Multiscale modeling		
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1. Introduction

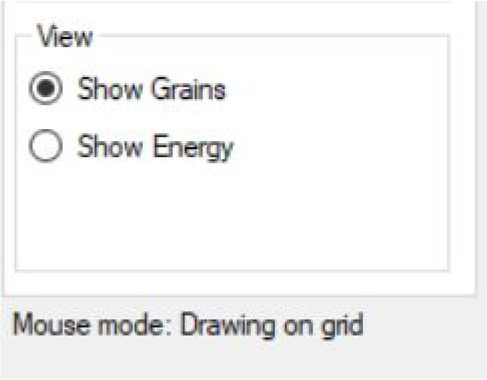
This report focuses on new functionalities developed to original program. As such, project was expanded upon which usage of C# language and Visual Studio 2019 as IDE. This time there was no need to use additional libraries. Full change history is available on GitHub under the following link: https://github.com/SlowikowskiMichal/MultiscaleModeling.

During this report I will present Monte-Carlo grain growth (with dual-phase), and flow combining this new method with cellular automata. At last simple example involving energy distribution and recrystallization will be shown.

Thanks to thought out design and object oriented programming all changes to the original code, for example to expand on visualization, went rather smoothly.

2. Graphical User Interface Overview

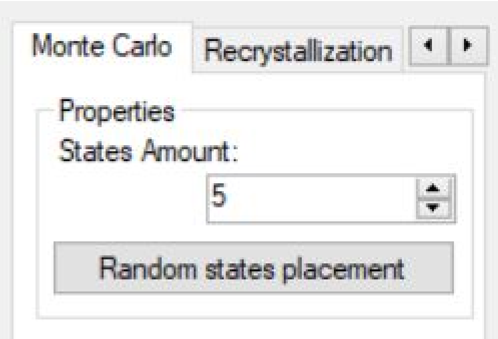
Application retained most of its original design. Two new tabs were added: Monte Carlo and Recrystallization [1]. On Properties tab new group was added, it contains new visualization modes [2].



● Show Grains

○ Show Energy

Mouse mode: Drawing on grid



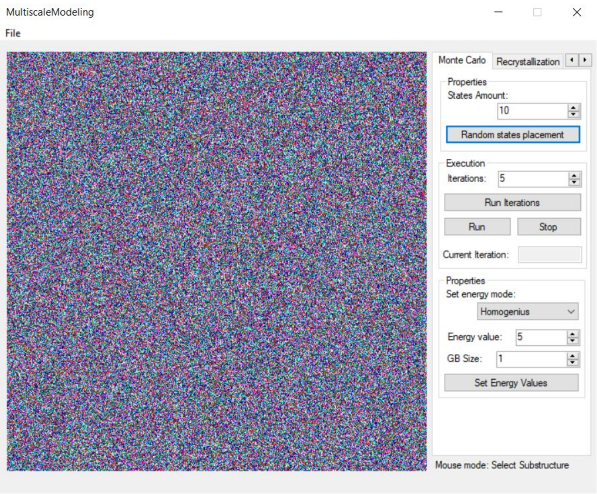
States Amount: 5

Pic.1 Visualization group

Pic. 2 New tabs added to menu

3. Features

In case of Monte Carlo user can choose number of initial states. After confirmation all grains will be assigned id from range of selected states [3]. Next user can determine how to run simulation. Available options are: run predeterminate number of operations, run one iteration or if user want, simulation can be stopped. At the bottom of this group current iteration is displayed.



States Amount: 10

Iterations: 5

Current Iteration:

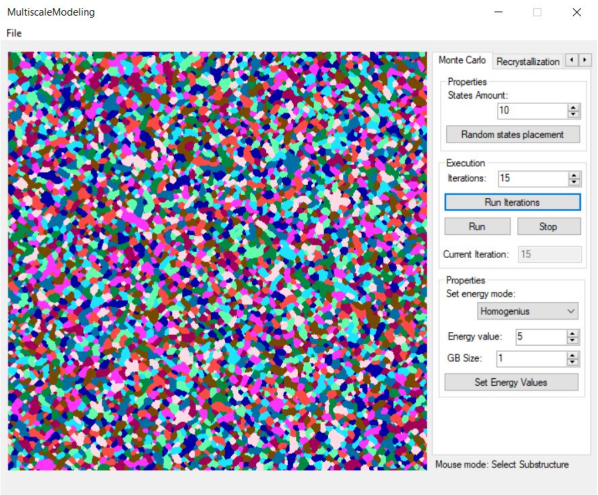
Set energy mode: Homogenius

Energy value: 5

GB Size: 1

Mouse mode: Select Substructure

Pic. 3 Initial placement of 10 IDs



States Amount: 10

Iterations: 15

Current Iteration: 15

Set energy mode: Homogenius

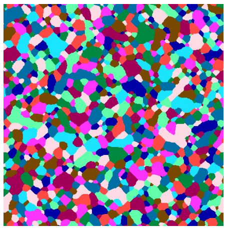
Energy value: 5

GB Size: 1

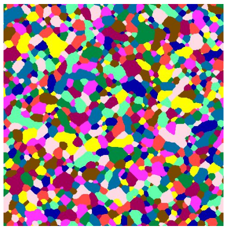
Mouse mode: Select Substructure

Pic. 4 Grid after 15 iterations

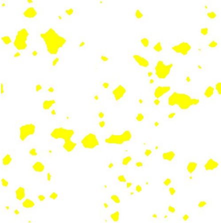
Because new functionalities were built upon already existing one and core of Monte Carlo method is the same as CA generated grid can be processed further with dual-phase functionality. For example user can start with structure generated from Monte-Carlo [5] then choose grains which will be preserved [6], clear grid [7] and start MC from beginning or use CA [8][9]. Result from Ca can be also used in MC in similar fashion. Furthermore all other functionalities also will work, like saving and loading, generating boundaries etc.



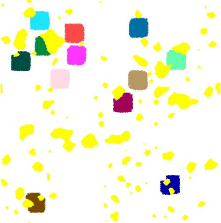
Pic. 5 Structure generated with MC



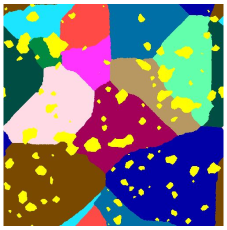
Pic. 6 Selected DP



Pic. 7 Grid after clearing unwanted grains



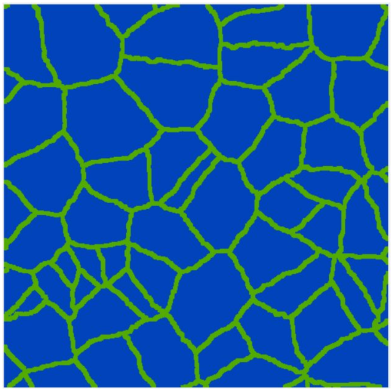
Pic. 8 Grid during growth using CA



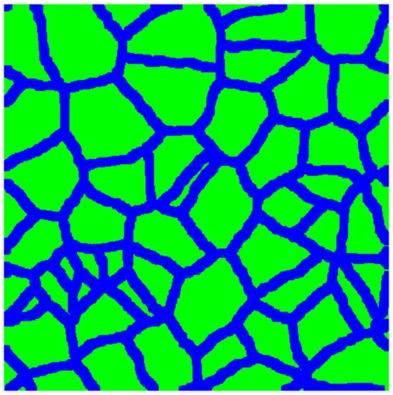
Pic. 9 Final structure

Second new feature is energy distribution and visualization. All cells now their own energy which can be set and visualized. Energy can be set in three different modes: homogeneous [10], on grain boundaries [11] and everywhere but grain boundaries [12]. Grain boundaries size can be set [11] [12]. User can view energy value by changing visualisation settings, recrystallized grains are visualized as red [16]

Pic. 10 All grains have energy equal to 0

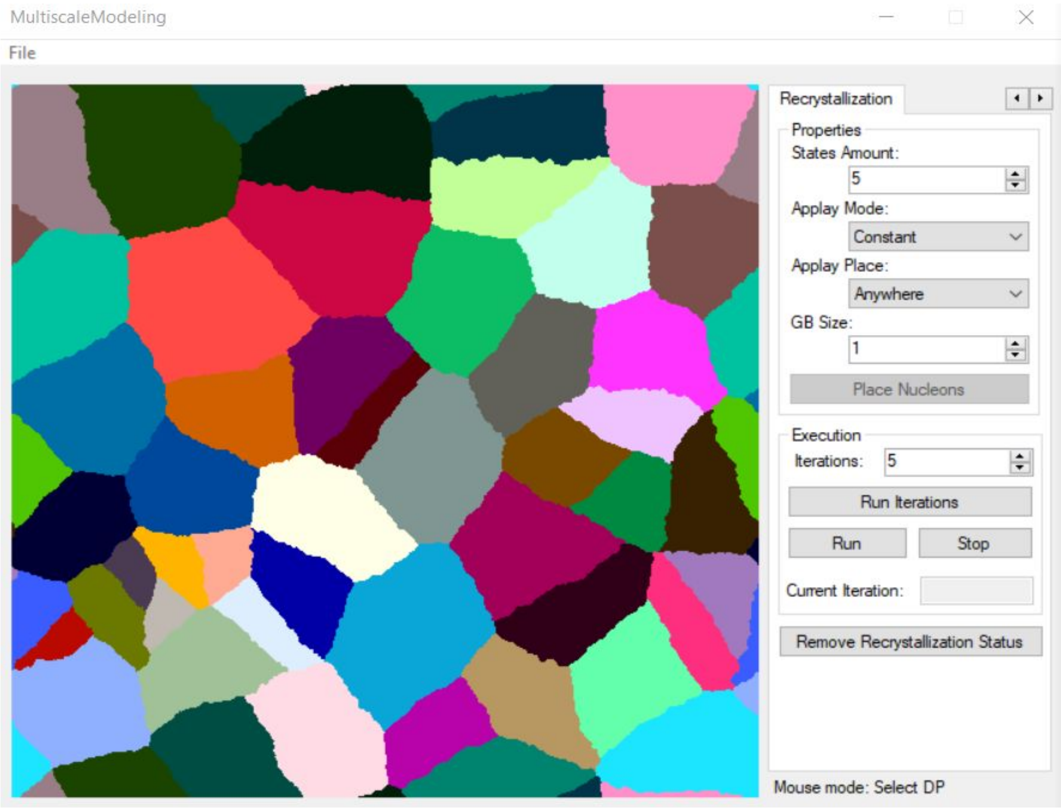


Pic 11 Grain boundaries have energy set to 3, boundary size is set to 3



Pic 12 Grain boundaries have energy equal to 0 and rest cells have energy set to 5, boundary size is set to 6

Fainal tab contains recrystallization settings [13].



States Amount: 5

Applay Mode: Constant

Applay Place: Anywhere

GB Size: 1

Iterations: 5

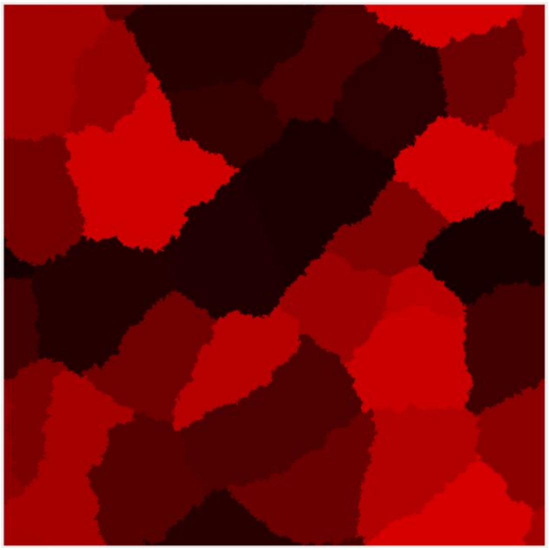
Current Iteration:

Mouse mode: Select DP

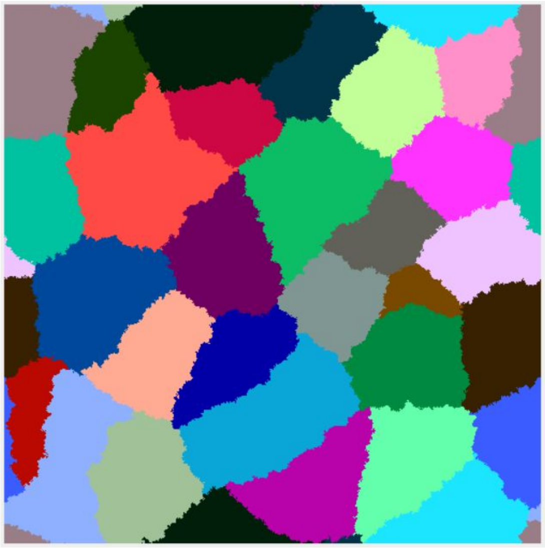
Pic. 13 Recrystallization options.

This menu is divided into two sections. Properties of recrystallization and its execution. In the first group user can decide states amount, how they should be applied and where. Placement of recrystallized grains is easy, they can be placed anywhere or on grain boundaries (size of boundary is determined by user). As for mode how should be applied user have three modes to choose from: manual - user determine where and how many new recrystallized nucleons should be added [14] [15], constant - each iteration constant amount of recrystallized nucleons is added (count of new nucleons is pulled from States Amount textbox), last but not least Increasing - amount of new nucleons is calculated: current iterations * States Amount TextBox [16] [17] [18] [19].

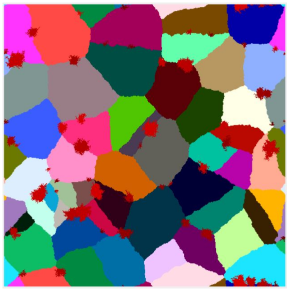
Execution menu is the same as in the case of Monte Carlo menu.



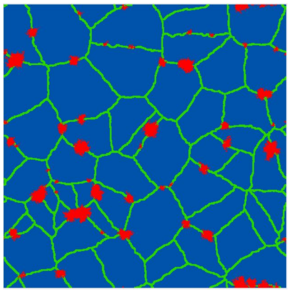
Pic. 14 Recrystallized grid from Pic 13, homogeneous energy, recrystallized nucleons (50) added at the beginning of simulation.



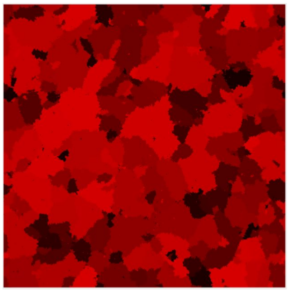
Pic. 14 with recrystallization status removed. This structure is ready for further processing.



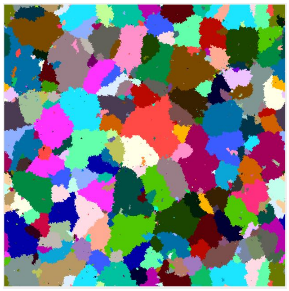
Pic. 16 Grid from Pic 13 during recrystallization, bigger energy on boundaries, increasing mode (amount equal to 10)



Pic. 17 Previous picture, but with energy visualization.



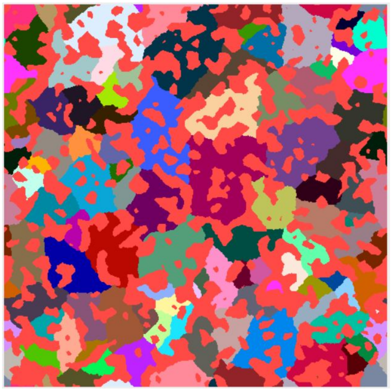
Pic. 18 Recrystallized structure with setting as described in Pic 16.



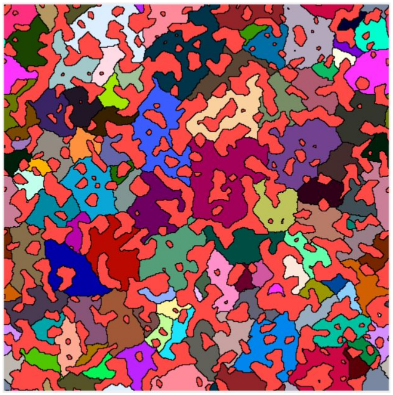
Pic. 19 Removed recrystallization status from structure in Pic. 18

4. Comparison with real microstructures

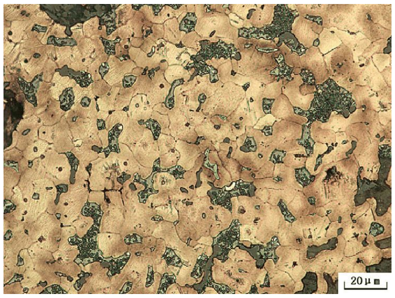
In the first comparison I have tried to recreate “microstructure of partly annealed casting bronze” [22].



Pic. 20 Generated structure.



Pic. 21 Generated structure with grain boundaries.



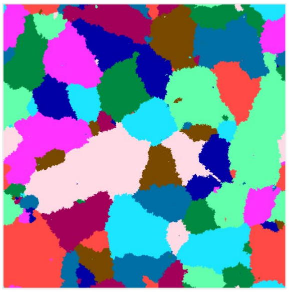
Pic. 22 Actual microstructure. Source:https://www.researchgate.net/figure/Microstructure-of-partly-annealed-casting-bronze-of-the-zun-HZ003-with-the-remaining-a_fig4_223374066

Structure generated by application [20][21] share some similarities with actual microstructure. Although not perfect I think it can be used for further processing. At first Monte Carlo simulation was conducted (3 nucleon ids). One of ids was selected as sub-structure and then microstructure was put through CA, when I have generated finished result. To enhance finished result I have generated grain boundaries.

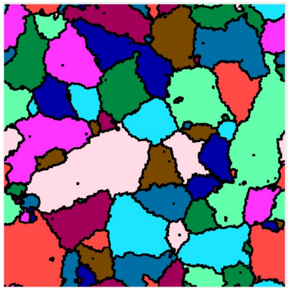
Monte Carlo algorithm helped with creating grains of various size and “rounded” boundaries seen in original microstructure. Thanks to further processing with usage of CA final result also shows more “straight” boundaries as seen in bronze structure.

Second microstructure chosen to recreate was homogenized 6026 aluminum alloy [26].

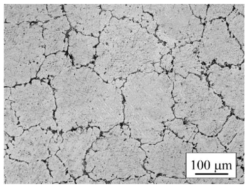
Pic. 23 Generated structure from recrystallization.



Pic. 24 Generated structure with recrystallization status removed.



Pic. 25 Generated structure with added inclusions and boundaries.



Pic. 26 Original microstructure https://www.researchgate.net/figure/Microstructure-of-the-homogenized-6026-aluminum-alloy_fig1_273579005

To generate this microstructure first I prepared grid in Monte Carlo method, then I have run recrystallization algorithm with this settings: nucleons amount: 10, apply mode: constant, apply place: Anywhere [23] [24]. Then I have added couple inclusions and set grain boundaries [25].

During simulation I have successfully recreated jagged grain boundaries as seen in original microstructure. Thanks to adding new recrystallized nucleons each iteration grains have various sizes.

Overall, even if not entirely accurate, generated microstructures share more than enough similarities to real structures to be viable in further processing.