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Multiscale Modelling

2st report

1. Introduction

The second report concerned implementation of Monte Carlo algorithm which is a method which after randomly selection of element, calculate energy of surrounding concerned element, calculate cell energy and and change it state or not - depending on energy value. Next implemented method was to give possibility to after calling CA algorithm run on the same cell space MC algorithm and similarly after MC algorithm run CA on the same space. Last part concerned implementation initial part of SRXMC algorithm, which on a generated space allows dividing into Homogenous and Heterogenous.

2. Functionalities

A. Monte Carlo algorithm

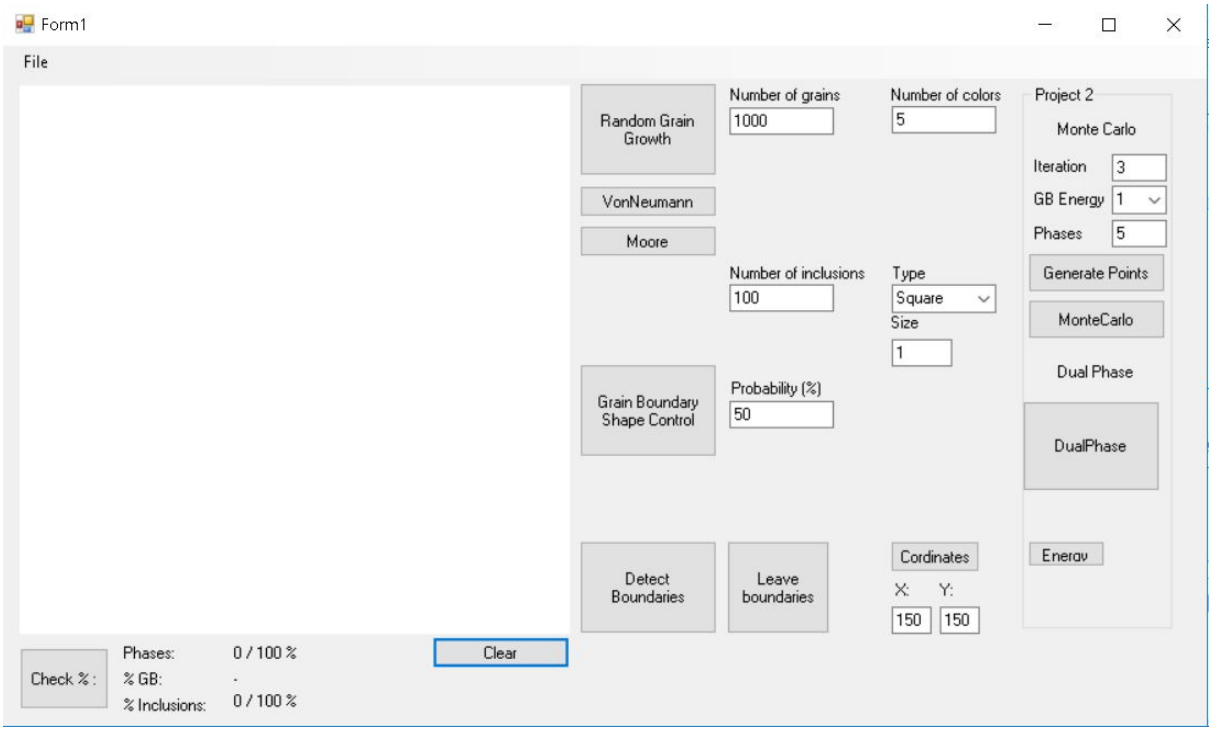
B. CA -> MC

C. MC -> CA

D. SRXMC

A.Monte Carlo algorithm

Picture 1 shows user interface of application



Picture 1. GUI

After randomly selection of element with specifically orientation energy of lattice site surrounding concerned element is being calculated using following formula:

$$E = J_{gb} \sum \left(1 - \delta_{S_i S_j}\right)$$

where:

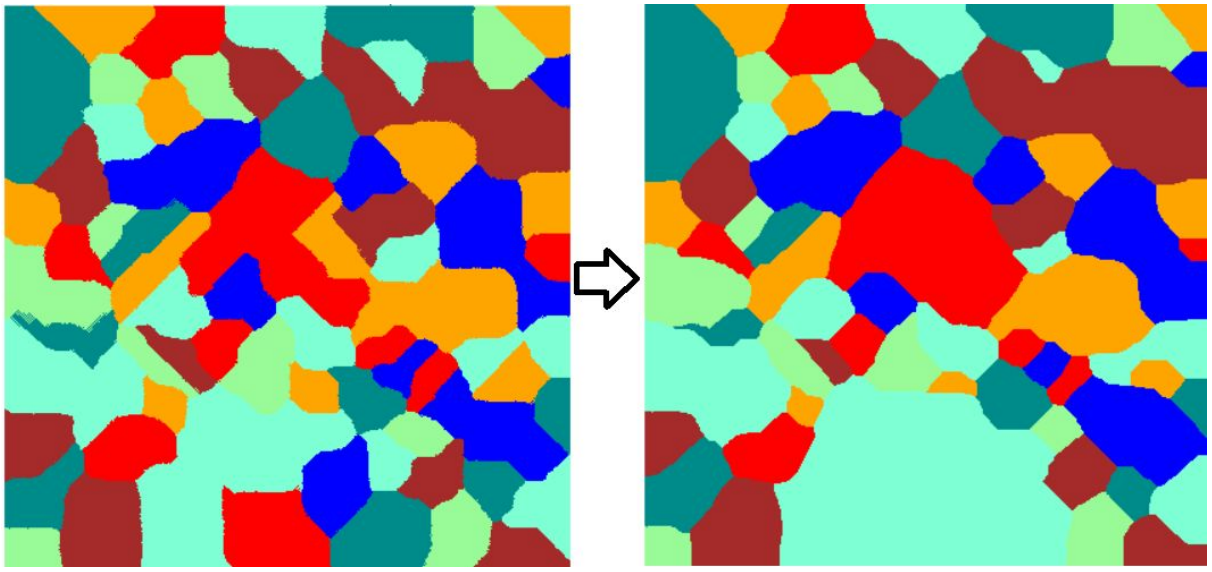
J- Grain boundary Energy <0.1 – 1.0>

Σ <i,j> - Surrounding neighbors points

δ Kronecker delta

The investigated cell changes the state to one of the available states. The state is randomly generated from available states. Next part is calculate the change in energy caused by orientation changes Grain Growth Algorithm. Last part of algorithm(Picture 2) is to change the state after if probability p equals 1.

In the example below (Picture 2) was:
Iteration: 15
GB Energy: 1

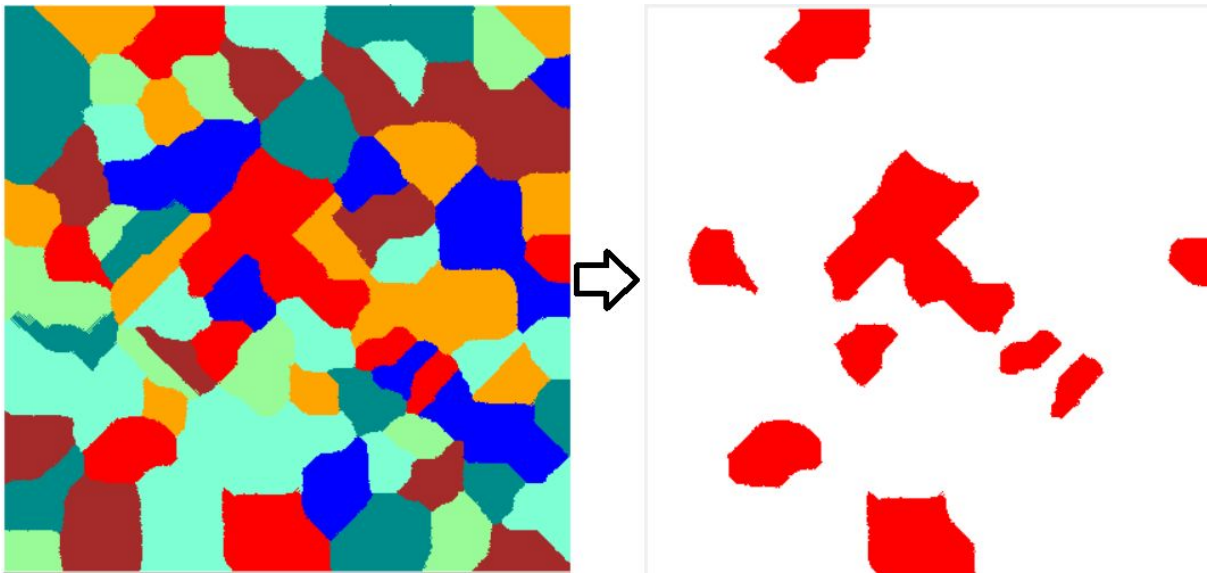


Picture 2. Successfully done Growth simulations

B. CA -> MC

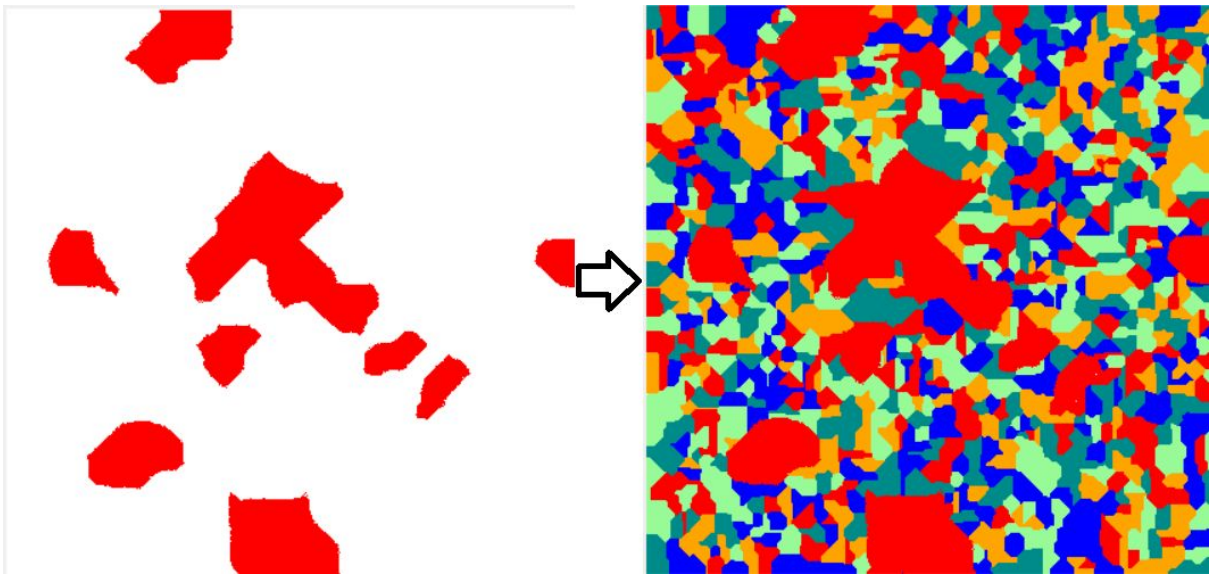
This part of implemented method was to give possibility to after calling CA algorithm run on the same cell space MC algorithm.

First part is to choose a color from coordinates. After this user can start simulation (Picture 3)



Picture 3. Selected phase

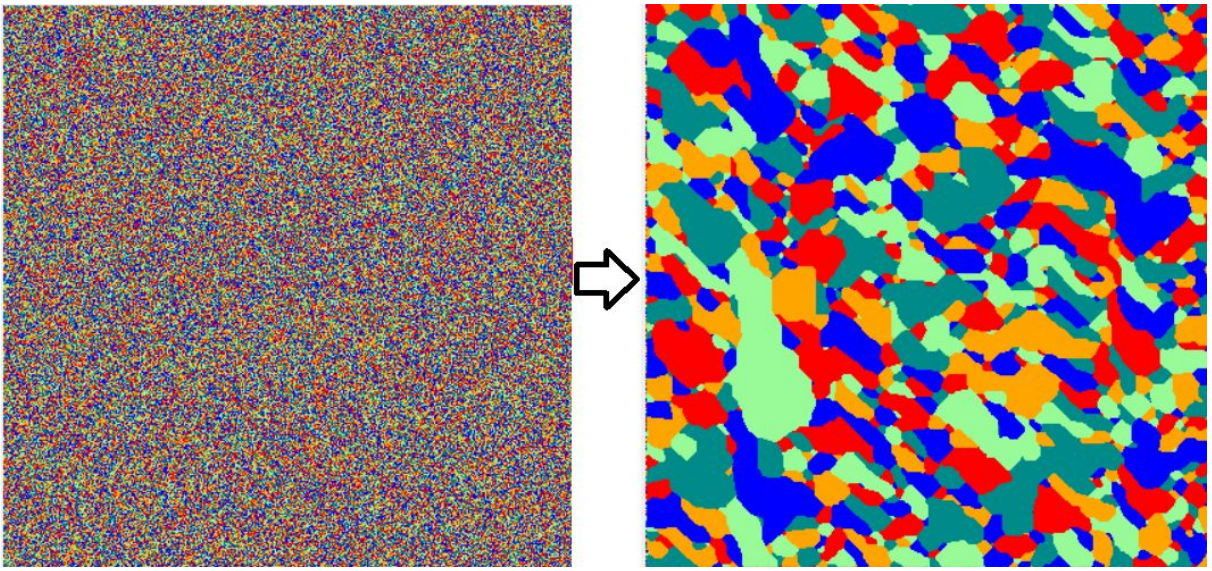
Picture 4 shows what the microstructure looks like after performing the MC simulation, selecting the dual phase and performing the next simulation of the CA.



Picture 4. CA -> MC

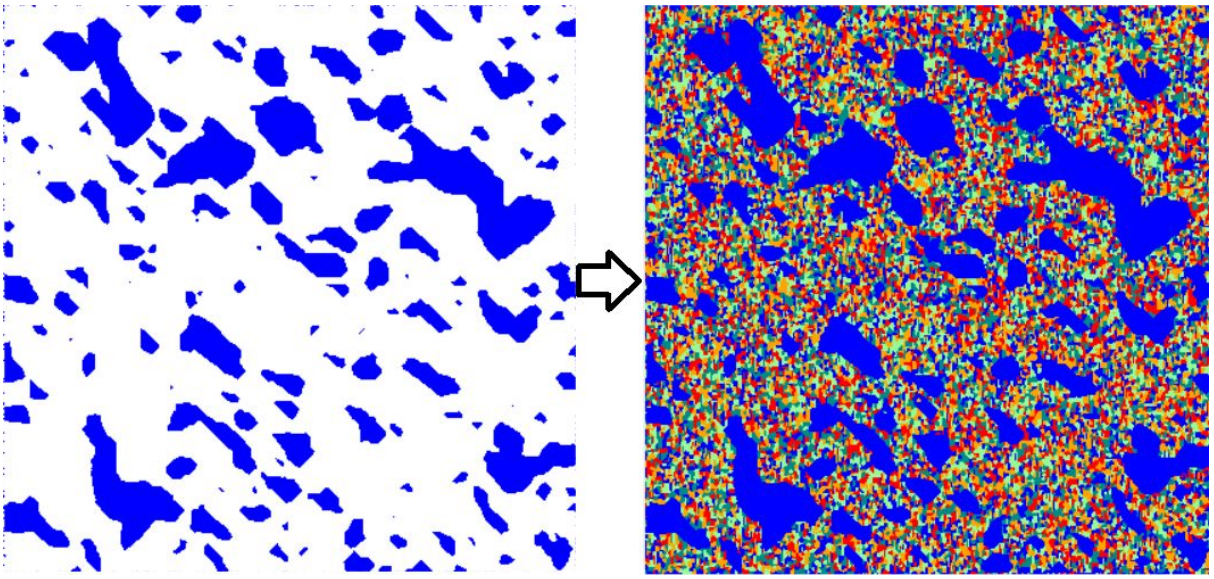
C. MC -> CA

First step is to generate whole space with randomly generated cell stated and run Monte Carlo simualtion (Picture 5)



Picture 5. MC simulation

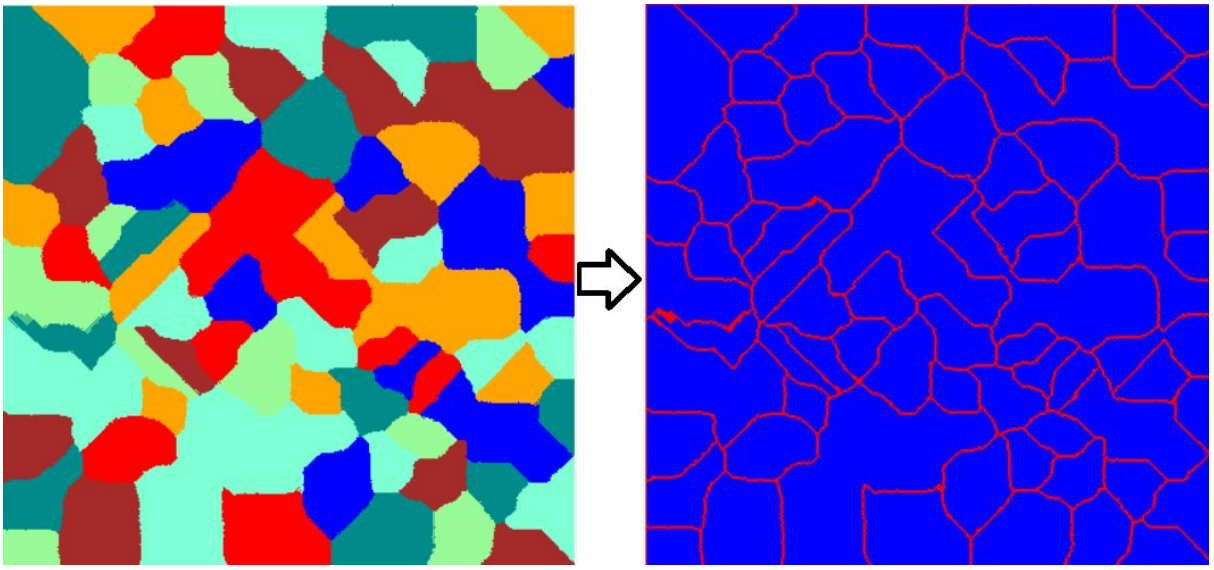
After MC simualtion user can start new CA growth (Picture 6)



Picture 6. MC -> CA simulation

D. SRXMC

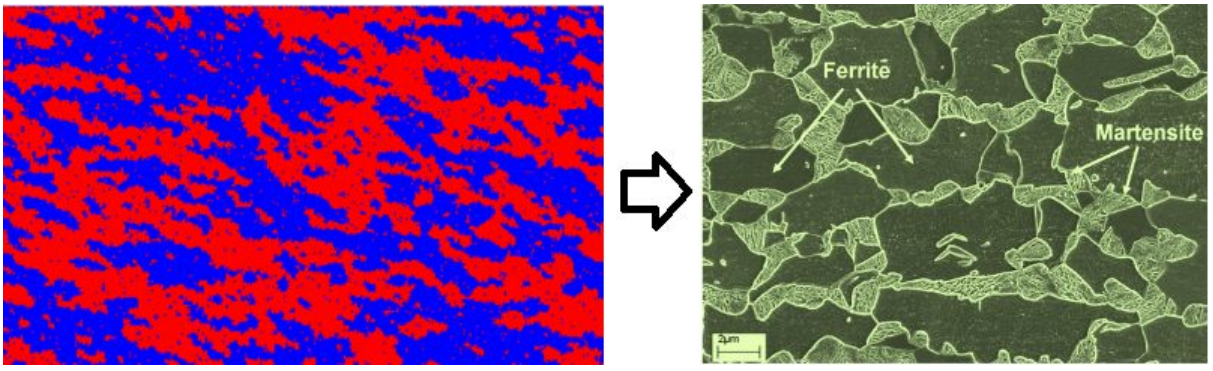
In the example below (Picture 7) in order to see heterogenous energy distribution view user can Energy button



Picture 7. Heterogeneous energy distribution.

3. Comparison

The following picture 8 presents a comparison of the microstructure created in the program and the microstructure of a Ferrite / Martensite microstucture. The growth in the created application is not as accurate as the real one. The microstructure created in the program has a more of grains in different phase and identifiers. It does look more realistic in comparison to the simple CA grain growth.



Picture 8. Comparison of a generated microstructure and real dual phase microstructure

4. Conclusions

In this report was presented software designed to implement simulation of the grain growth. The program is based on the Monte Carlo method. There is no single Monte Carlo method – the term describes a large and widely-used class of approaches characterized by common assumptions. Monte Carlo is algorithm that can implemented in many ways. It can be used in many of different areas such as computer science, mathematics, physics, biology, microstructure modelling.

The software has a lot of functionality such as MC grain growth simulation, dual phase microstructure and it can be used in four different ways, possibility of change size, sight of distribution energy, choosing distribution type.