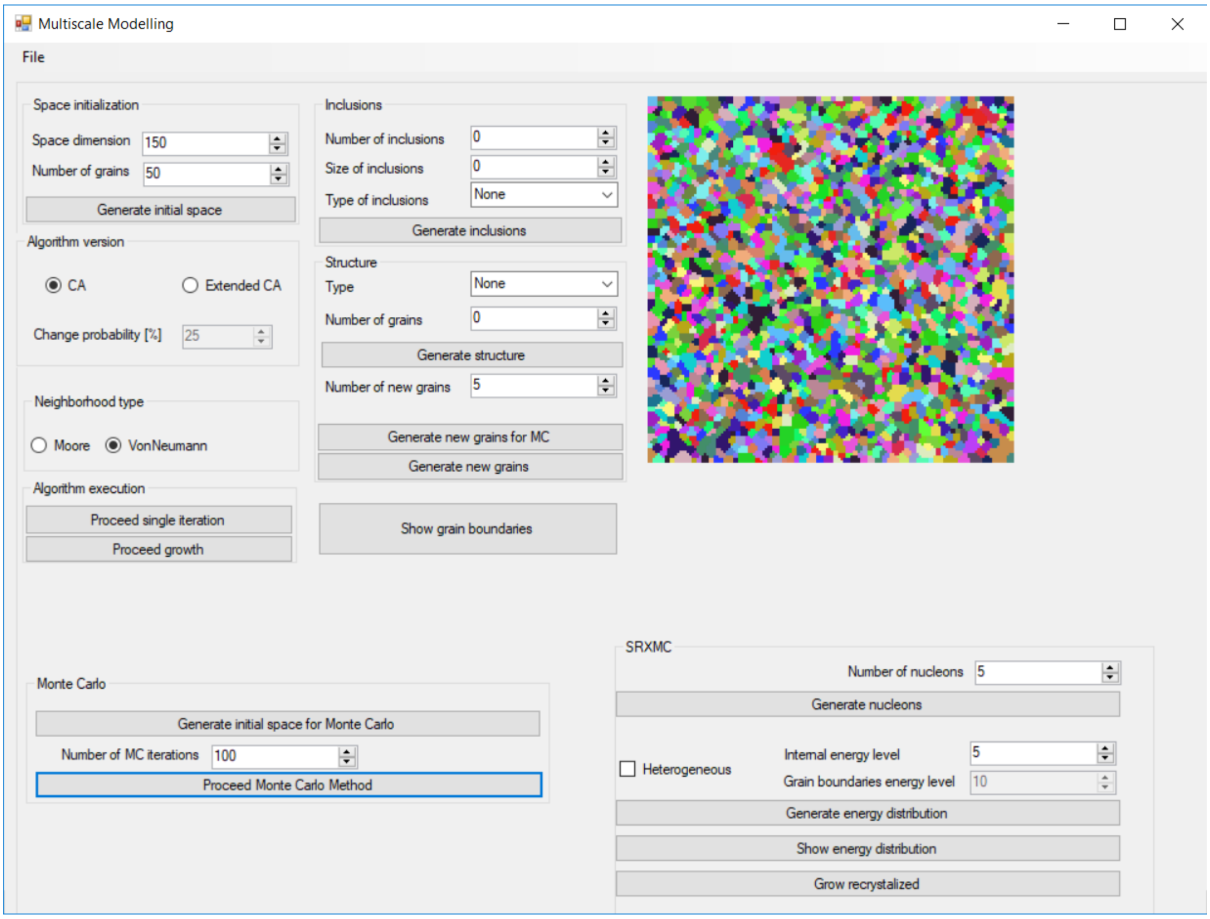
Post-Lab Multiscale Modelling Report 2 **Krzysztof Belcarz**
Raport Date: 18/12/18

1 Graphical User Interface

Program's graphical user interface is presented in figure 1



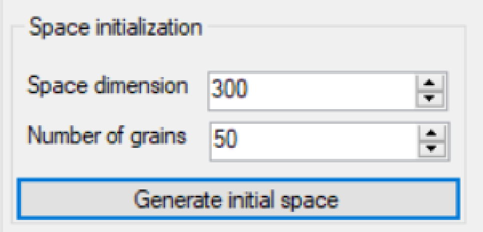
Space dimension 150
Number of grains 50
● CA ○ Extended CA
Change probability [%] 25
○ Moore ● VonNeumann
Number of inclusions 0
Size of inclusions 0
Type of inclusions None
Type None
Number of grains 0
Number of new grains 5
Number of MC iterations 100
Number of nucleons 5
□ Heterogeneous
Internal energy level 5
Grain boundaries energy level 10

Figure 1: GUI

2 Algorithm

2.1 Space generation

In order to proceed with Monte Carlo algorithm one needs to define dimension and number of types of grains, as depiceted in 3

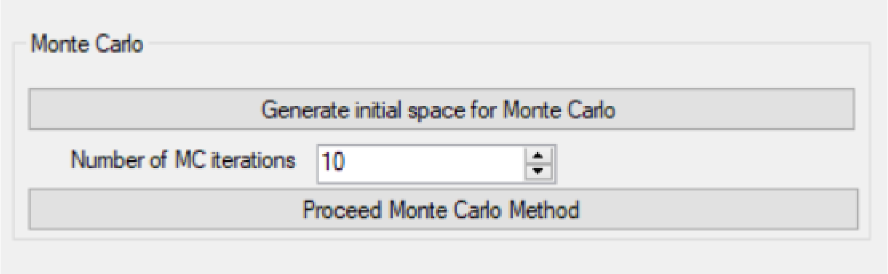


Space dimension 300

Number of grains 50

Figure 2: Space initialization group box

Next step is to generate the space using button from Monte Carlo group box **??**


Monte Carlo
Generate initial space for Monte Carlo
Proceed Monte Carlo Method

Number of MC iterations 10

Figure 3: Monte Carlo group box

In contrary to previous part of the project generated space has no ”empty” places. Each cell is occupied by a particular grain. An exemplary space can be observed in 4

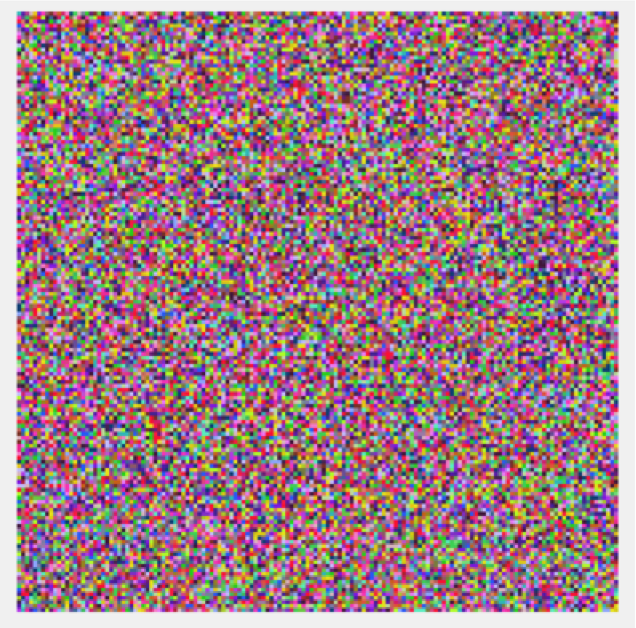


Figure 4: Exemplary Monte Carlo space

2.2 Monte Carlo execution

2.3 Exclusive Monte Carlo

After the space is generated one can proceed with Monte Carlo algorithm. Button Proceed Monte Carlo Method allows user to execute defined number of iterations on generated space. Result for presented exemplary space after ten iterations is shown in figure 5.

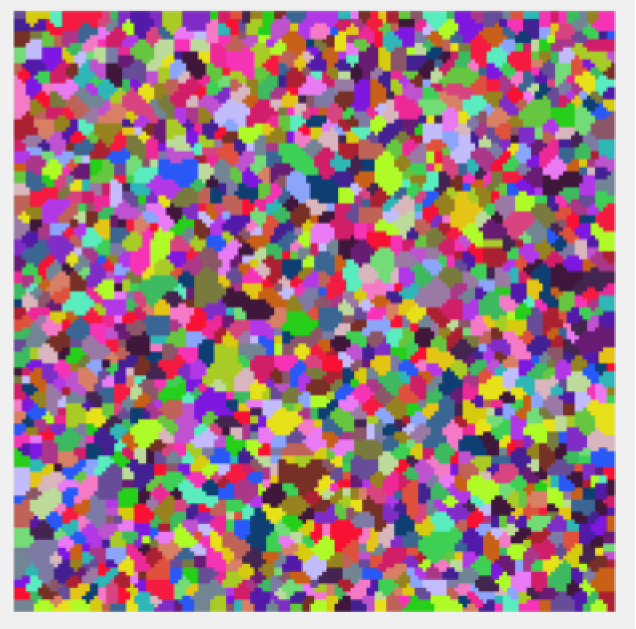


Figure 5: Result after 10 iterations

2.4 CA->DP->MC

User can choose to generate space ”the classical way”, proceed with growth using e.g. extended Cellular Automata algorithm, then generate dual phase, generate space for Monte Carlo method and proceed with Monte Carlo growth. Dual phase structure with Monte Carlo generated initial grains is presented in figure 6.

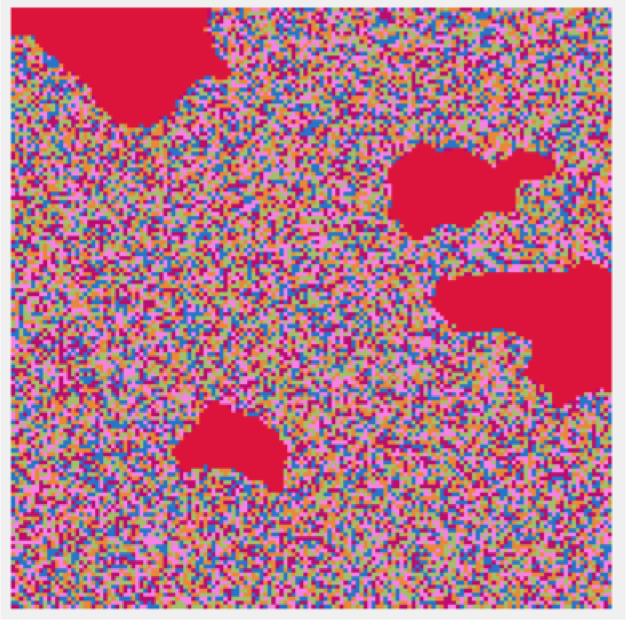


Figure 6: Dual phase

After twenty Monte Carlo iterations the space looks as shown in figure 11.

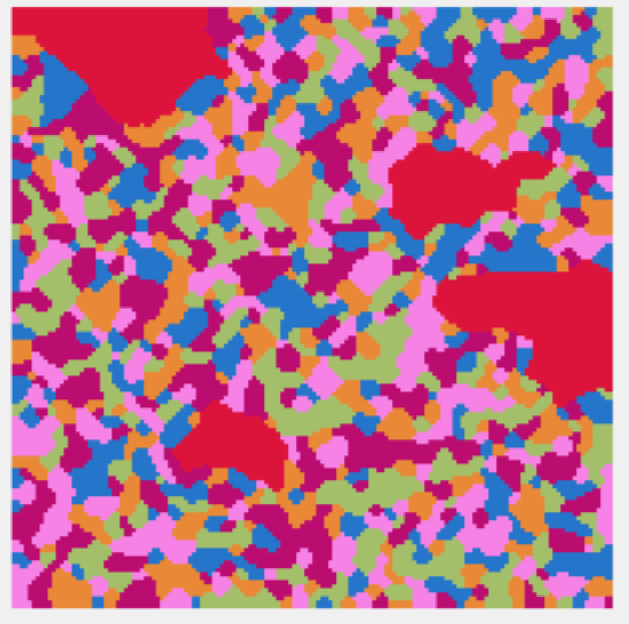


Figure 7: Monte Carlo with dual phase

2.5 Energy distribution

After growth is complete user can calculate energy distribution according to preferences. There are two possibilities either homogeneous energy distribution or heterogeneous. When homogeneous energy distribution is selected all grains get the same amount of energy, thus they are illustrated with the same colour. Whereas in heterogeneous energy distribution grain boundaries have different energy value. Described situations are depicted in figures 8 and 9.

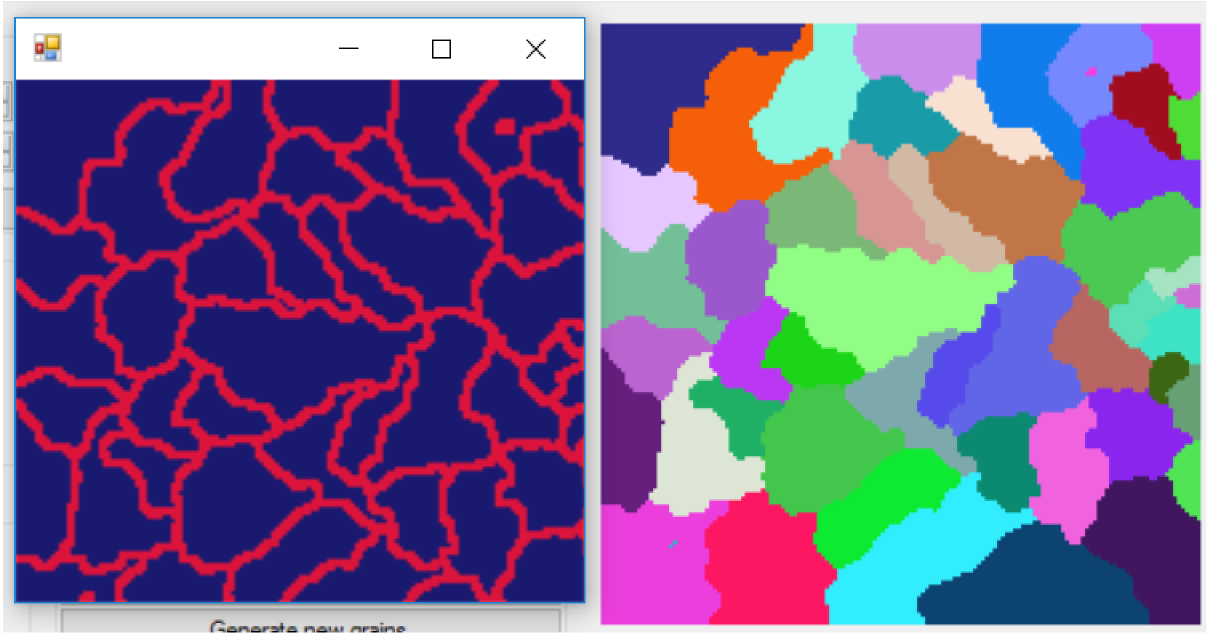


Figure 8: Heterogeneous distribution

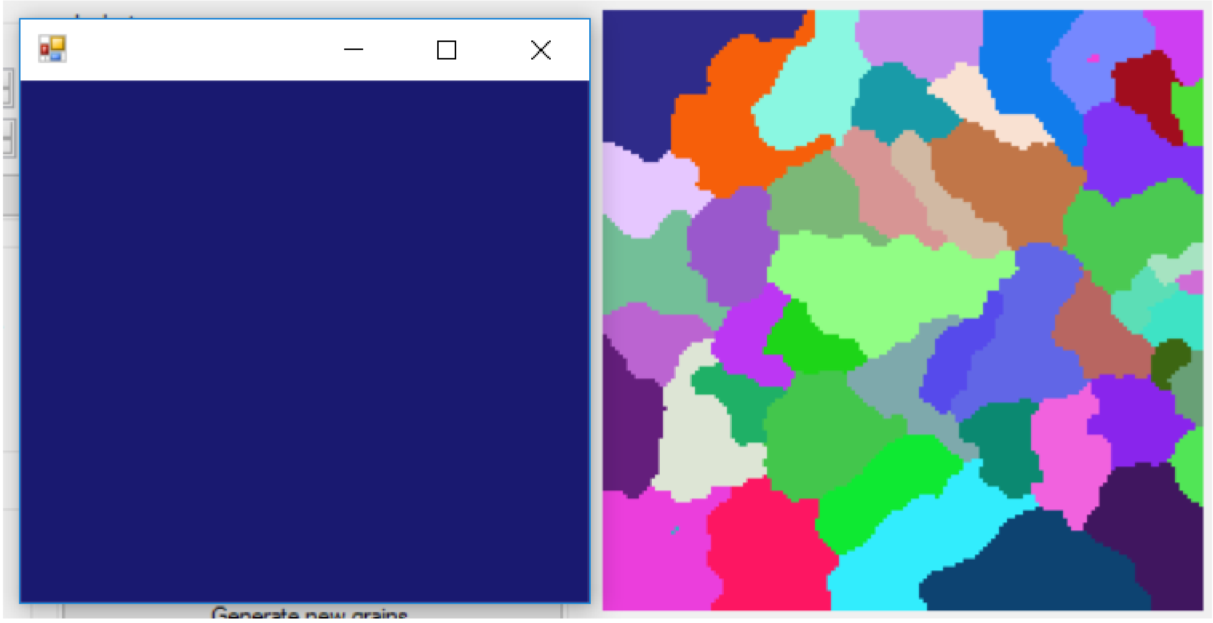
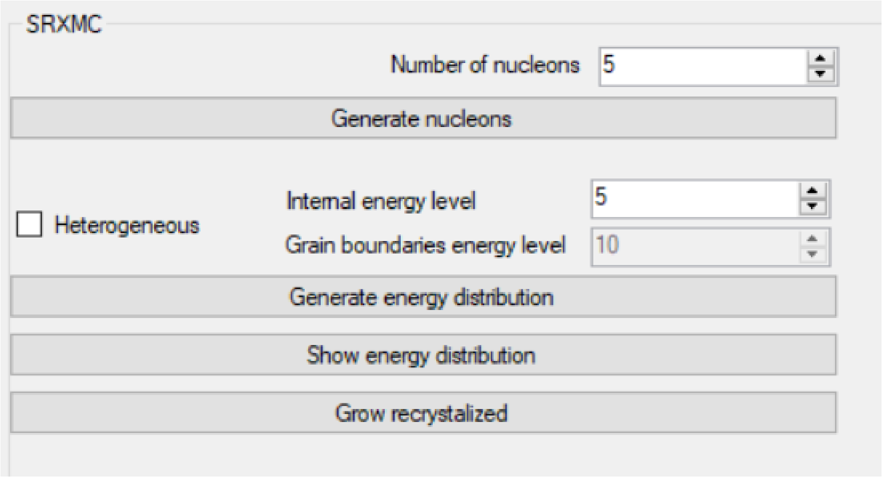


Figure 9: Homogeneous distribution

Parameters regarding energy distribution, such as type of distribution and energy levels can be configured using dedicated group box 10.


SRXMC

Number of nucleons 5

☐ Heterogeneous

Internal energy level 5

Grain boundaries energy level 10

Figure 10: SRXMC group box

3 Comparison

In order to evaluate results it is good to compare them with real structure 11 and 12.

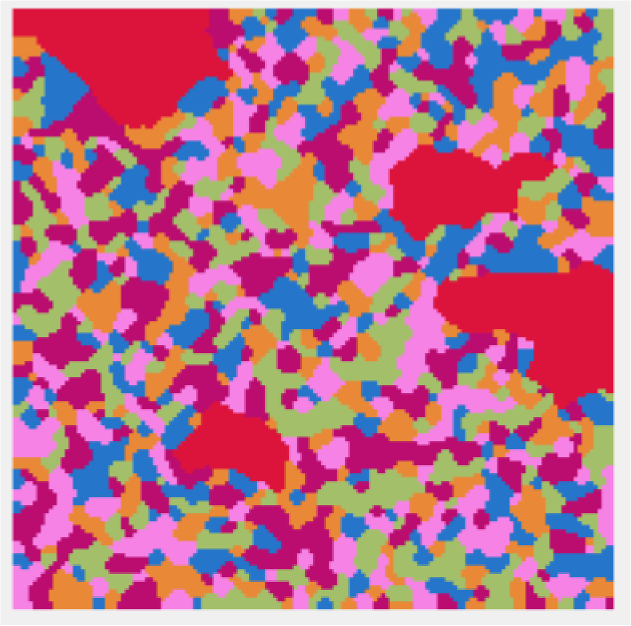


Figure 11: Monte Carlo with dual phase

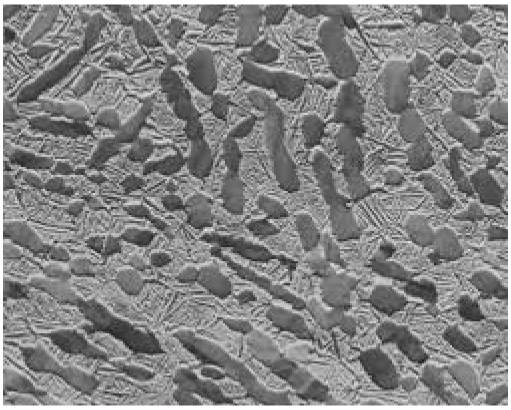


Figure 12: Real DP structure

As can be observed structures are in general consistent. Of course number and size of grains differs a lot, but all of those parameters can be adjusted provided that there was enough time for parameter tuning. Configuring parameters such as number of grains to be preserved while generating dual phase structure and number of grains generated for initial space for Monte Carlo method it is possible to achieve any desired result.

4 Conclusions

Parts of the project regarding Monte Carlo algorithm and initial energy distribution were implemented sucessfully. Part regarding recrystalization with newly added nucleons is not fully implemented, but is a good starting point for future work.

As stated in previous paragraph, provided that there is a good process of parameters tuning program can give satisfying results. In conjunction with that it proves to be useful.

Project was a good incentive to get acquainted with Monte Carlo algorithm. It turned out to be a indeed a great method for posed problem and what is more it seems to have good flexibility in terms of adjusting its operation for other uses.

For a software engineer who works mostly with computer vision based algorithm implementation and not with GUIs it's a refreshing experience to deal with all issues emerging from user interactions. It definitely allowed to widen the knowledge regarding both the mechanism of grain growth and C Sharp programming.

5 Attachments

All source files as well as pdf version of the raport are accessible through repository: https://github.com/krsonetbg/MultiscaleModelling Zdjęcie struktury stali pozyskane z: https://www.worldautosteel.org/steel-basics/steel-types/dual-phase-dp-steels/