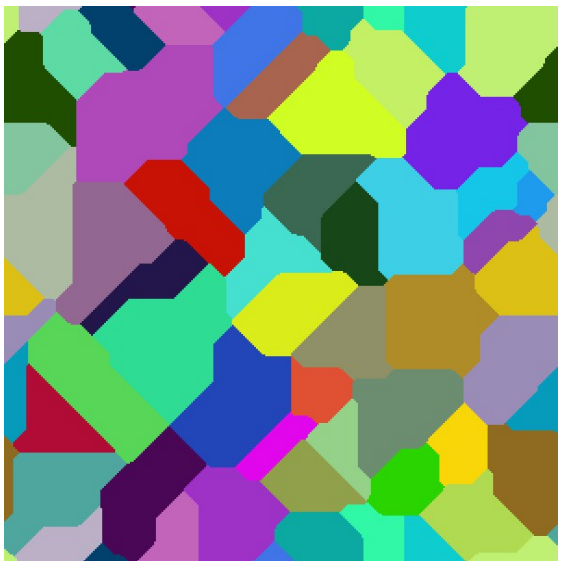
Picture 4. Microstructure generated with 15 Monte Carlo steps.



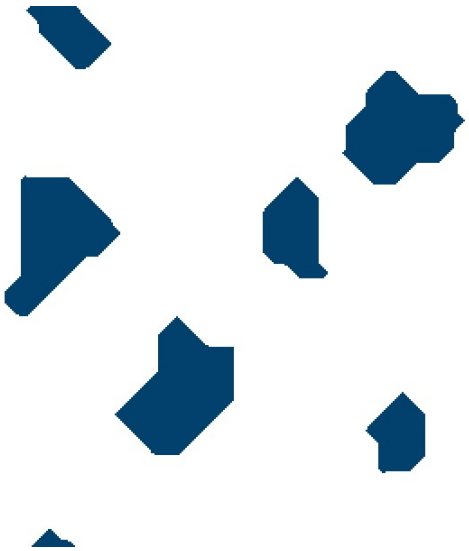
Picture 5. Microstructure generated with 20 Monte Carlo steps.

2.2 Dual phase microstructure

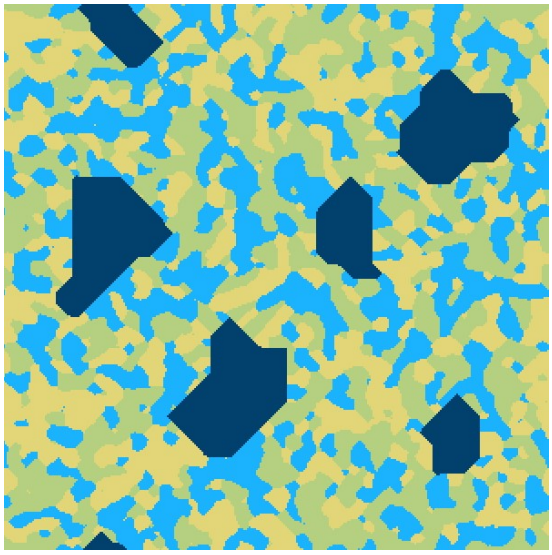
Another feature is when the process of growth is finished. The user can choose the dual phase structure from the combobox, which makes that selected grains are united – they have the same id and color. What is more, the user can unselect selected grain by clicking on this grain again. When the user selects all the grains which he wants, he has to press the “Show selected” button which makes the non selected grains deleted. After that the user can start the process of growth again. But the most important thing is the fact that the user can combine the methods of growth. That means that the user can make simple grain growth with Cellular Automata method, select grains and then start the process of growth again but with the Monte Carlo method. It also applies the other way round. Pictures 6, 7, 8, 9, 10, 11, 12 and 13 show the full process of creating dual phase with two scenarios.



Picture 6. Simple grain growth with CA method.

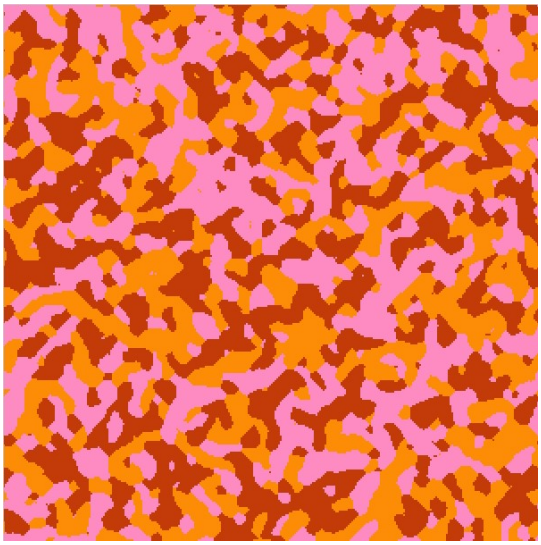


Picture 7. Selected grains for dual phase.

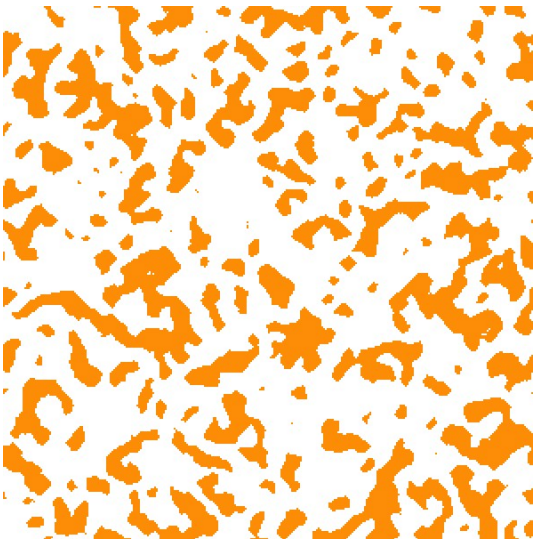


Picture 8. Dual phase after regrowth with MC method.

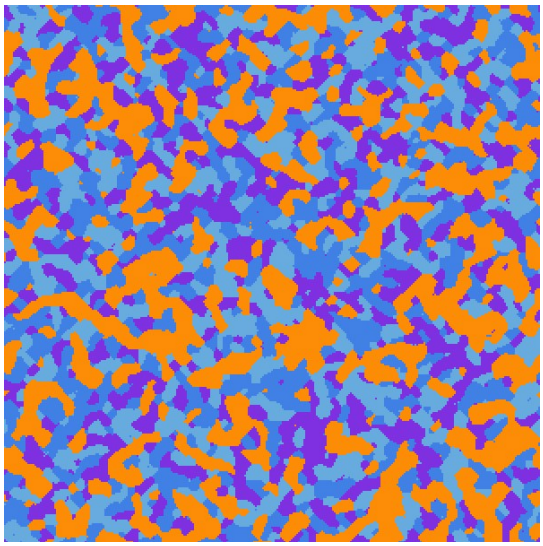
Picture 9. Dual phase after regrowth with CA method.



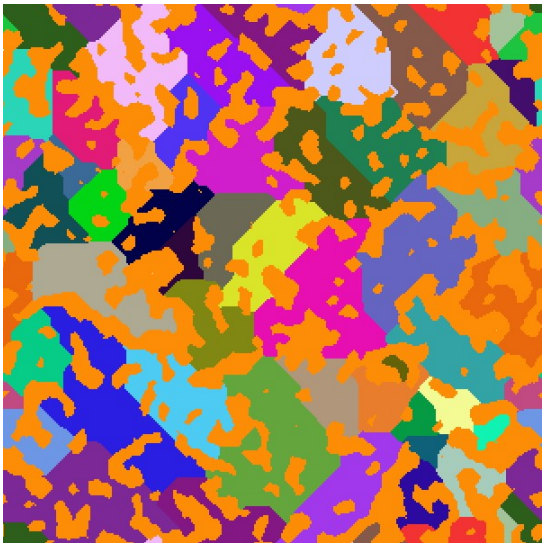
Picture 10. Simple grain growth with MC method.



Picture 11. Selected grains for dual phase.



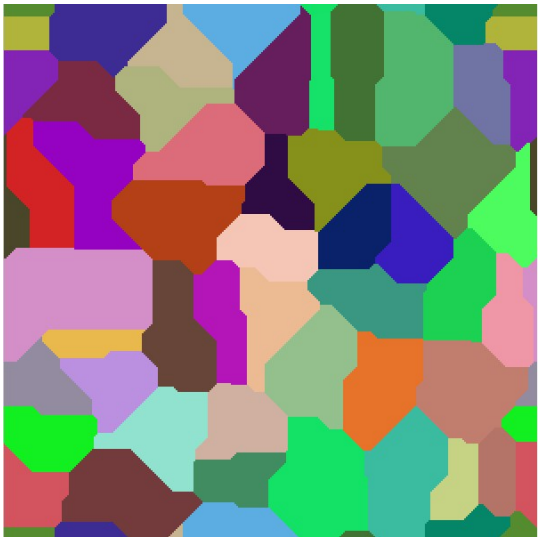
Picture 12. Dual phase after regrowth with MC method.



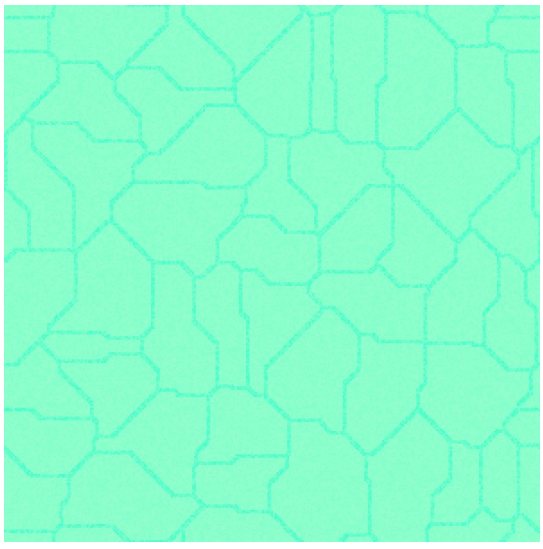
Picture 13. Dual phase after regrowth with CA method.

2.3 SRX Monte Carlo

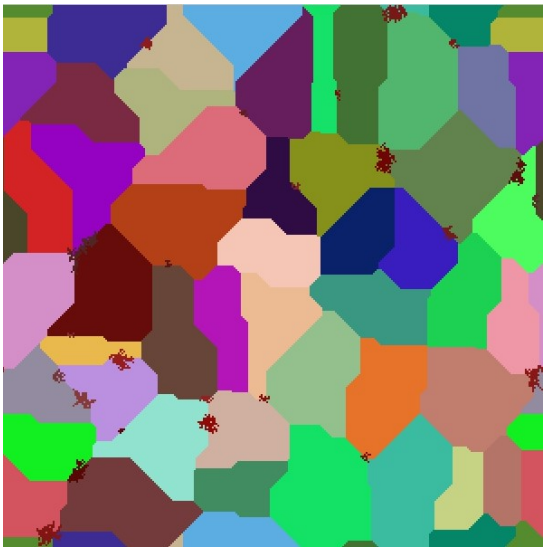
The last feature allows the user to make nucleation and grain growth of recrystallized grains. First of all the user has to generate the initial material morphology – using Cellular Automata or Monte Carlo method. The second step is distribution of stored energy. To realize that step the user has to select from the combobox the way of the energy distribution – homogenous or heterogenous. Homogenous means that distribution of energy is evenly and heterogenous means that on boundaries is more or less energy – distribution of energy is unequal. After that the user has to define the values of energy inside, energy on the edges and threshold energy. But when we are taking into consideration the heterogenous distribution, the user does not have to input the value of energy on the edges, because that energy is equal to energy inside. To see result of that step, the user has to press the 'Distribution button'. The last step is nucleation and grain growth of recrystallized grains. The user has to select from the comboboxes two important issues: nucleation location – anywhere or on boundaries, and nucleation type – constant, increasing or at the begging. To make growth of recrystallized grains the user has to input the number of nucleons on start and the number of iteration. After pressing the 'Growth SRX' button the user will see the result. Pictures 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24 and 25 show the full process with different parameters selected.



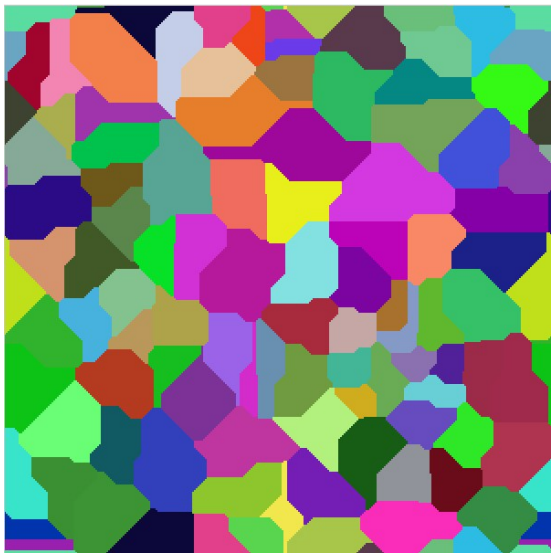
Picture 14. Simple grain growth with CA method with 50 grains, periodic boundary conditions and von Neumann neighbourhood.



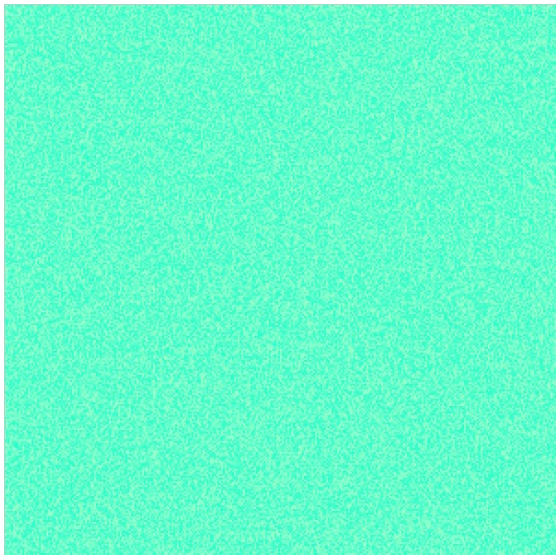
Picture 15. Heterogenous energy distribution with 15 energy inside, 5 energy on the edges and 50 energy threshold.



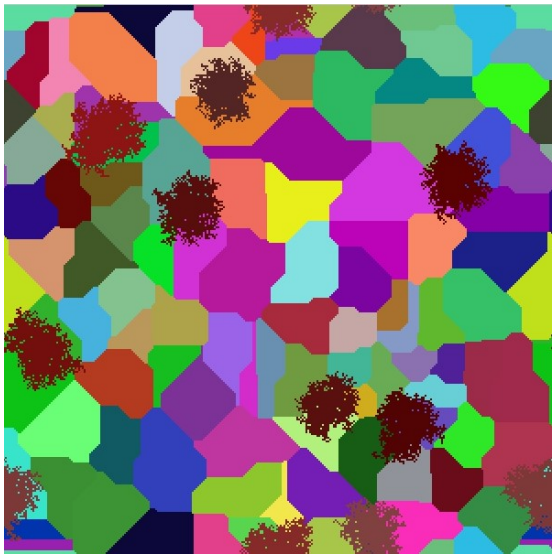
Picture 16. Nucleation location on boundaries, with nucleation type constant and grain growth with 5 nucleons on start and 5 iterations.



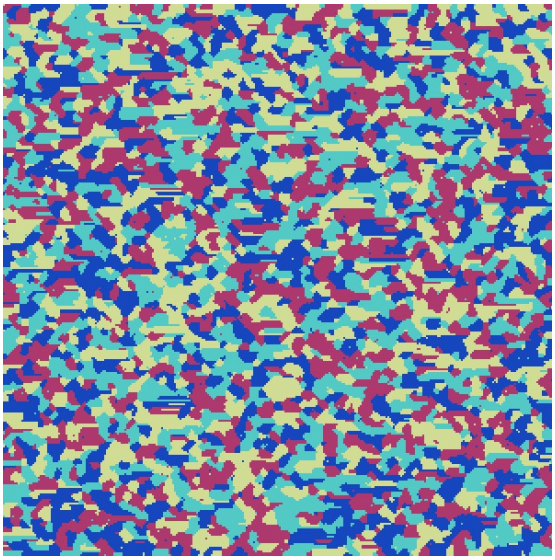
Picture 17. Simple grain growth with CA method with 100 grains, periodic boundary conditions and von Neumann neighbourhood.



Picture 18. Homogenous energy distribution with, 15 energy inside and 100 energy threshold.

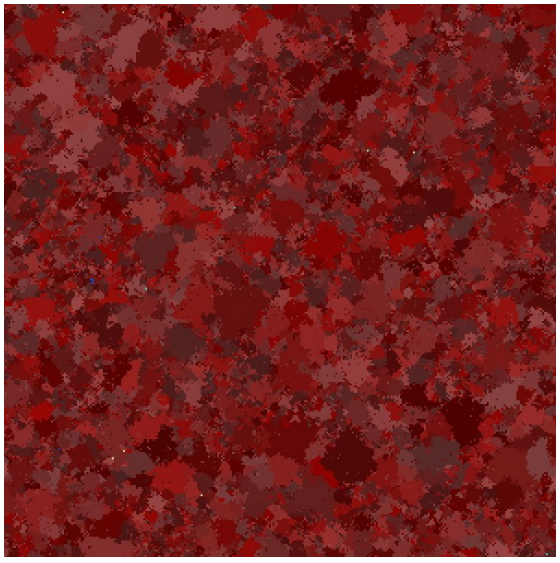


Picture 19. Nucleation location anywhere, with nucleation type at the begging and grain growth with 10 nucleons on start and 10 iterations.

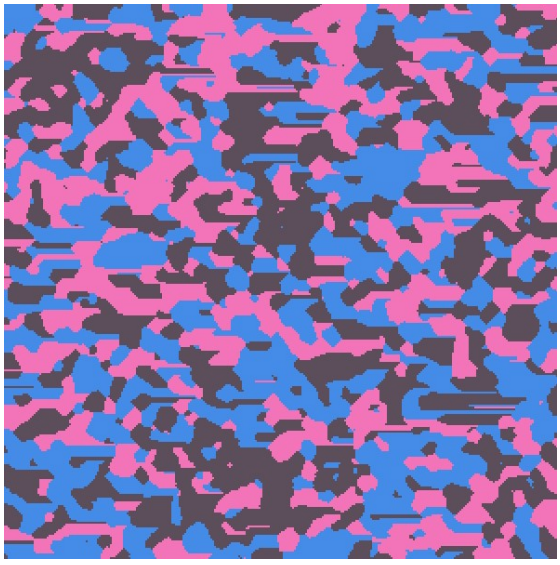


Picture 20. Simple grain growth with MC method with 5 grains and 20 monte carlo steps.

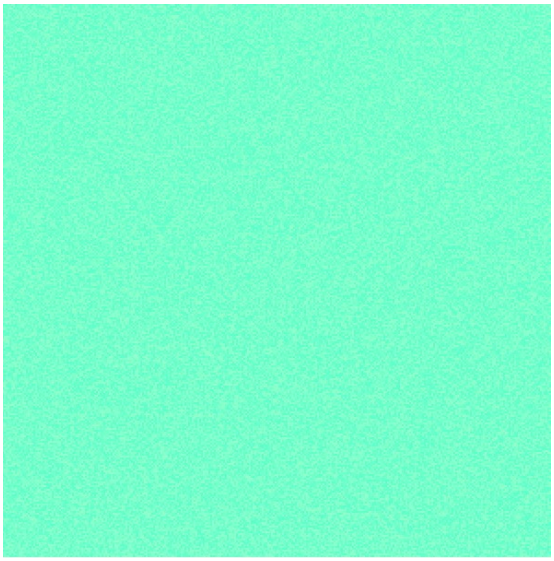
Picture 21. Heterogenous energy distribution with 4 energy inside, 10 energy on the edges and 20 energy threshold.



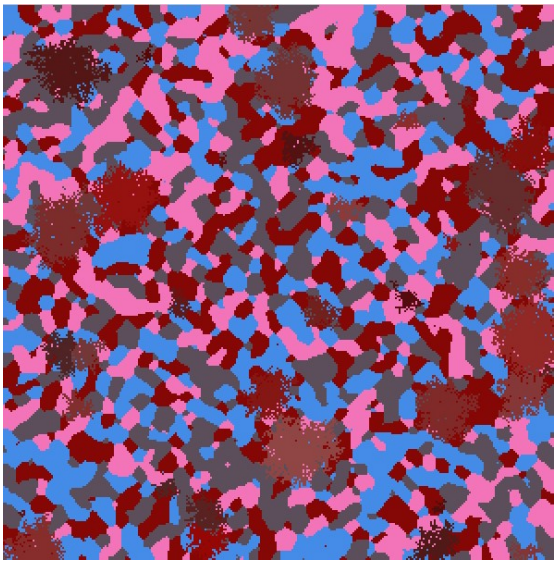
Picture 22. Nucleation location on boundaries, with nucleation type increasing and grain growth growth with 5 nucleons on start and 20 iterations.



Picture 23. Simple grain growth with MC method with 3 grains and 40 monte carlo steps.



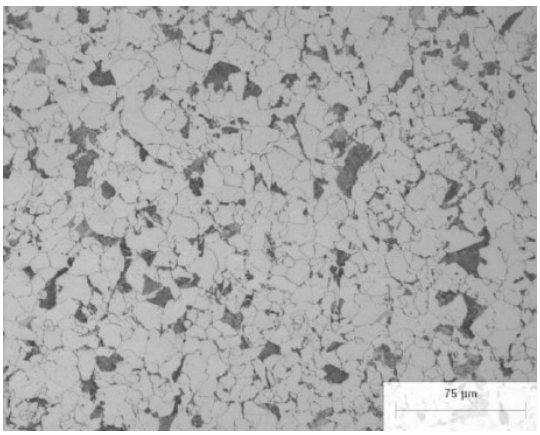
Picture 24. Homogenous energy distribution with 10 energy inside and 75 energy threshold.



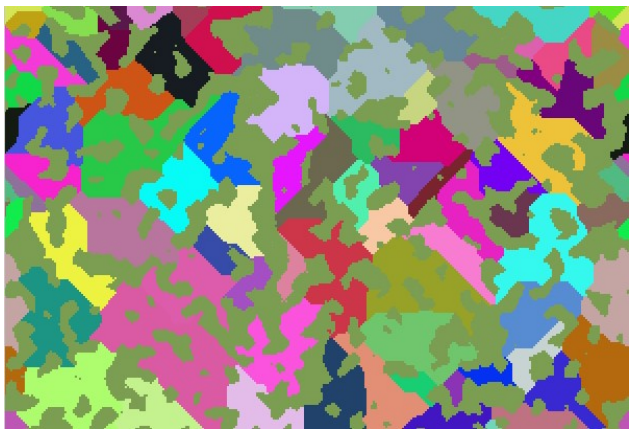
Picture 25. Nucleation location anywhere, with nucleation type constant and grain growth with 4 nucleons on start and 10 iterations.

3. Summary

The application allows the user to generate many different microstructures. In fact, the real-life microstructures are very similar to them. Pictures below show the comparison between the program results and genuine microstructures.

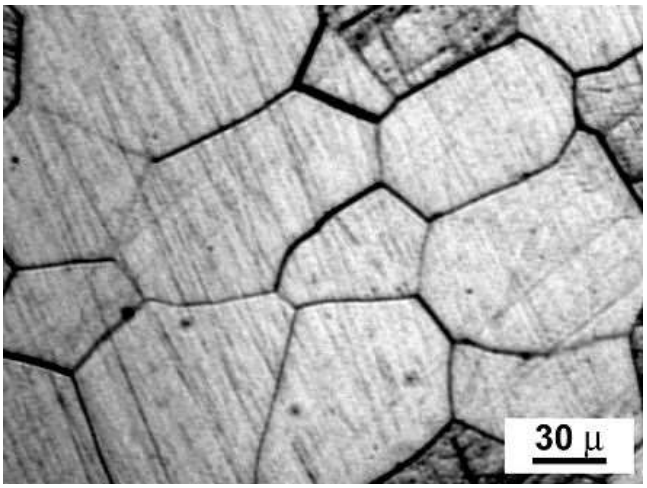


Picture 26. Microstructure of API 5L X-52 steel. [1]



Picture 27. Microstructure generated with Monte Carlo method, and dual phase after regrowth with Cellular Automata method.

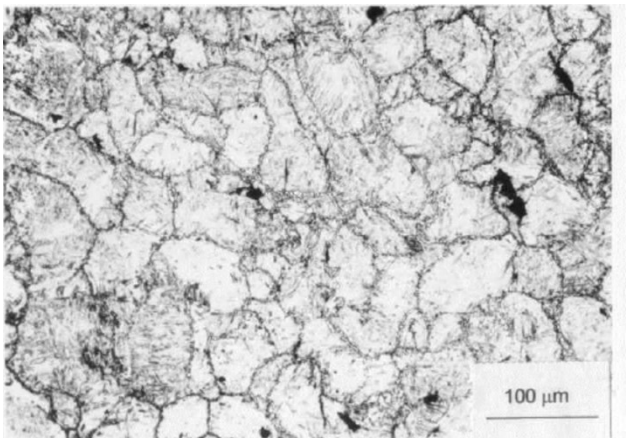
Picture 27 was generated by using Monte Carlo method with three number of grains and 20 steps. After grain growth process I have selected grains to make dual phase and then I have started process of the grain growth again but with the Cellular Automata method with Moore neighborhood, periodic boundary conditions and 50 number of grains. We can conclude that presented structures are very similar.



Picture 28. Microstructure of polycrystalline metal; grain boundaries evidenced by acid etching [2].

Picture 29. Heterogenous energy distribution with 15 energy inside, 5 energy on the edges and 50 energy threshold

Picture 29 was generated by using Cellular Automata method with 50 number, periodic boundary conditions and von Neumann neighborhood. After that was generated heterogenous energy distribution with 15 value of energy inside and 5 value of energy on the edges and 50 energy threshold. The generated microstructure is very similar to the genuine microstructure.



Picture 30. Microstructure of recrystallized fraction in austenite of steel [3].

Picture 31. Microstructure after nucleation and grain growth of recrystallized grains.

Picture 31 was generated with the SRX Monte Carlo. The first microstructure was generated using Monte Carlo method with 4 grains and with 40 steps. After that the heterogenous energy distribution was made with 4 energy inside, 10 energy on egdes and 60 energy threshold. The last step was nucleation with anywhere location and increasing nucleation type. The growth of recrystallized grains was generated with 4 nucleons on start and 30 iterations. The likeness to the real-life structure is marvelous.

4. References

[1] https://www.researchgate.net/figure/Microstructure-of-API-5L-X-52-steel_fig1_274072899

[2] https://www.wikiwand.com/en/Grain_boundary

[3] https://www.researchgate.net/figure/Microstructure-of-recrystallized-fraction-in-austenite-of-steel-used-Reheating_fig1_286286336