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17.01.2018

Multiscale Modelling

Report 2 - MC-based grain growth and static recrystallization simulation

Project description

Presented below user interface contains all updates performed during the whole process of system creation. User can choose between two methods used for microstructure generation,
which are Cellular Automata and Monte Carlo

This led to
implementation of following new features:

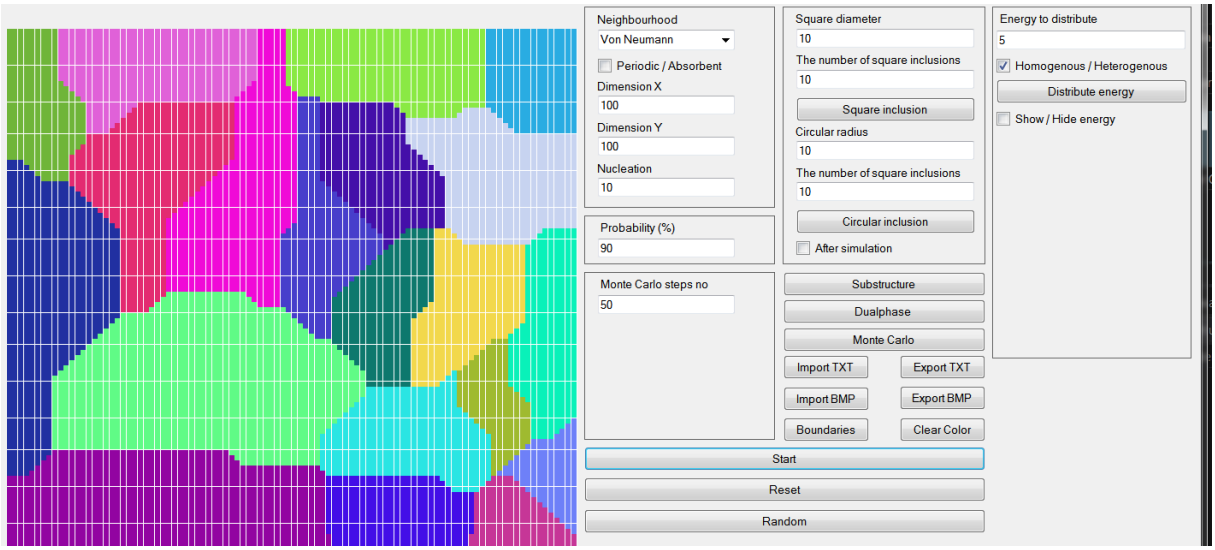
- MC-based grain growth can be used both in initial microstructure generation stage and in
substructure/DP growth stage- The dual phase structure can be generated using CA or MC method

- takes into account probability of accepting the new state based on energy change rather than fixed energy change threshold
Cell energy visualization
-additional energy distribution view

Technology

For the purpose of building this application the C# programming language (.Net Technology) was used. The user interface was created based on a Win Forms. This technology allows to easily create interactive user interface and implement required function.

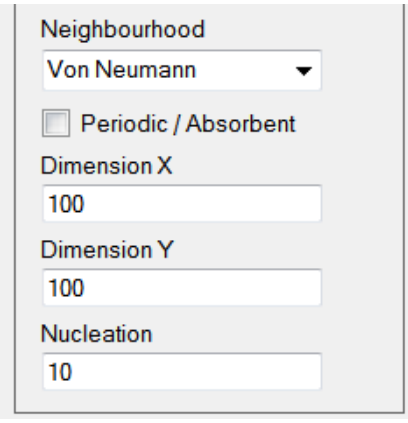
User interface



Img 1: Main app view

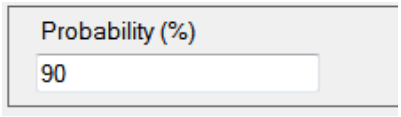
This image presented the main app view. On the right we can see all parameter what we set to generate microsubstructure, distribute and show energy and possibility to save/load to bmp and text format. On the left we have visualization us simulation.

User interface - application configuration



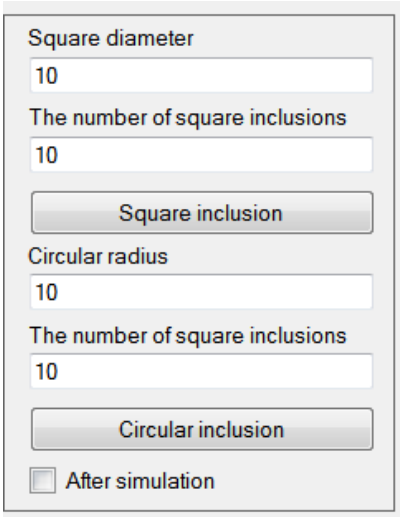
Img 2: paramaters view in main columns

First user set neighbourhood type. This parameter defines the change in shape of each grain and describes the slosest neighbors of a particular cell. Next user can set Periodic / Absorbent options. This parameter defines whether grains can grows without or with borders. Dimension tell about size window visualization of simulation in pixels/cells proportion . Number nucleation defines how many nucleations we can observe in the resulted structure.



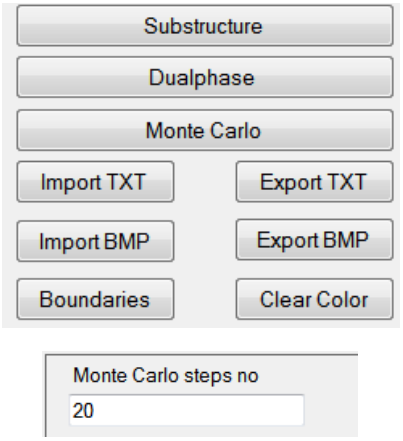
Img 3: Proballity columns for Moore Ext rule four view.

This parameter used in rule four Moore Ext method and tell about probality chance to change the particular cell.



Img 4: Inclusions column view.

In inclusions column user can generate
inclusions, set size, amount and their type (square
or circular. User can set when inclusion must be added before or after simulation inclusions.

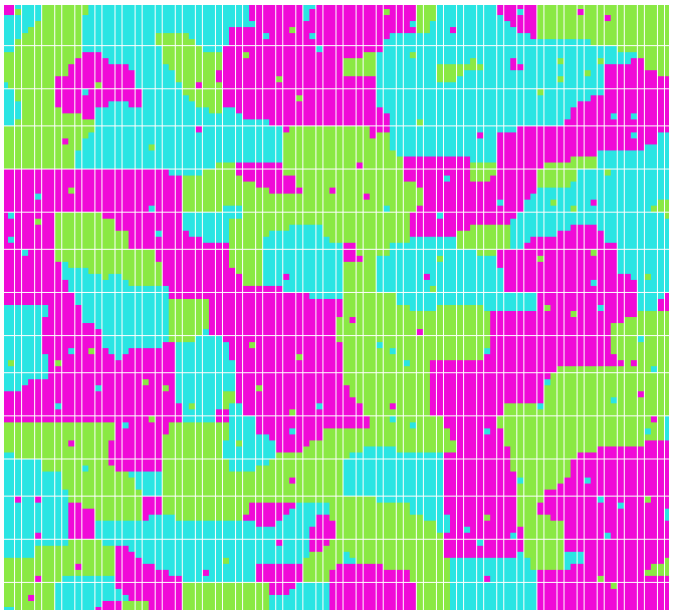


Img 5: function generation microstructure column view.

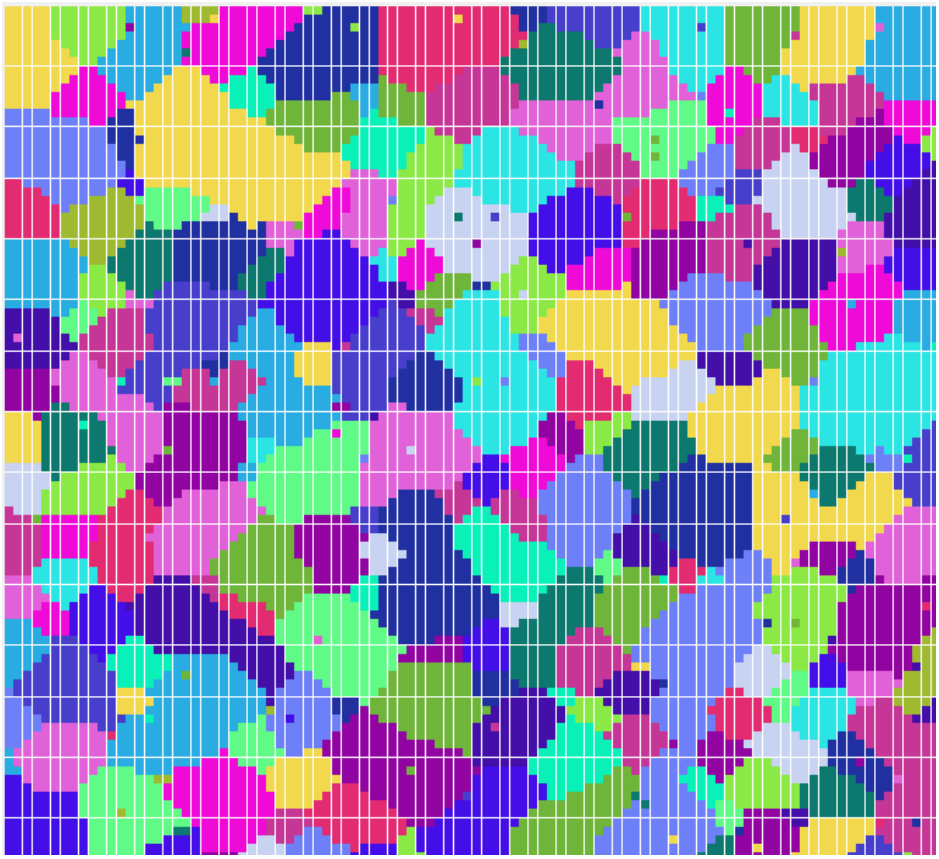
This column is about functions what we can generate. substructure makes that grains retain their IDs and color, but cannot grow.

Dual phase makes that grains cannot grow and have common ID and color assigned. After pressing *Boundaries* button on the current structure user can see black lines of the required size which represents the grains boundaries.

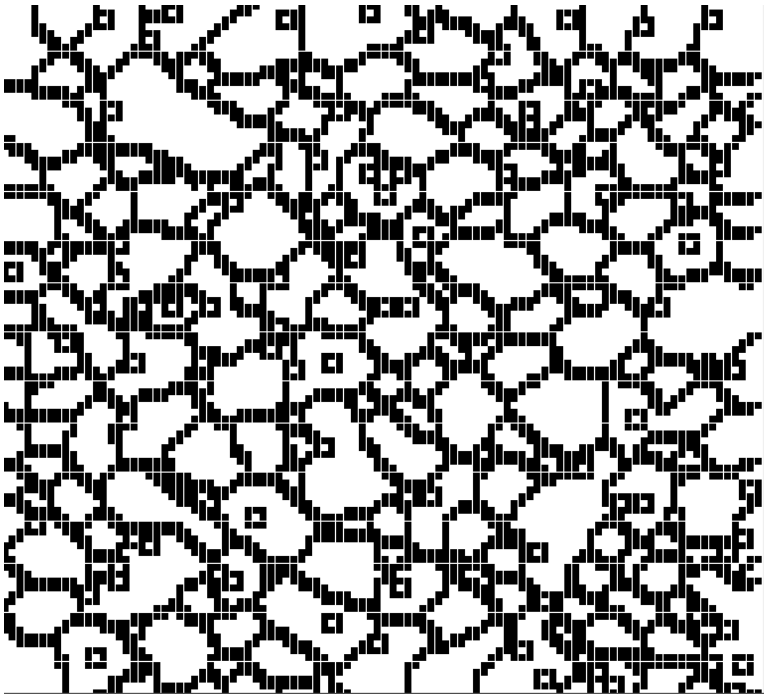
After used this option user can press the *Clear color* button which will result with the white board only containing grains boundaries. We add MonteCarlo function Basic parameters which user provides are *number of states* and *number of MC steps*. For this method the *Moore neighbourhood type* is a default one for the grain growth process. By pressing the *Monte Carlo* button user can start the process of grains growing. The growth process is carried out in accordance with assumptions of MC method. The resulting structures obtained after each MC step are displayed so the user can see how the whole process is performed. The belowing illustrations shows resulted structures processed accordingly to the certain parameters configuration.



Img 6: Generated microstructure (Number of nucleation: 3, Monte Carlo steps: 20,Type of neighborhood:Von Neumann)



Img 7: Generated microstructure (Number of nucleation: 20, Monte Carlo steps: 20,Type of neighborhood:Moore)

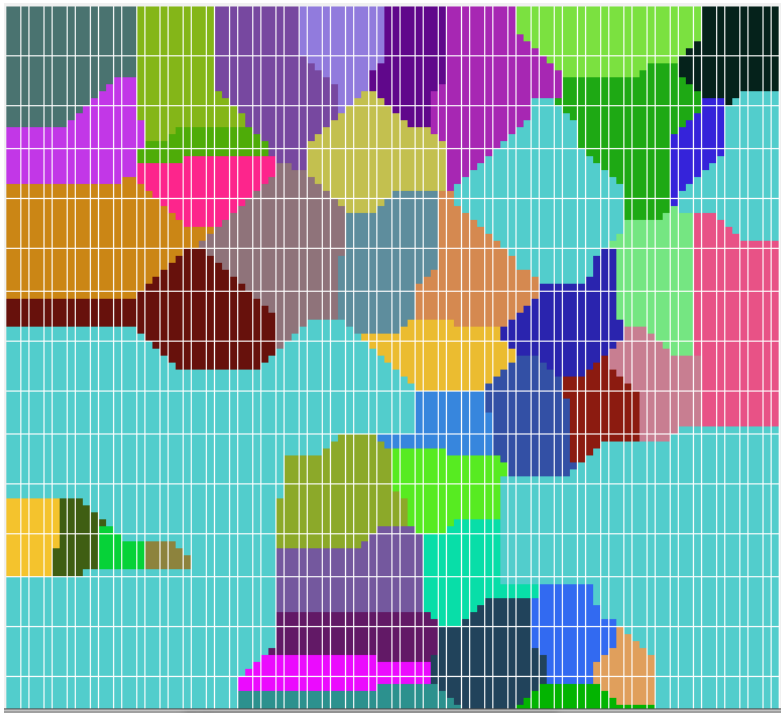


Img 8: Microstructure from img 7 with boundaries and after set functions clear color.

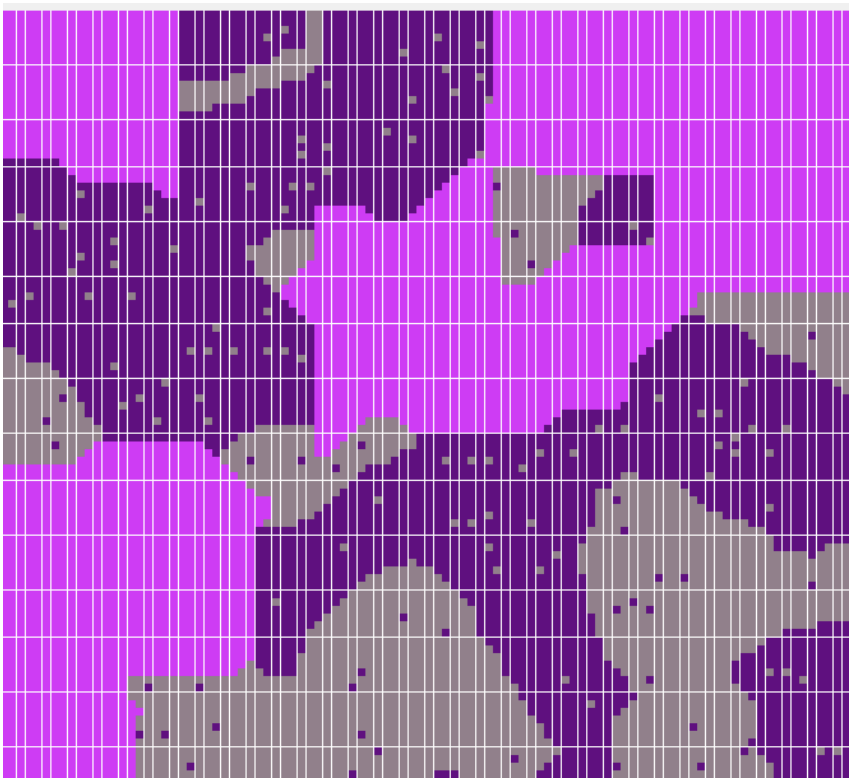
Dual Phase microstructure – CA -> (CA or MC)

or MC -> (CA or MC

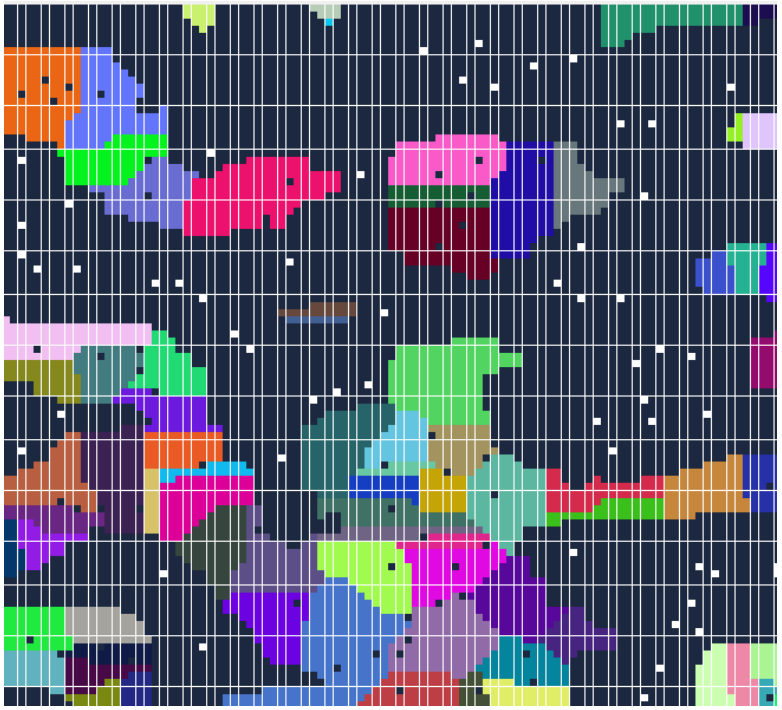
When structure generation (based on MC or CA method) is finished user can choose parameters of its modification. The dual phase structure can be generated using CA or MC method.
User can also specify number of remaining grains, which will become a second phase in resulted
structure.



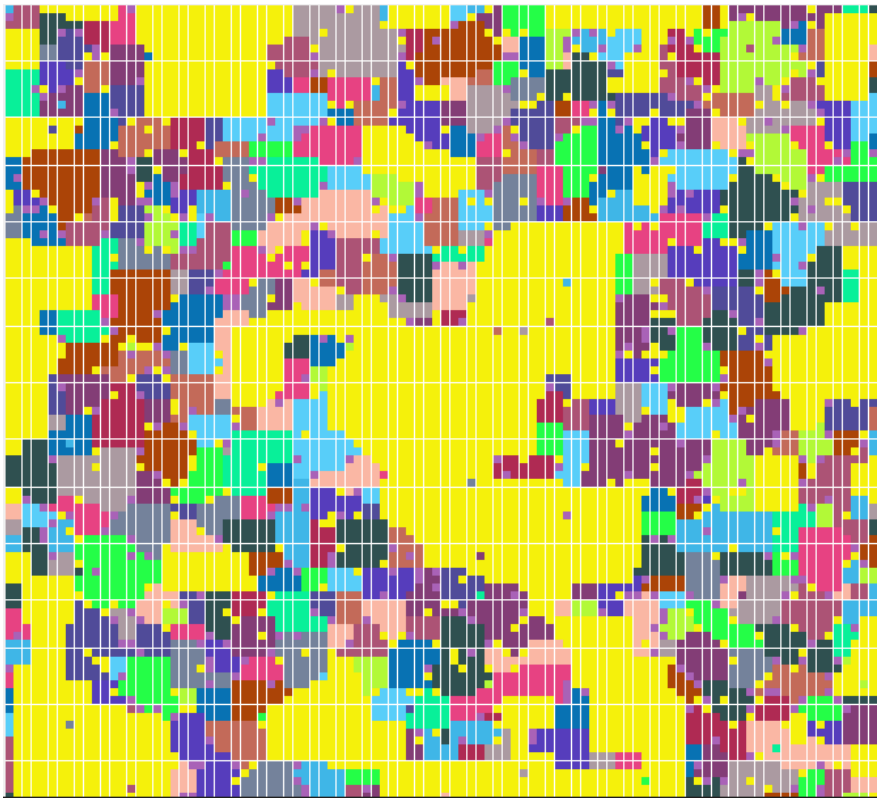
Img 9: CA -> CA



Img 10: CA -> MC



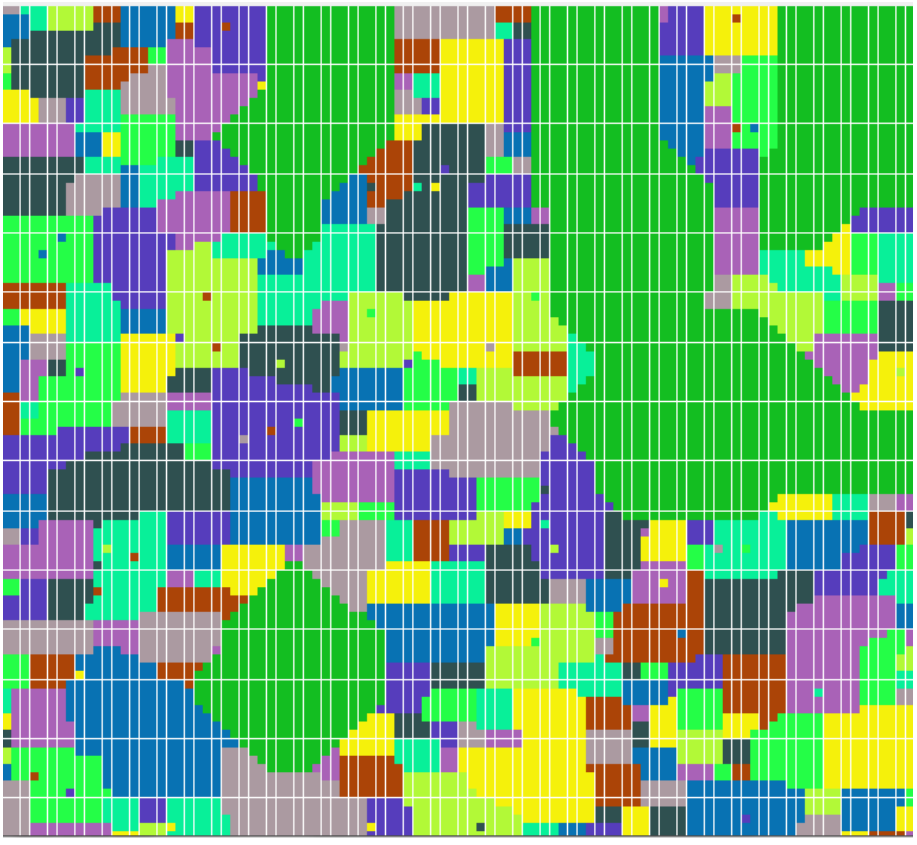
Img 11:MC->CA



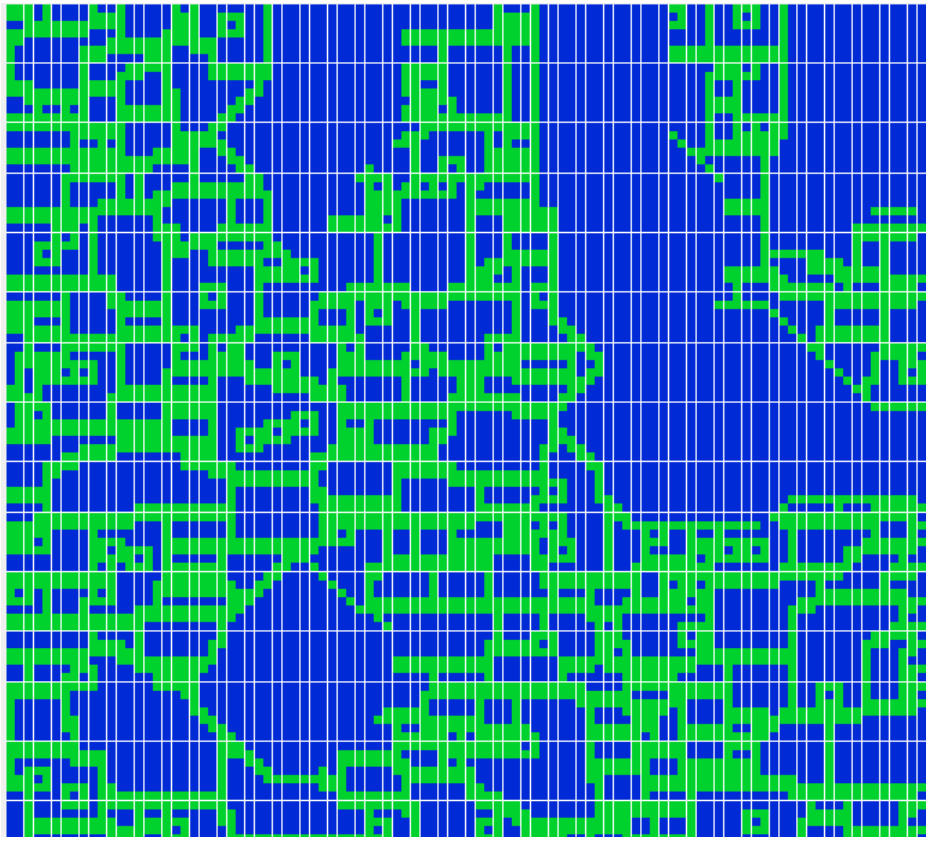
Img 12: MC->MC

Energy distribution

Energy distribution can be vizualized on the previously generated structure. User can choose if energy
distribution is *homogenous* or *heterogenous* an provide such information as *grain energy* and
boundary energy. After pressing *Vizualize* button, the figure presenting energy distribution is
displayed. To vizualize energy two colors were used: blue – represents
zero energy in cell, green – one to ten energy rate



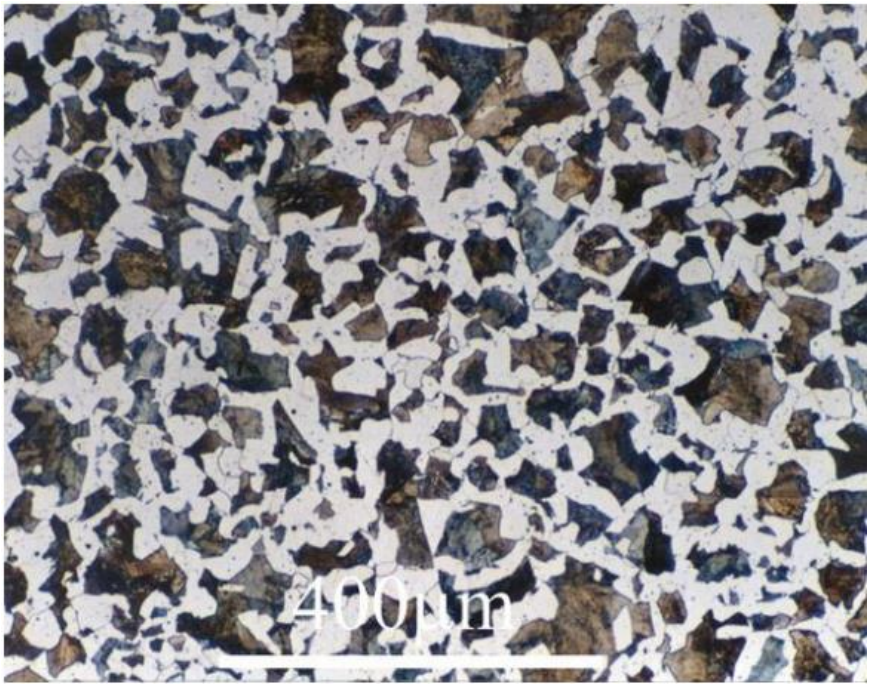
Img 14: Example generate microstructure



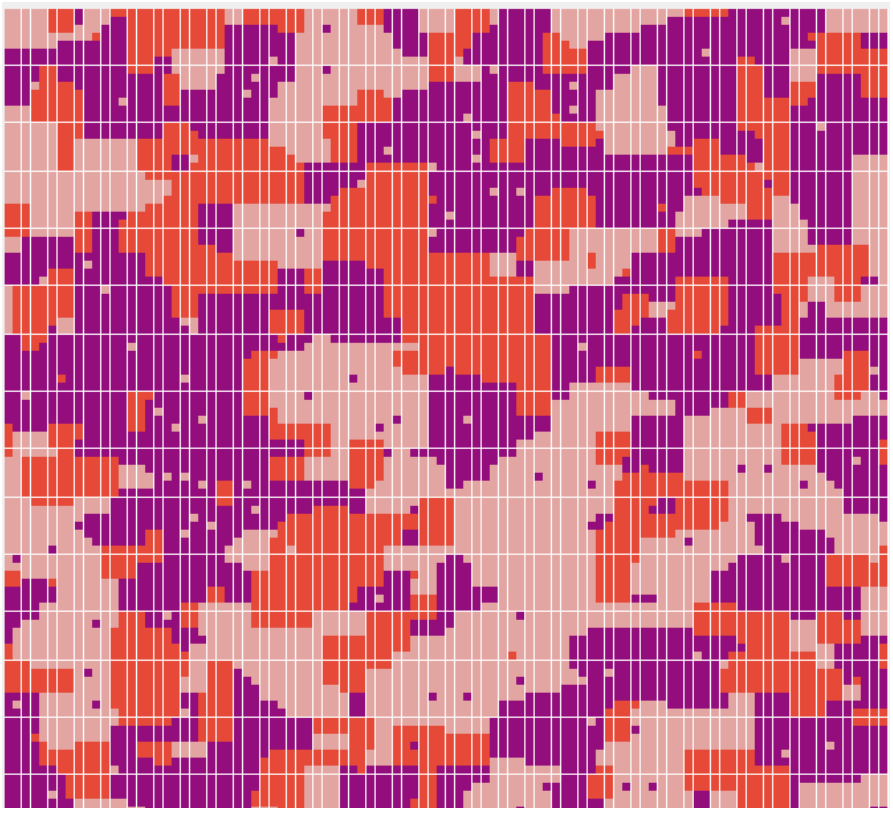
Img 15: Microstructure from img 14 showing heterogeneous energy distribution.

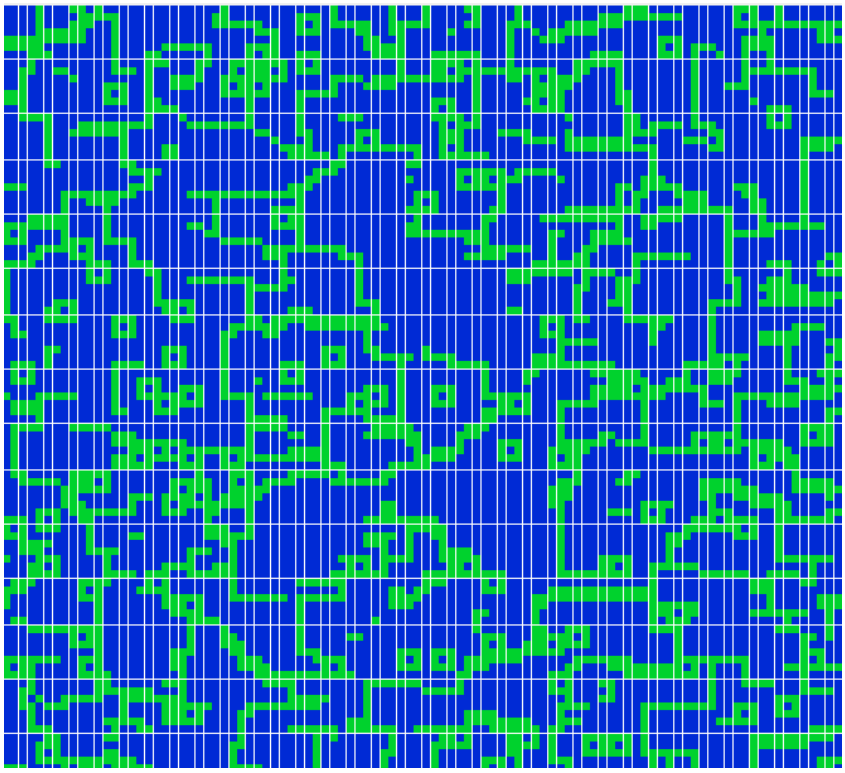
Microstructure comparison

I took two microstructures to compare them. First microstructure comes from my application, second microstructure is dual phase steel. Both of them are shown below.



Img 16: Allotriomorphic ferrite in a Fe-0.4C [1]





Img 17,18: Similar microstructure and energy distribution generated with the application.

Conclusions

- MC method give us more possibility to show more realistic microstructure

- MC method is helpful when grains have complex, no regular structure

- Energy distribution efficiently show how to energy distribution in microstructure.

- If we want to have complex and no regular microstructure with MC method we need more than 30 steps to have satisfy result. More steps higher complex and no regular but in example 100 steps we need wait one minute to complete generation in Intel i7 processor generation.

https://www.researchgate.net/figure/Initial-microstructure-of-CP-titanium-longitudinal-direction_fig1_267406005, 22.11.2018