Project 2

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Monte Carlo (MC) technique is becoming a very effective simulation method for prediction and analysis of the grain growth kinetics at mesoscopic level. The concept behind the Monte Carlo method in grain growth simulation is both simple and fascinating: its only basis is the thermodynamic of atomic interactions. There are no other experimental or theoretical inferences, nor mathematical approximations. The first step is to represent the material as a 2D or 3D matrix, in which each site corresponds to a surface or volume element. The content of each element represents its crystallographic orientation. During classes class algoritm was modified in accordance with the given guidelines. Additionally, new functionalities was made, such as: dual phase microstructures with CA simple growth and Monte Carlo; energy distribution and recrystalization.

Technology

Programming language: Python
Language version: 3.7
Visualization library: Tkinter

User interface

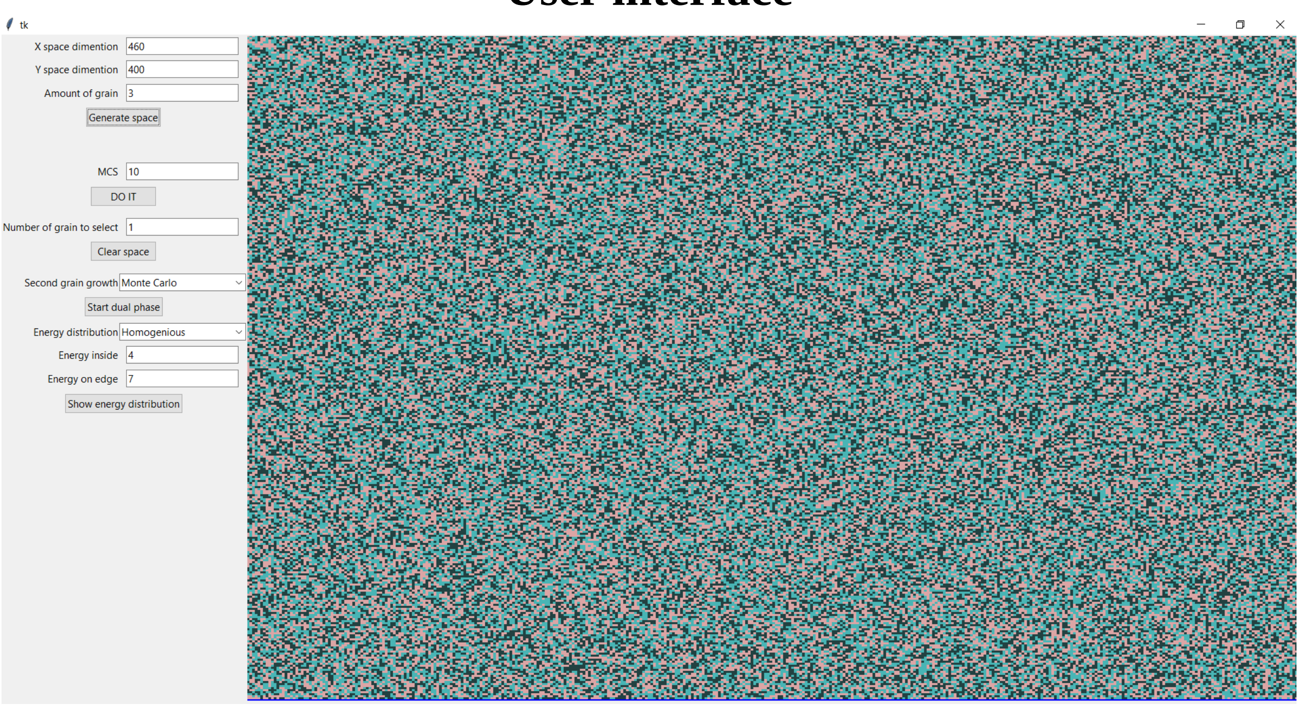

Image 1. User interface

In the Image 1 we can see main app view. On the left, there is main menu where we can start manipulate our simulation. On the right we have the main part of the application – microstructure visualization. The menu contain field with space generation, dualphase, and energy distribution.

App operating

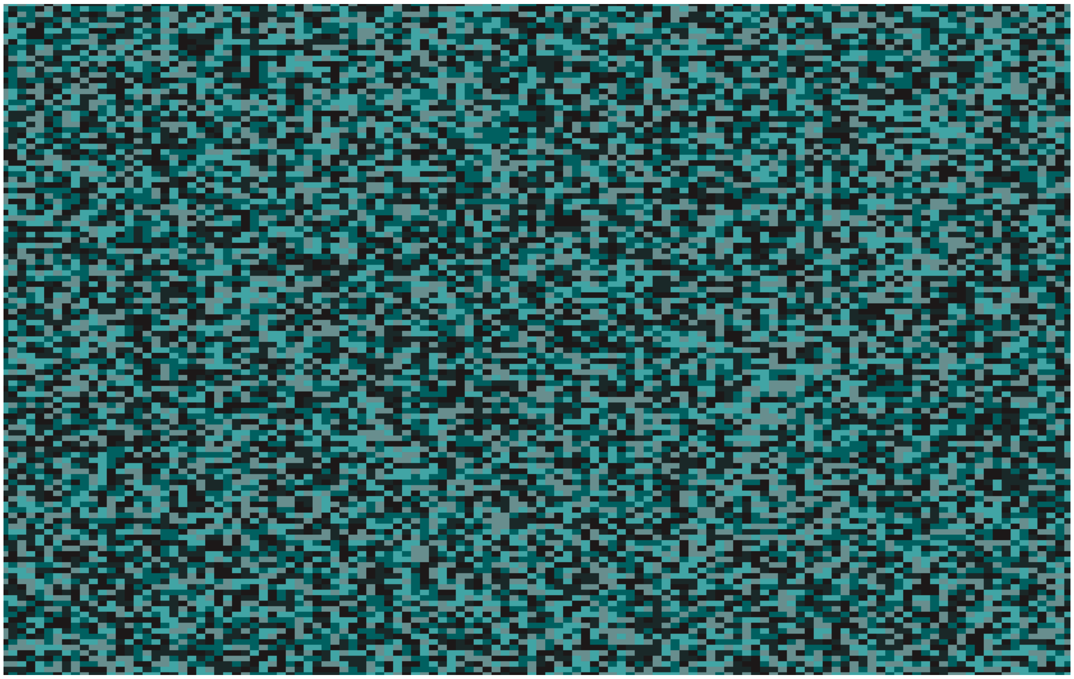

Image 2. Monte Carlo initialization – 130x130 field with 5 grains.

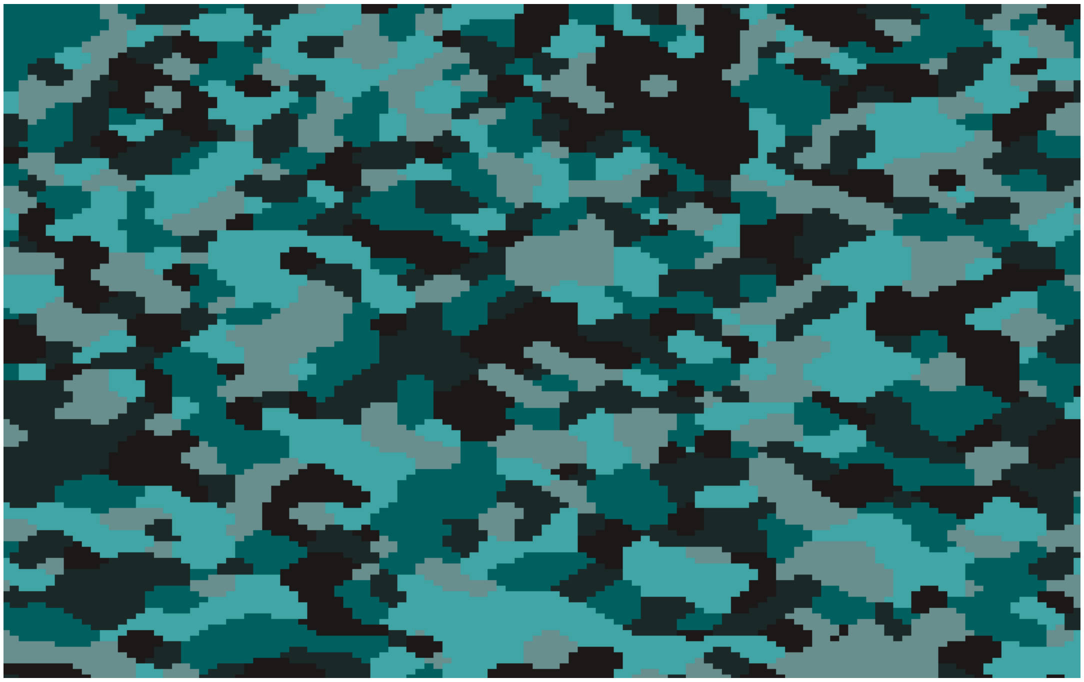

Image 3. Monte Carlo 130x130 field with 5 grains after 60 iterations.

Full example of all program options

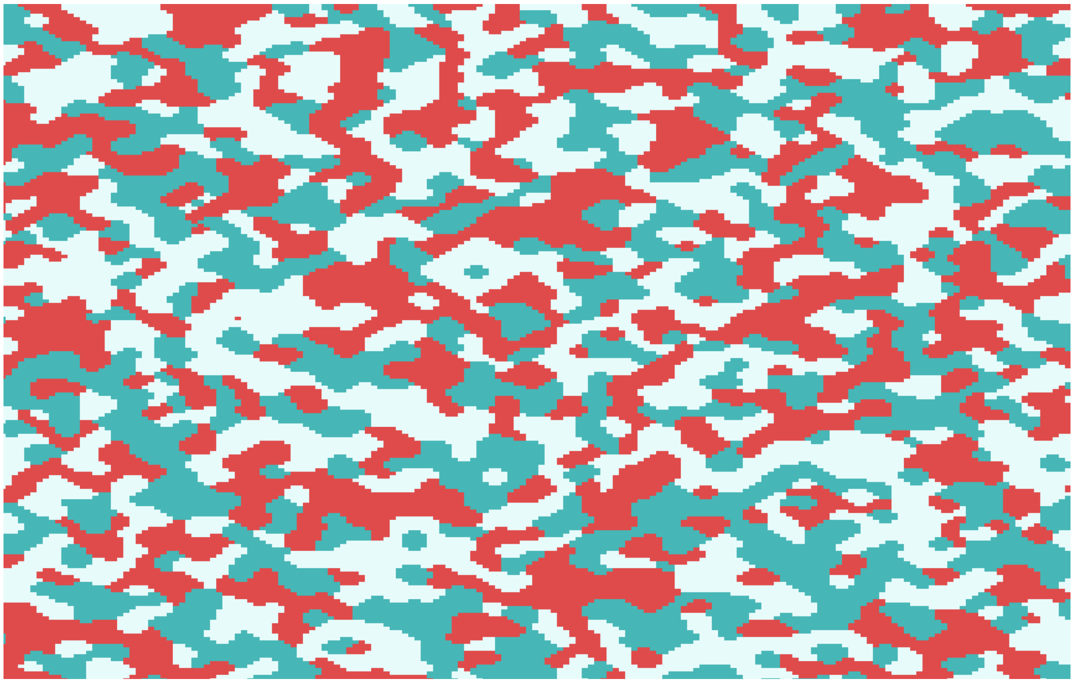

Image 4. Generate microstructure

First step of algorithm is generation of microstructure. Image 4 shows microstructure of 3 different grains on 120x120 field. Application give possibility to generate dual phase microstructure after generate grain structure. User can select remaining grains, numer of grains to generate and type of microsturcture.

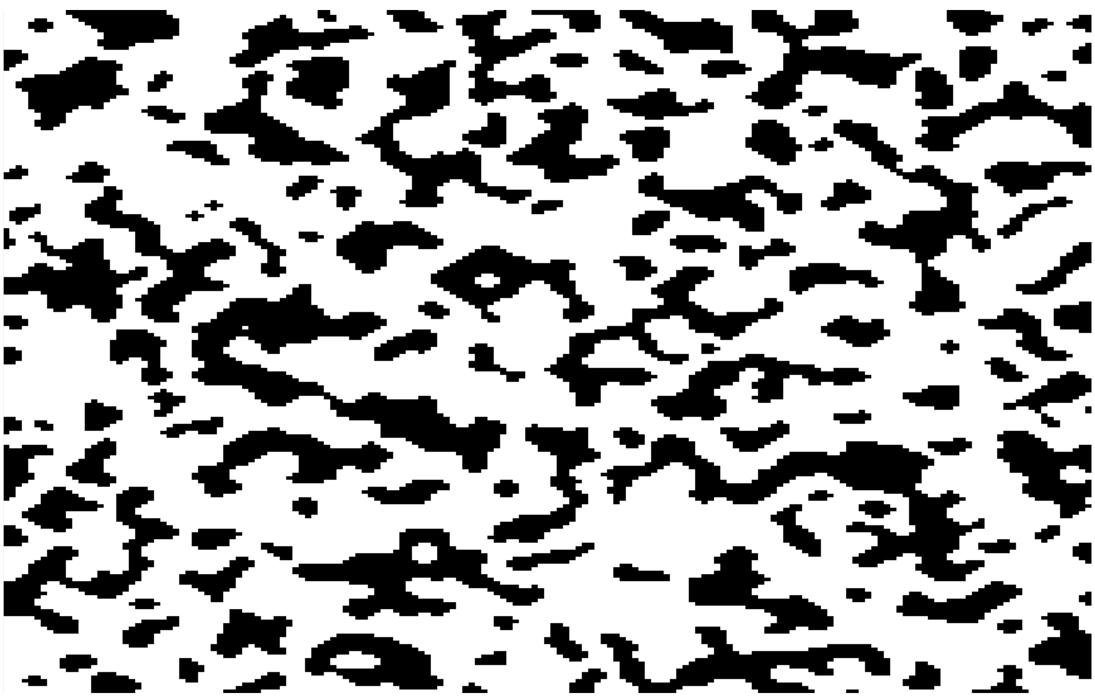

Image 5. Grain selection

Image 6 shows dual phase structure that can be generated using CA and image 7 shows dual phase MC method.

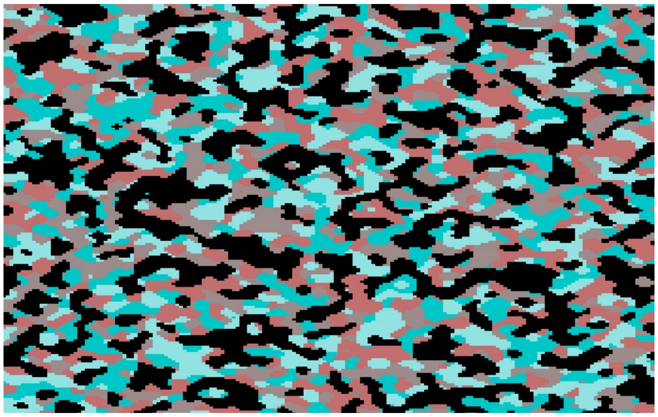

Image 6. Dualphase Monte Carlo

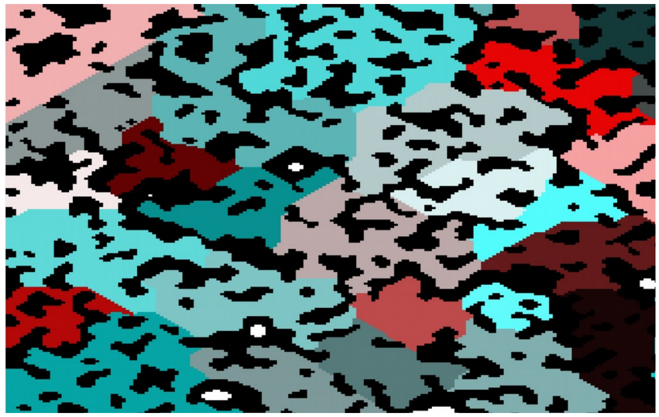

Image 7. Dualphase cellular automaton

Application gives opportunity to calculate and show Energy inside the structure. We can choose between heterogenous and homotenous energy distribution woth some small value perturbation (less than 10% of total energy value).

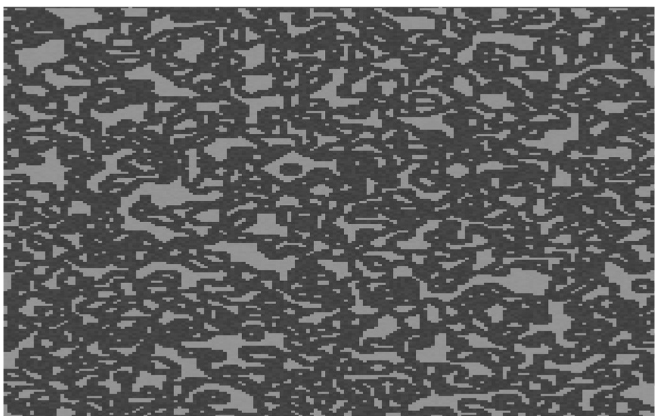

Image 8. Heterogenous energy distribution after Monte Carlo

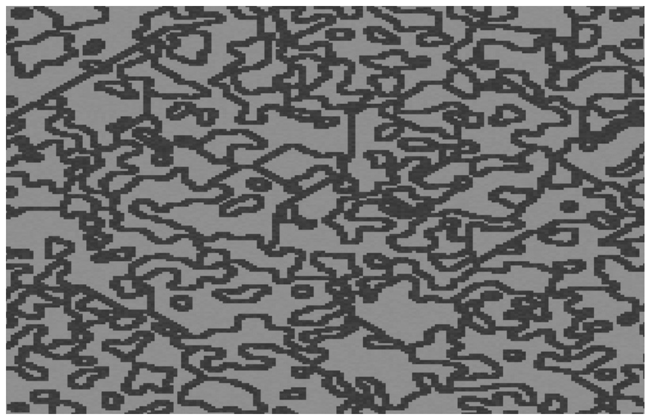

Image 9. Heterogenous energy distribution after cellular automation

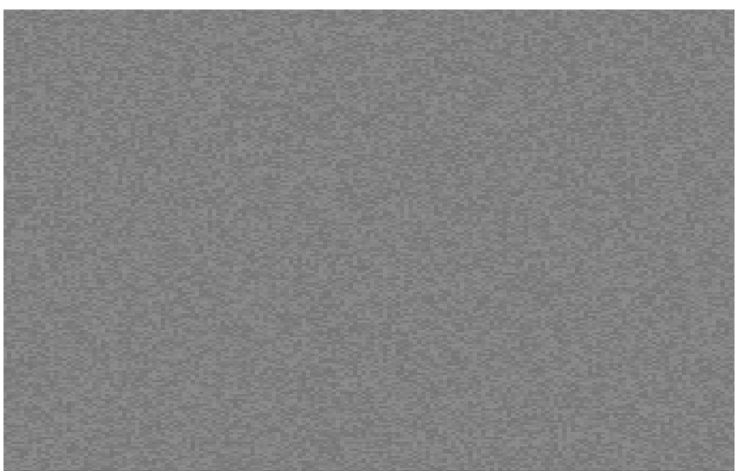

Image 10. Homogenous energy distribution

Real example

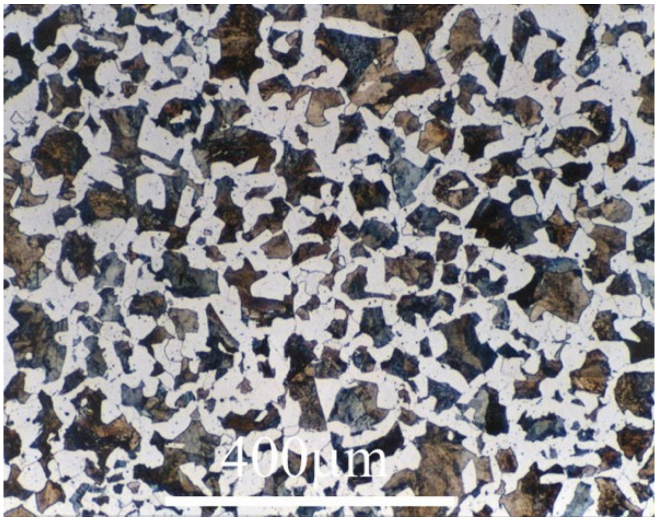

Image 11. Allotriomorphic ferrite in a Fe-0.4C steel which is slowly cooled.

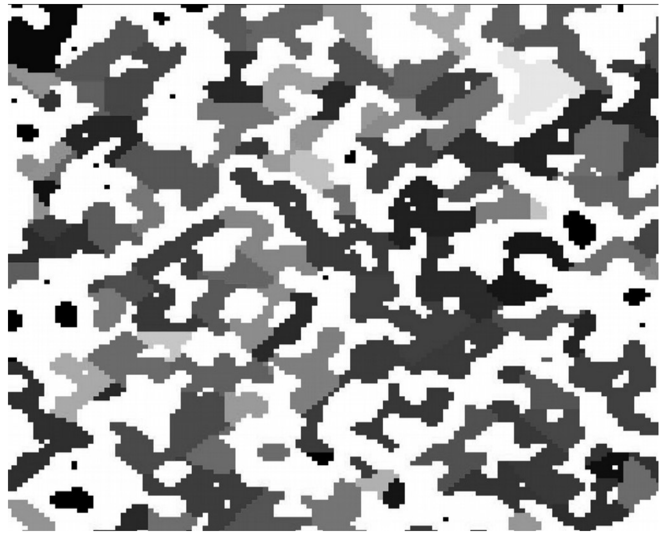

Image 12. Microstructure generated with dual phase Monte Carlo.

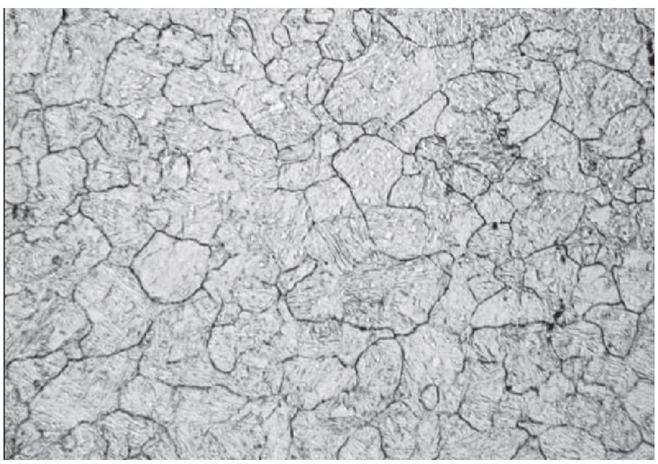

Image 13. S405 after 45 seconds of recrystallization.

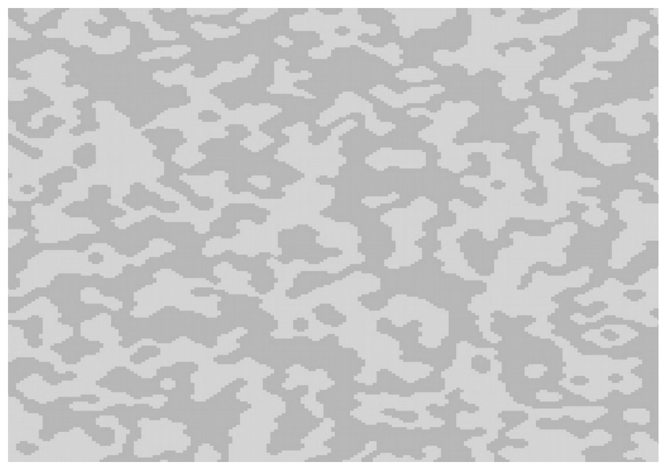

Image 14. Microstructure generated with MC

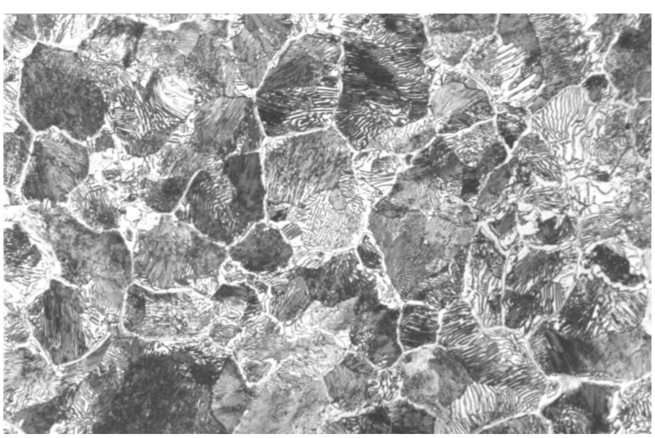

Image 15. Steel with 1,3% of carbon.

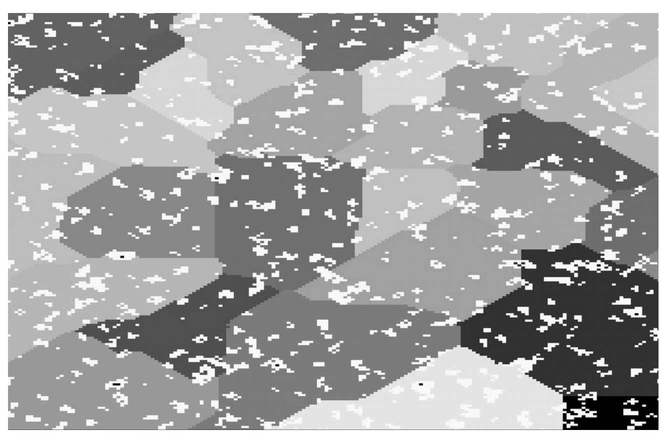

Image 16. Microstructure generated with MC and cellular automata.

In all examples we managed to achieve similar grains shape and size. Created image seems to be quite good attempt of simulating this kind of material but there are some small inaccuracy. In the image 14 we wasn’t able to create good enaught grain boundaries and in the image 15 grains should be a little smaller.

Conclusions

Simulations give results which are similar to real microstructures. Application can be used to solve real problems, is expandable if new functionalities will be needed, Monte Carlo method is slower than CA but its possible to imporving some parts of algorithm. Monte Carlo method is working completely random. The most important thing is amount of iterations and good random number generator. It is hard to generate big grains using that method.