AGH University of Science and Technology

Multiscale Modelling

Mateusz Sitko

Faculty of Metals Engineering and Industrial Computer Science
Department of Applied Computer Science and Modelling

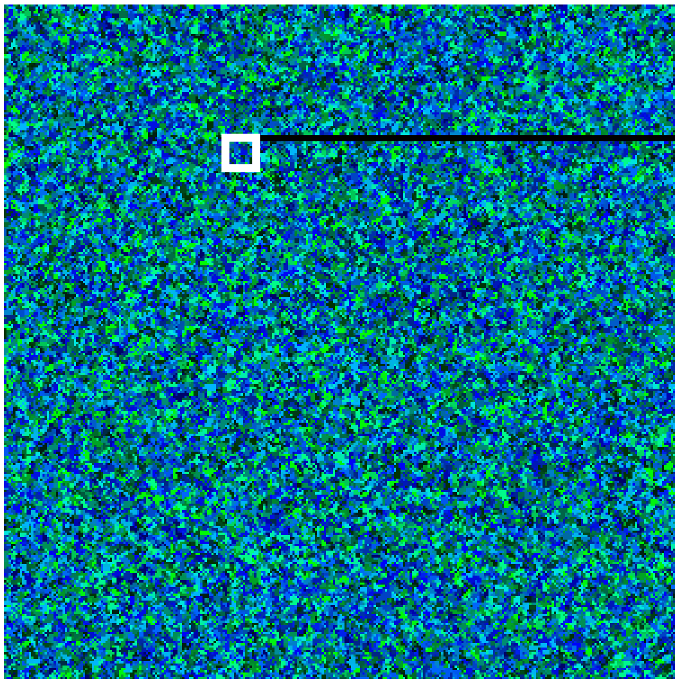
Kraków 2017

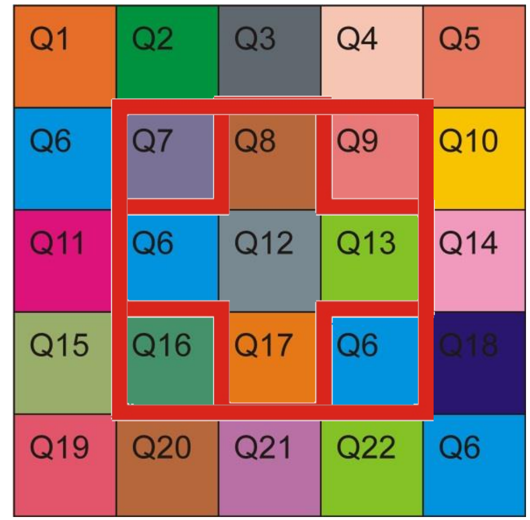
Classes calendar

	Issues
1	Organizational class - simple grain growth CA + visualization
2	Microstructures export/import to/from txt files, pictures.
3	Modification of cellular automata grain growth algorithm- inclusions (at the beginning/end of the simulation)
4	Modification of CA grain growth algorithm - influence of grain curvature
5	Modification of CA grain growth algorithm - substructures CA
6	Modification of CA grain growth algorithm - boundaries coloring
7	**Reports 1st part**
8	Monte Carlo grain growth algorithm
9	Modification of MC grain growth algorithm - substructures CA, MC
10	**MC static recrystallization algorithm - energy distribution**
11	MC static recrystallization algorithm - nucleation
12	MC static recrystallization algorithm - growth
13	**Reports 2nd part**
14	Final degree

MC method assumptions

$n = 50$

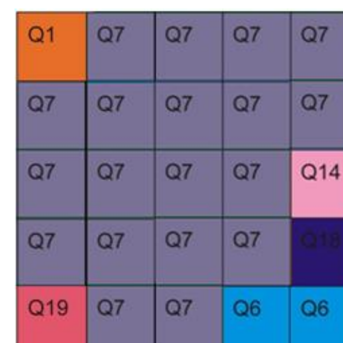




1 MCS

Cells in the same state represent particular grain

$$\Omega = \{Q_0, \ldots, Q_{n-1}\}$$



Grain Growth Algorithm steps:

Step 1: Random selection of element with specifically orientation.

Step 2: Calculate the energy of lattice site surrounding concerned element Q_i. Energy is calculated using following formula:

$$E = J_{gb} \sum_{<i,j>} \left(1 - \delta_{S_i S_j}\right)$$

Kronecker delta

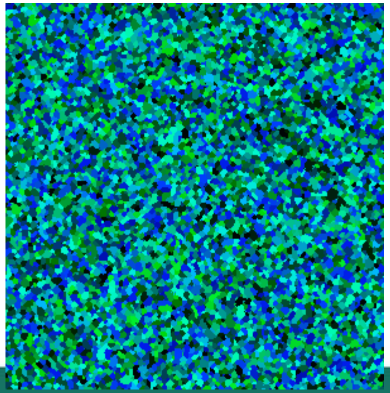
Grain boundary energy

Surrounding neighbors points

Q1	Q1	Q2
Q3	Q3	Q2
Q3	Q2	Q2

Q1	Q1	Q2
Q3	Q4	Q2
Q3	Q2	Q2

Step 3: The investigated cell changes the state to one of the available states/orientation.
The state/orientation is randomly generated from Ω available states/orientations.

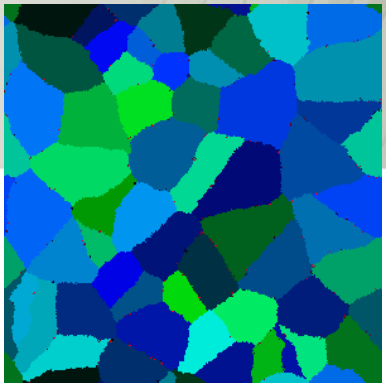


Step 4: Calculate the change in energy Q_i caused by orientation changes

Step 5: The orientation change is accepted with the probability p:

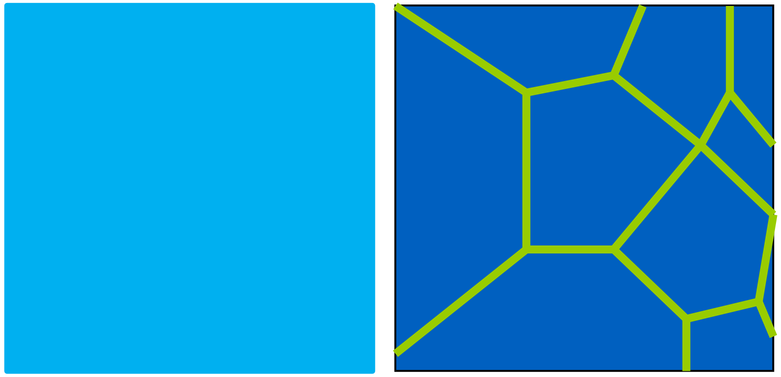
$$p(\Delta E) = \begin{cases} 1 & \Delta E \leq 0 \\ 0 & \Delta E > 0 \end{cases}$$

Monte Carlo SRX

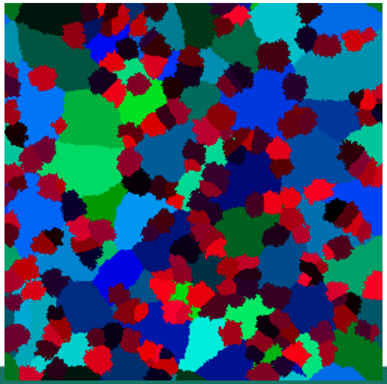


Generation of initial material morphology (CA or MC grain growth)

Distribute stored energy - *H*

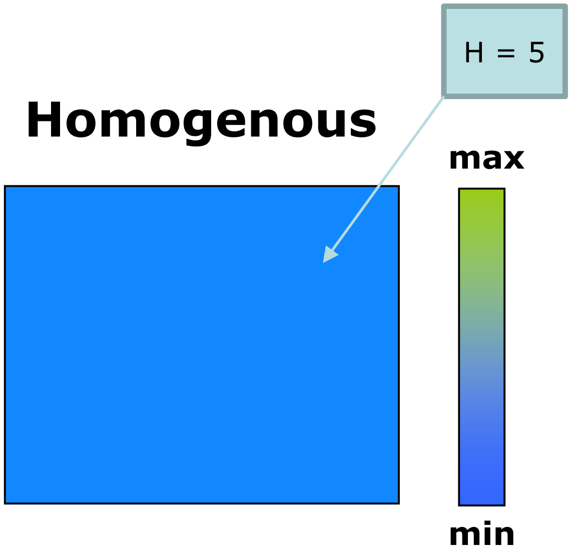


Nucleation and grain growth of recrystallized grains

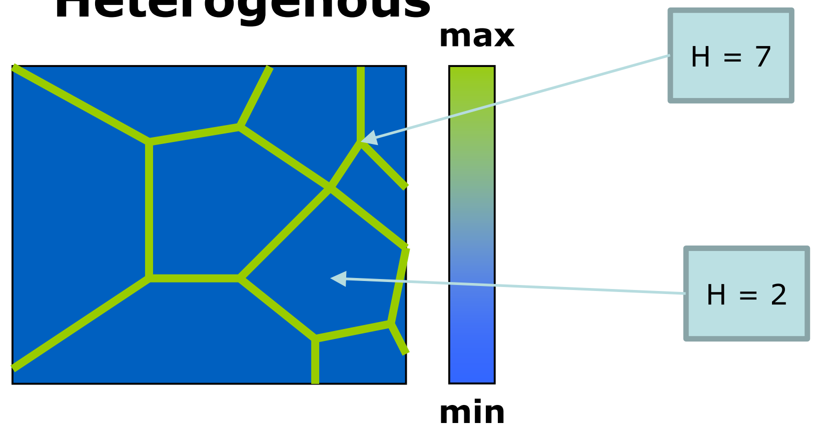


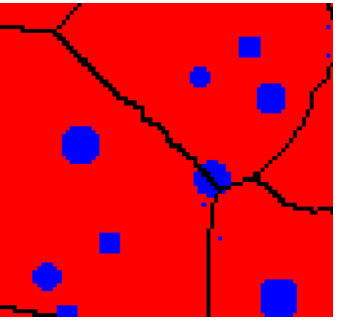
1st step of SRXMC - Energy distribution *H*

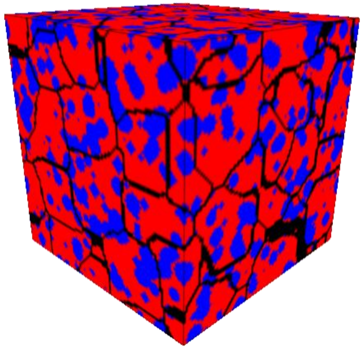
Homogenous

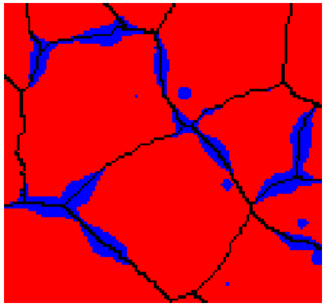


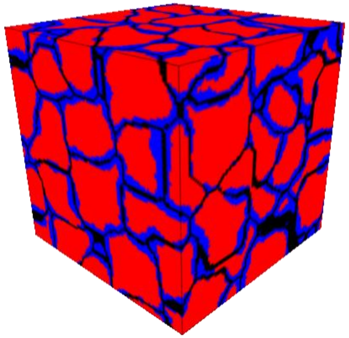
Heterogenous



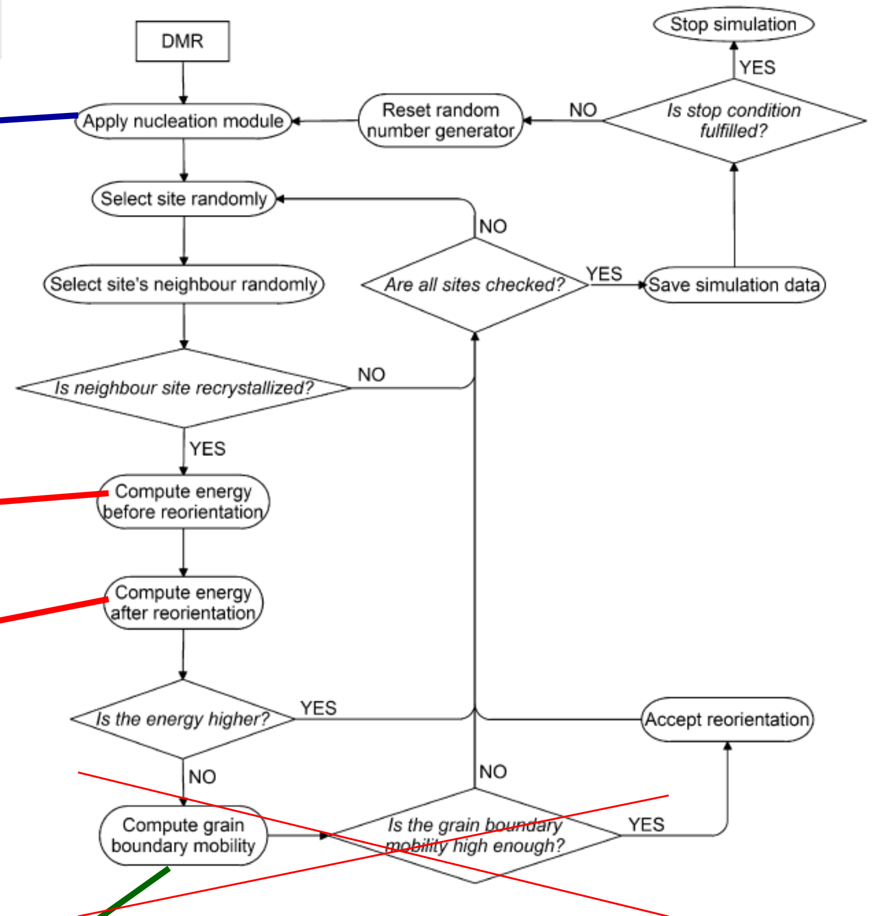








SRXMC - Algorithm steps:



Number of nucleons:

- Constant (e.g. 10, 10, 10 ,10)
- Increasing (e.g. 10, 20, 30 ,40)
- At the begining of simulation (e.g. 100)

Location:

GB or Anywhere

Driving force – Energy minimization

$$E_i^{beforeSRX} = J\sum_{j=1}^{Z}\left(1-\delta_{S_iS_j}\right)+H_i$$

$$E_i^{afterSRX} = J\sum_{j=1}^{Z}\left(1-\delta_{S_iS_j}\right)$$

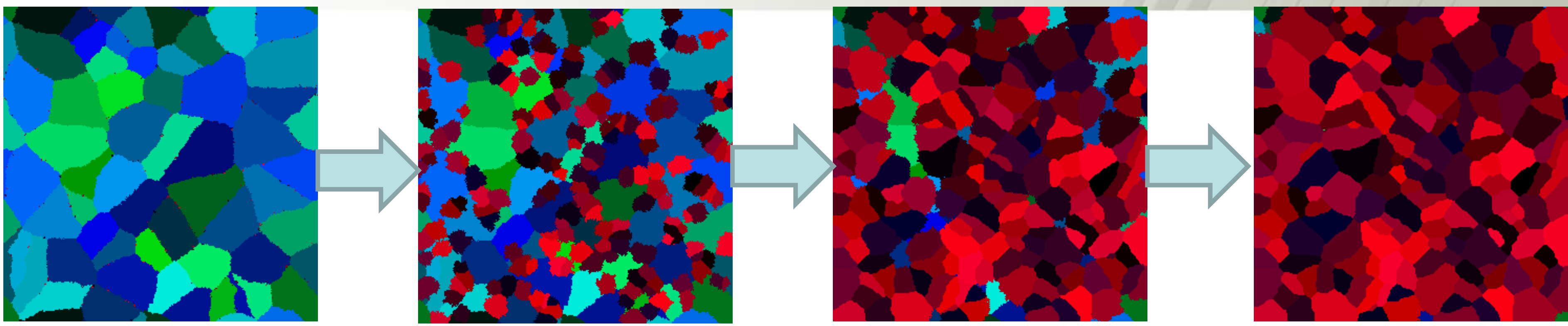
$$\Delta E_i = E_i^{afterSRX} - E_i^{beforeSRX}$$

Driving force – grain boundary mobility

$$M(\theta) = M_m\left[1-\exp\left(-B\frac{\theta}{\theta_m}\right)^n\right]$$

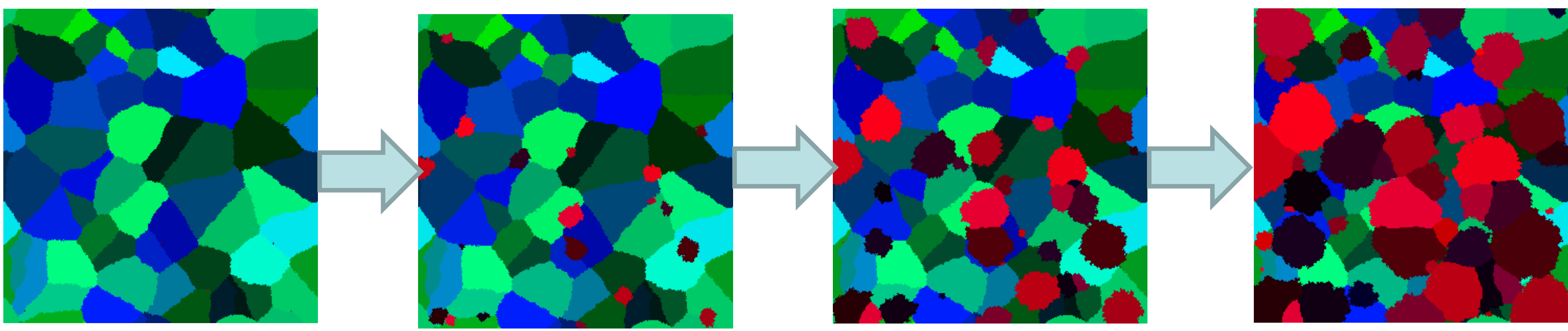
Result obtain with different nucleation modules:

Site saturated nucleation



0MCS 20MCS 40MCS 60MCS

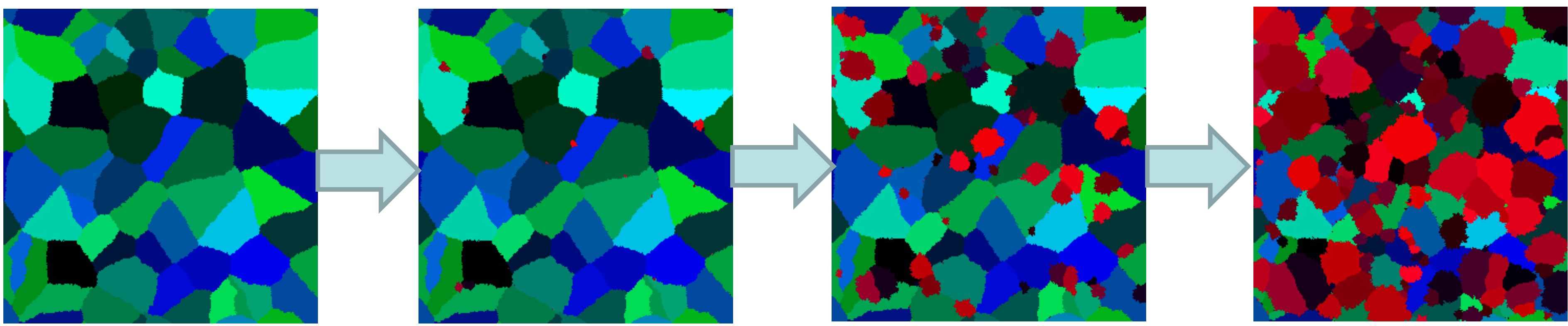
Constant



0MCS 20MCS 40MCS 60MCS

Result obtain with different nucleation modules:

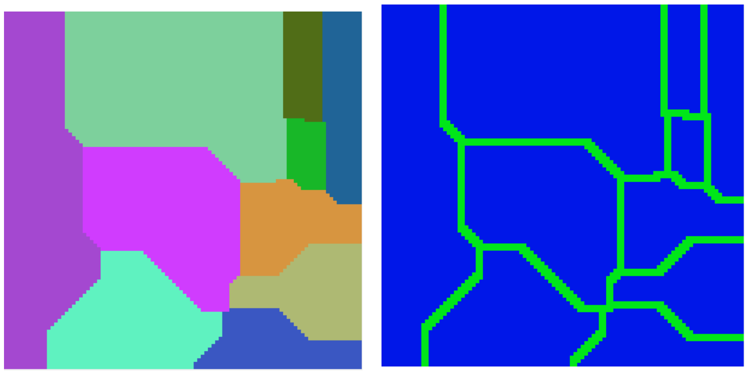
Increasing nucleation



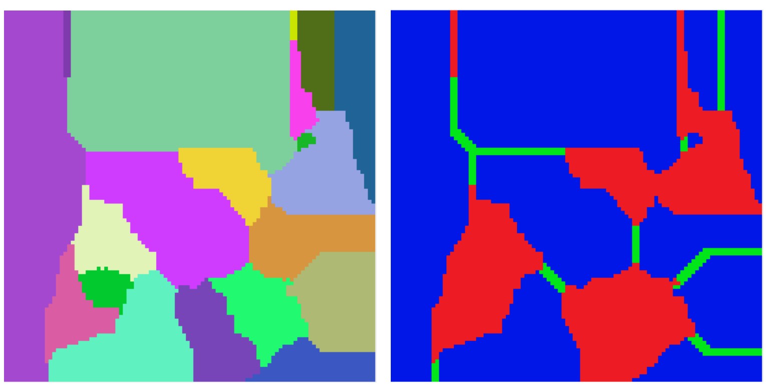
0MCS 20MCS 40MCS 60MCS

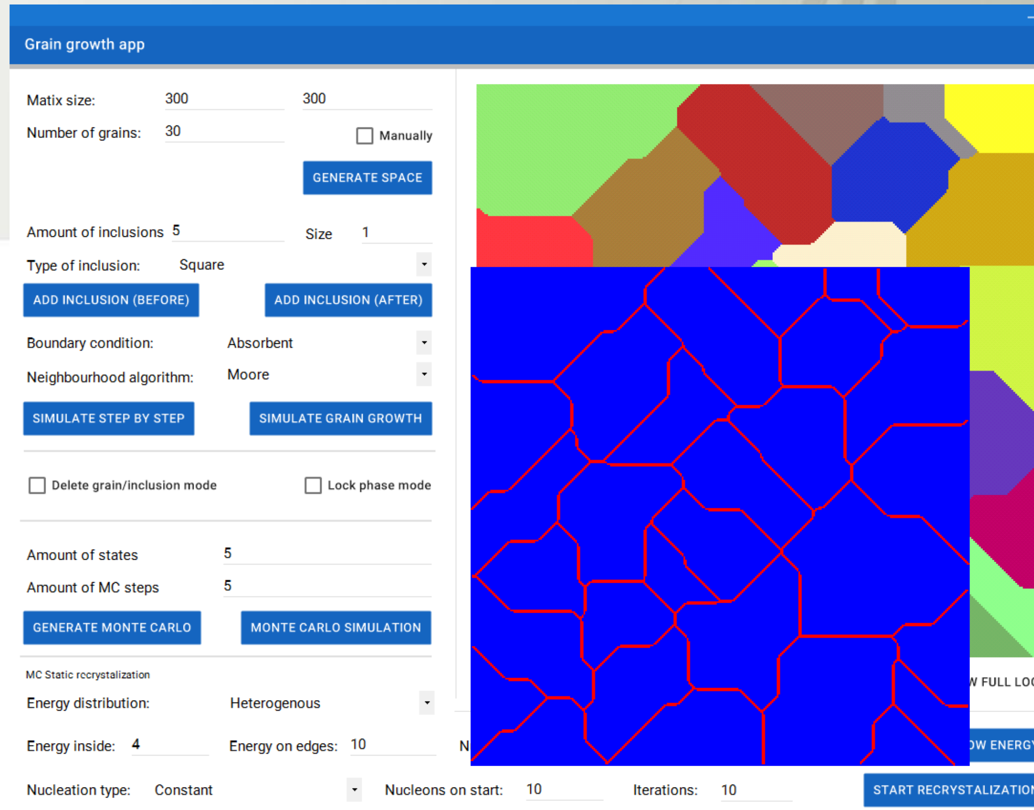
Results:

Initial micro:



15 MSC:





10MSC:

100MSC: