AGH

AKADEMIA GÓRNICZO-HUTNICZA
IM. STANISŁAWA STASZICA
W KRAKOWIE

Multiscale modelling

2st report: Monte Carlo grain growth algorithm

Katarzyna Fornal
WIMiIP, IS, 2nd grade
MiTI, gr. 4

INTRODUCTION

Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. This report presents software designed to implement a simulation of the Monte Carlo grain growth. Program contains also other features such as generating different microstructure types and distributing stored energy.

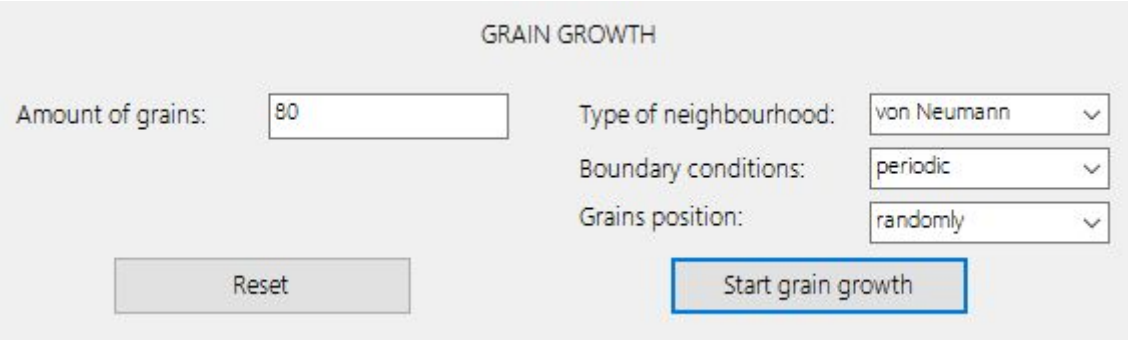
The simulation of MC grain growth algorithm was implemented in C# using Microsoft Visual Studio. GUI was created using Windows Forms Application.

FUNCTIONALITY

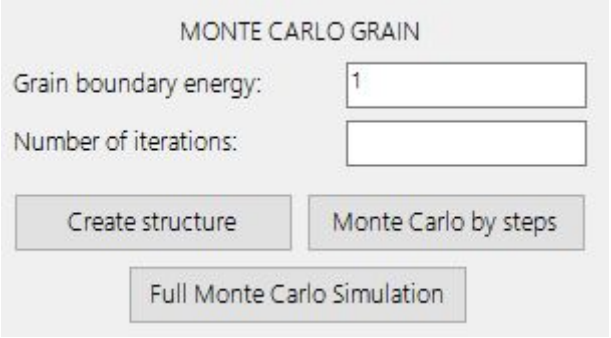
1. MONTE CARLO GRAIN GROWTH

To start simulation of Monte Carlo grains growth, grains need to be located in the CA grid (picture 3). User has to input amount of grains and click 'Create structure' button. Every cell is defined, by setting state's value, choosing randomly a value from 1 to inputed number of grains (picture 1).

Next, user has to input value of grain boundary energy <0.1 - 1.0>. There are two ways to start simulation of Monte Carlo grains growth (picture 2). First one, by clicking on 'Full Monte Carlo Simulation' button - full simulation starts, iteration by iteration, until the CA grid will be containing only one grain or reseting the grid. Second one, by inputting number of iteration and clicking 'Monte Carlo by steps'. It generates the Monte Carlo microstructure after defined iteration.



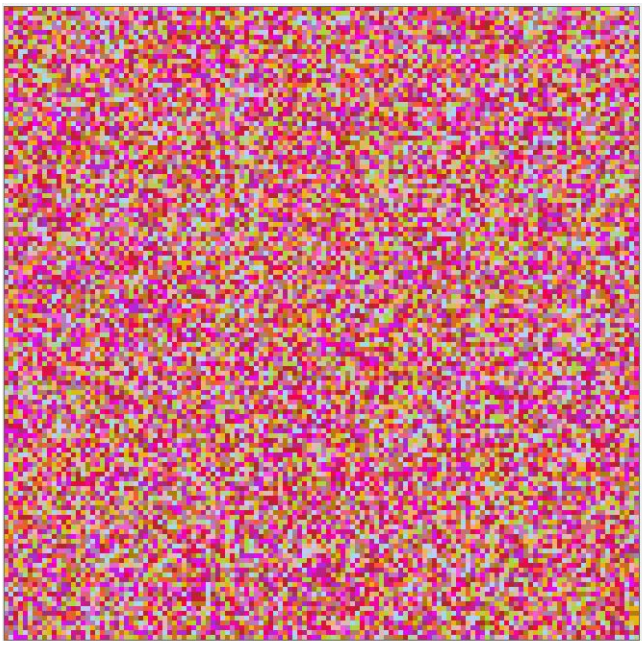
Picture 1: Grain growth algorithm parameters



Picture 2: Monte Carlo grain growth algorithm parameters

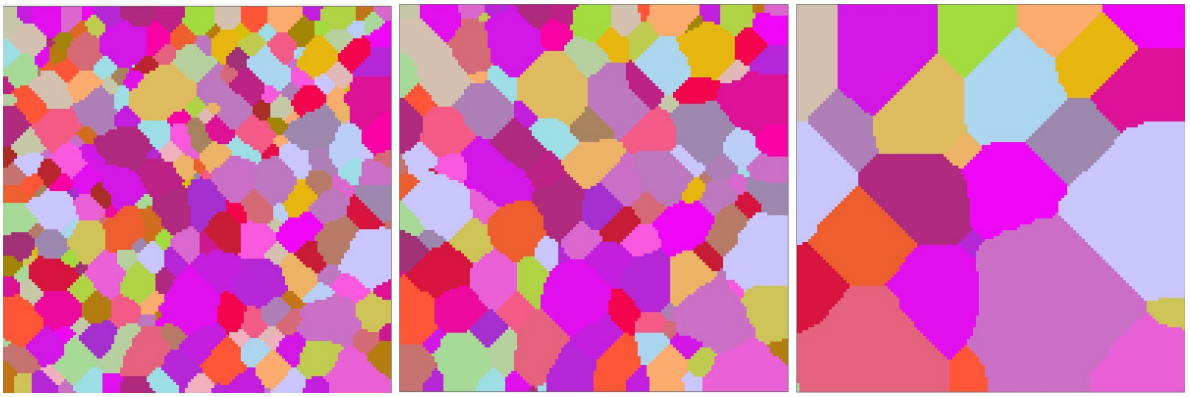
MONTE CARLO GRAIN GROWTH ALGORITHM

One value from defined scope of grains amount was assigned randomly to every state of cell in the grid (picture 3). Algorithm goes through the grid, cell by cell, calculating its energy. Calculation is made by checking how many of its neighbours have other state value and multiplying returned value by number of grain boundary energy <0.1 - 1.0>. After that, state of concerned cell is replaced by one of its neighbour and energy is calculated for the new state of the grid. If the present energy value is higher than the previous one, the state is replaced by its previous value. When all of the cells are checked, image of the grid is updated and next iteration begins. The simulation is running until the grid contains only one grain or if user stops it.



Picture 3: Location of cells in Monte Carlo

Picture 4: Monte Carlo grain growth by steps



a. after 50 iteration **b. after 100 iteration** **c. after 500 iteration**

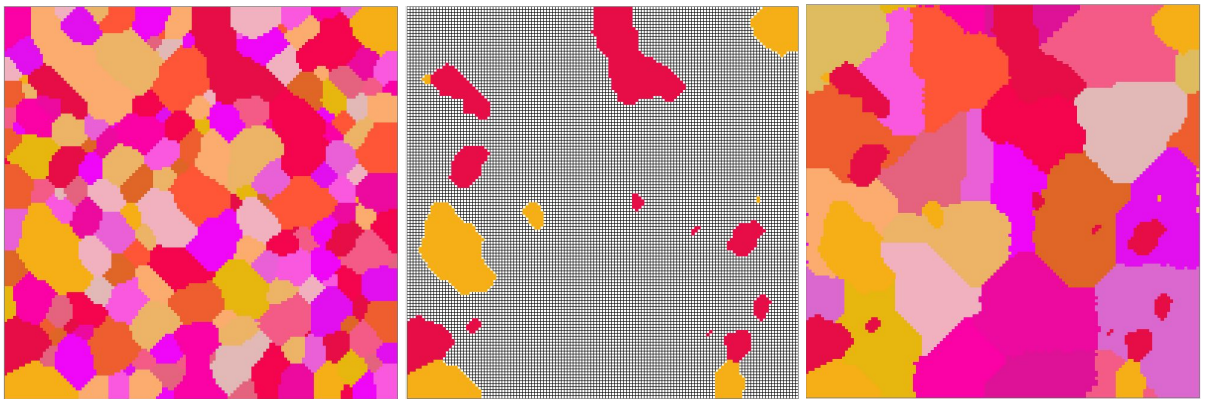
2. DIFFERENT MICROSTRUCTURE TYPE

To achieve different microstructure type, user needs to only click on chosen grains of generated CA grid, select type of structure and click ‘Generate structure’ button (picture 10).

Picture 5: Microstructure type parameters

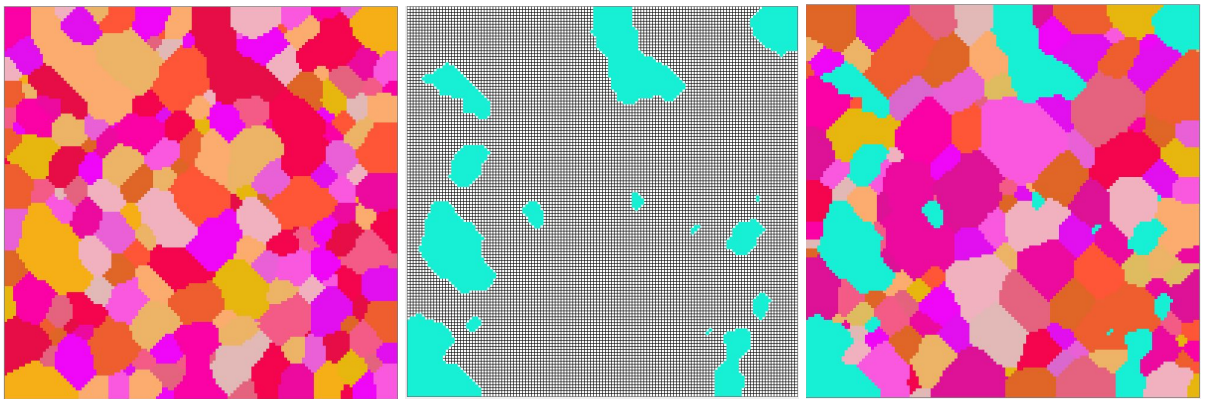
In addition, the phase value of chosen grains increase. Under the generated structure user can start a new simulation. Picture 6 presents Monte Carlo grains growth (6a), generated substructure (6b) after choosing two grains, by clicking on them, then generating new structure of simple grain growth under the substructure (6c). Picture 7 presents similar operation, but after Monte Carlo grains growth (7a), dual phase structure is generated (7b) and then new Monte Carlo structure under the dual phase (7c).

Picture 6: Substructure - Monte Carlo → Simple Grain Growth



a. MC grains growth **b. generated substructure** **c.Simple GG under substructure**

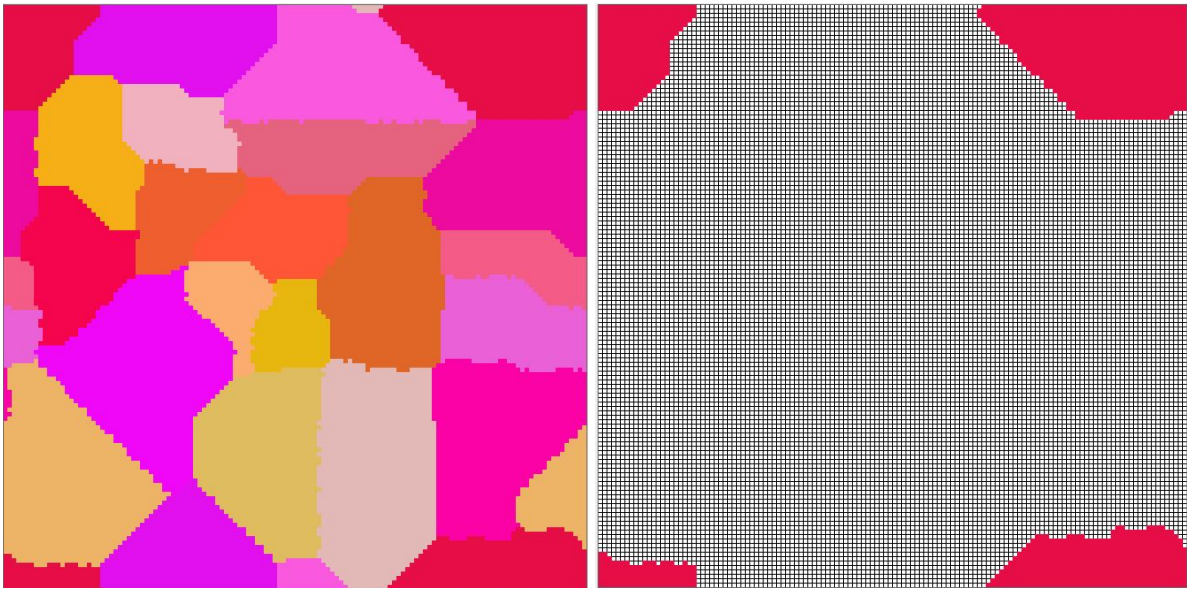
Picture 7: Dual phase - Monte Carlo → Monte Carlo Grain Growth



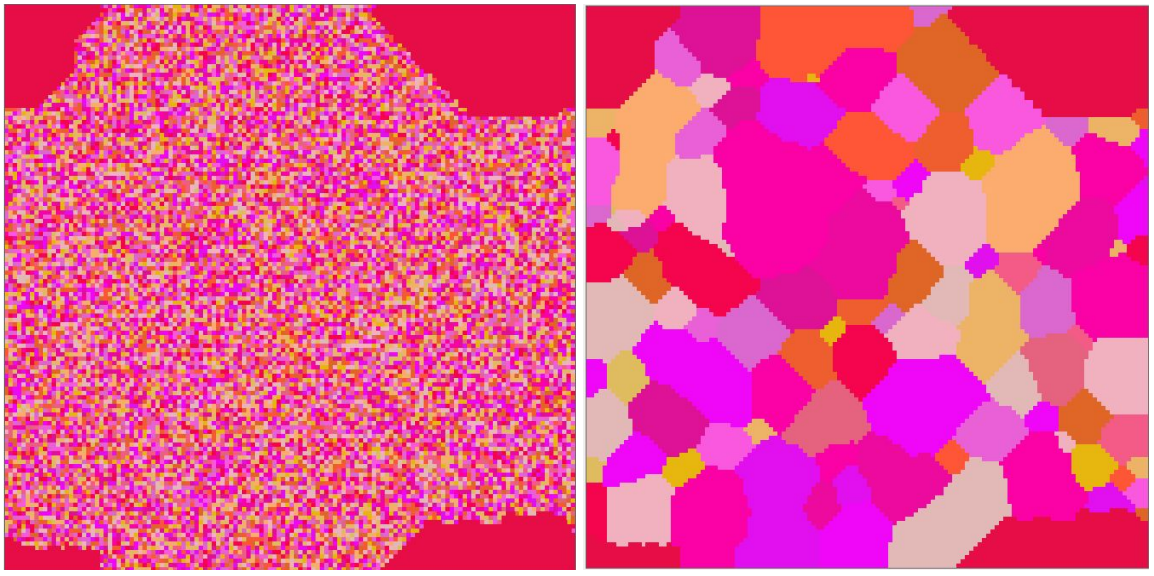
a. MC grains growth **b. generated dual phase** **c.MC grain growth under dual phase**

Picture 8 presents simple grains growth (8a), generated substructure (8b) after choosing one grain, by clicking on it, then locating new grains according to Monte Carlo algorithm (8c) and then generating new structure of Monte Carlo grain growth under the substructure (8d). Picture 9 presents simple grains growth (9a), next dual phase structure is generated (9b) and then new simple structure under the dual phase (9c).

Picture 8: Substructure - Simple Grain Growth → Monte Carlo

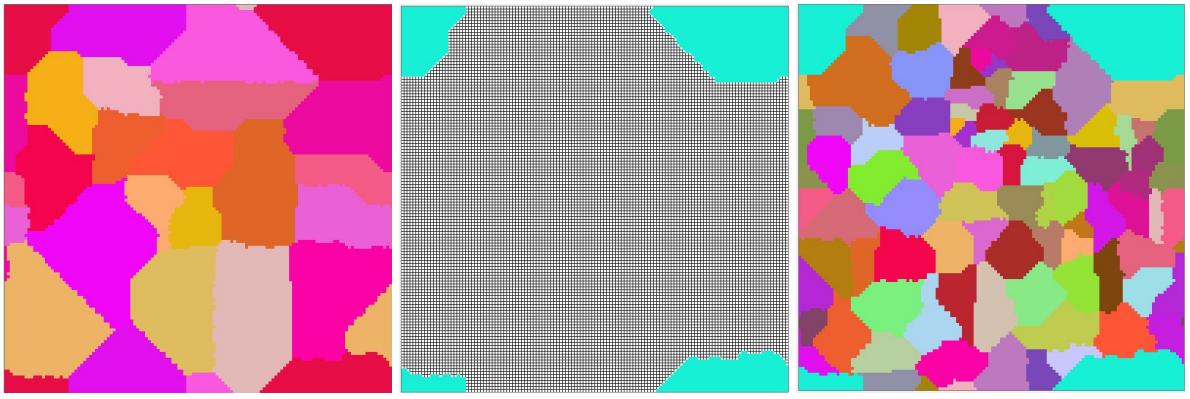


a. Simple grains growth **b. generated substructure**



c. Location of MC grains **d. Simple grains growth under generated substructure**

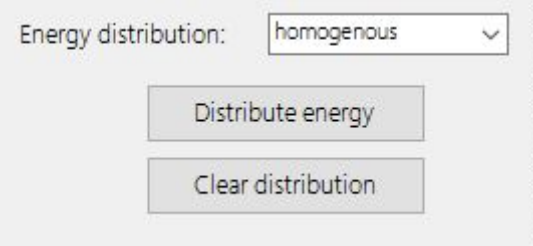
Picture 9: Dual phase - Simple Grain Growth → Simple Grain Growth



a. Simple grains growth **b. generated dual phase** **c.Simple GG under dual phase**

3. ENERGY DISTRIBUTION

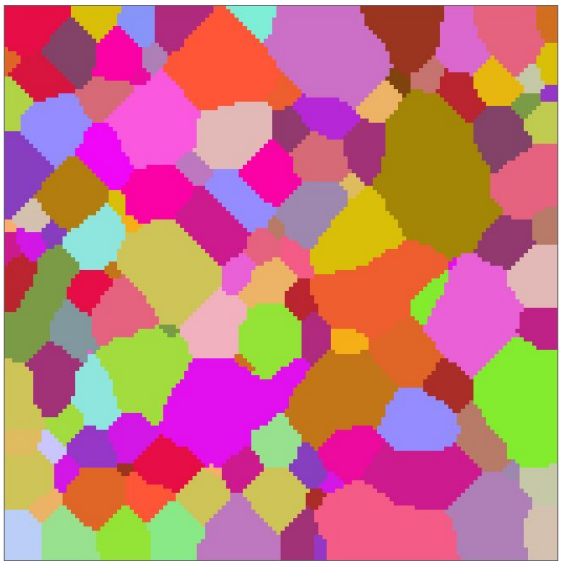
To achieve distribution of stored energy, user has to select what type of energy distributions he wants - homogenous or heterogenous (picture 10). If its homogeneous type, value of the stored energy is the same in every cell, in case of heterogeneous type, value of the stored energy is higher on the edges of grains. After clicking 'Distribute energy' user gets the visualization of energy distribution.



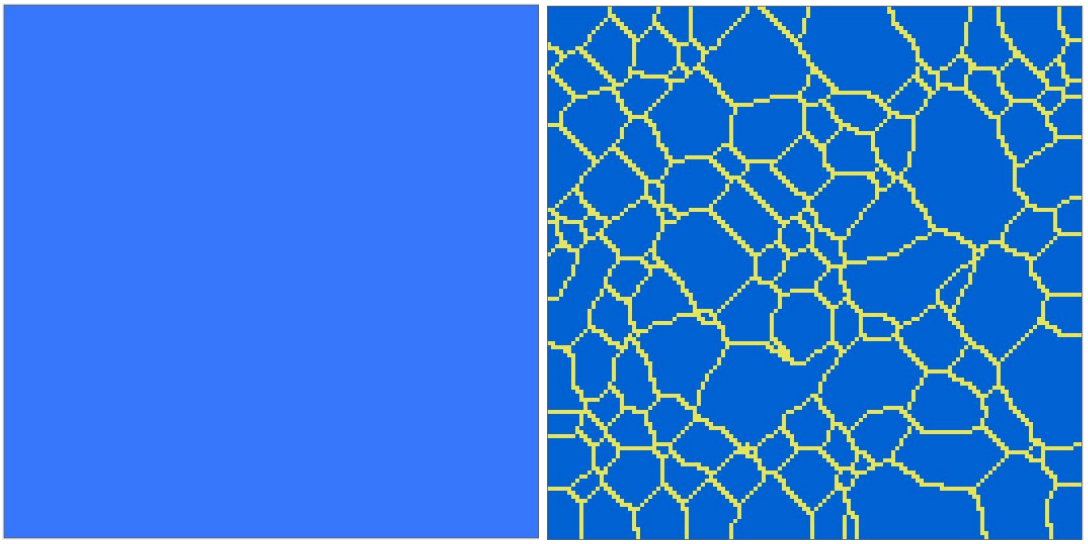
Picture 10: Energy distribution parameters

Simulation of distributing energy made on generated Monte Carlo grid (picture 11a). Sequentially, energy was distributed in homogeneous way (11b), then after restoring generated grid, energy was distributed in heterogeneous way (11c).

Picture 11: Simulation of energy distribution on Monte Carlo grain growth



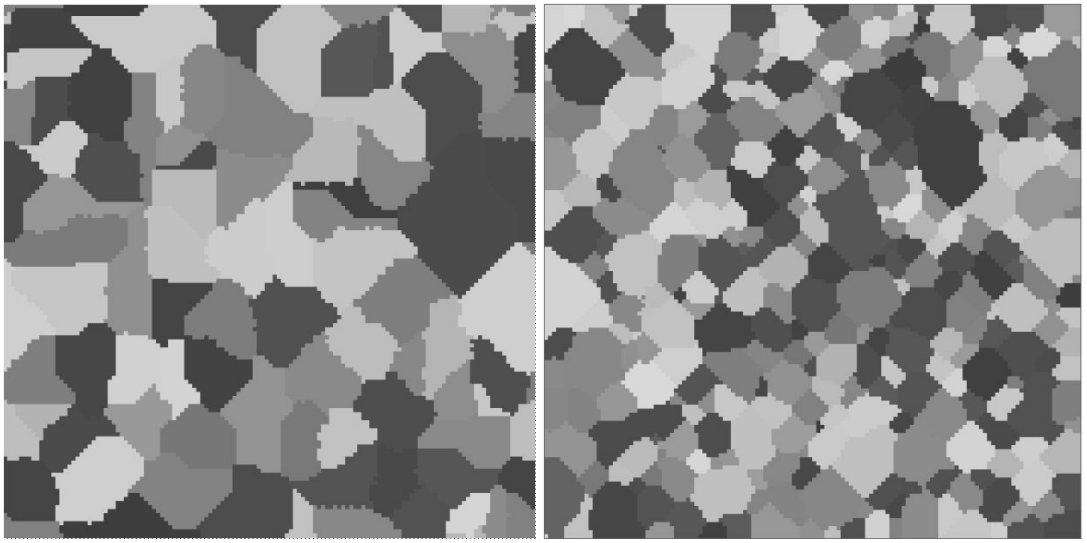
a. Monte Carlo grain growth in 100th iteration



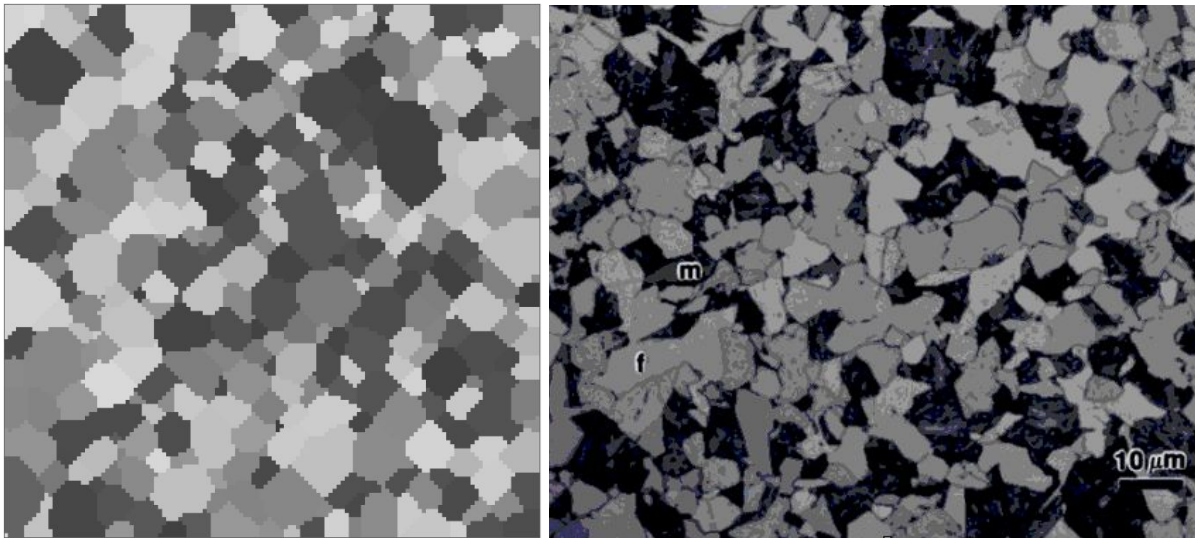
b. Homogeneous distribution on MC structure **c. Heterogeneous distribution on MC structure**

COMPARISON OF REAL LIVE AND SIMULATED MICROSTRUCTURES

Picture 12 presents comparison between the simple grains growth structure and the Monte Carlo one. Both images of these structures are grayscale to make better comparison. Picture 13 shows comparison between the Monte Carlo microstructures generated by program and the microstructure of a malleable cast iron after conversion to nodular graphite.



Picture 12: Comparison of grayscale, generated CA microstructure vs. MC microstructure



Picture 13: Comparison of grayscale, generated CA microstructure vs. real microstructure

Monte Carlo structure seems to be more similar to the real microstructure, especially by looking at its shape and size of grains. Also to present some single, bigger grains which are appearing in real structure, using a dual phase feature would be a good solution.