



**AGH UNIVERSITY OF SCIENCE
AND TECHNOLOGY**

Multiscale Modelling

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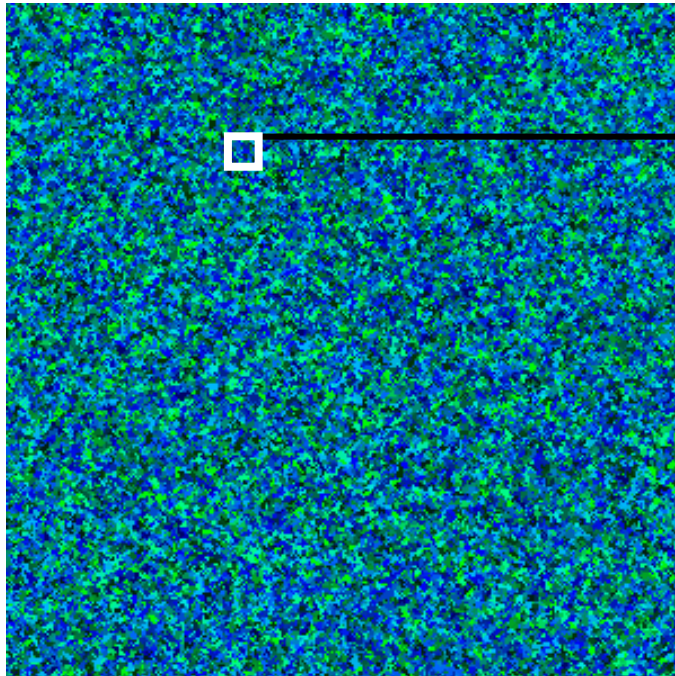
**Faculty of Metals Engineering and Industrial Computer Science
Department of Applied Computer Science and Modelling**

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| 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

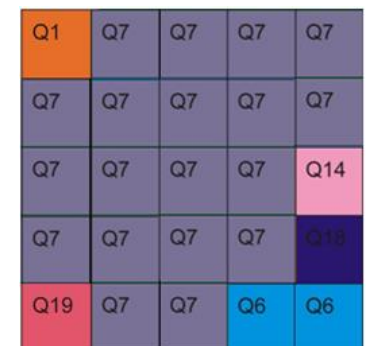
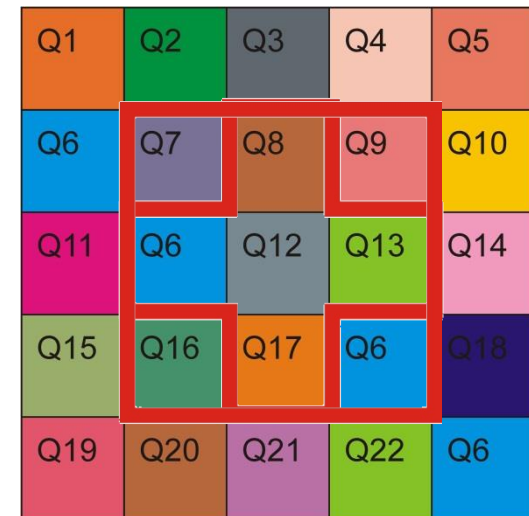
$n = 50$



1 MCS

Cells in the same state represent particular grain

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



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:

$$E = J_{gb} \sum_{\langle i,j \rangle} (1 - \delta_{S_i S_j})$$

Grain boundary energy

Kronecker delta

Surrounding neighbors points

| | | |
|----|----|----|
| Q1 | Q1 | Q2 |
| Q3 | Q3 | Q2 |
| Q3 | Q2 | Q2 |

| | | |
|----|----|----|
| Q1 | Q1 | Q2 |
| Q3 | Q4 | Q2 |
| Q3 | Q2 | Q2 |

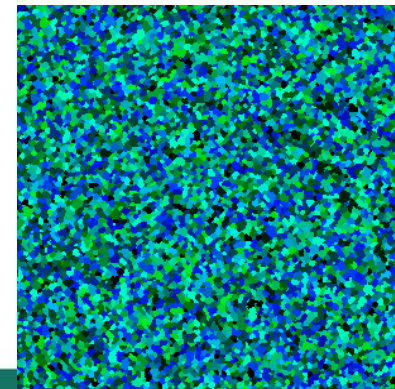
Step 3: The investigated cell changes the state to one of the available states/orientation.

The state/orientation is randomly generated from Ω available states/orientations.

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

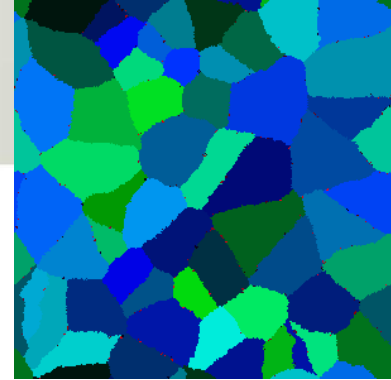
Step 5: The orientation change is accepted with the probability p :

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

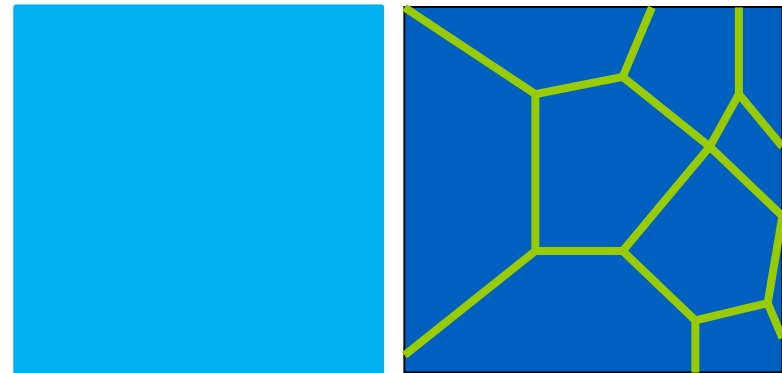


Monte Carlo SRX

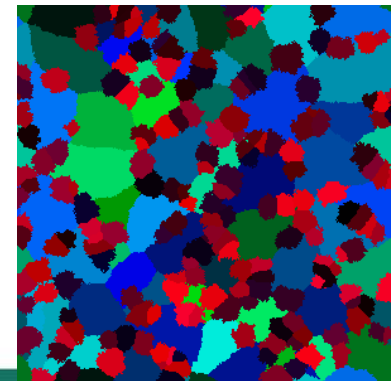
Generation of initial material morphology (CA or MC grain growth)



Distribute stored energy - H

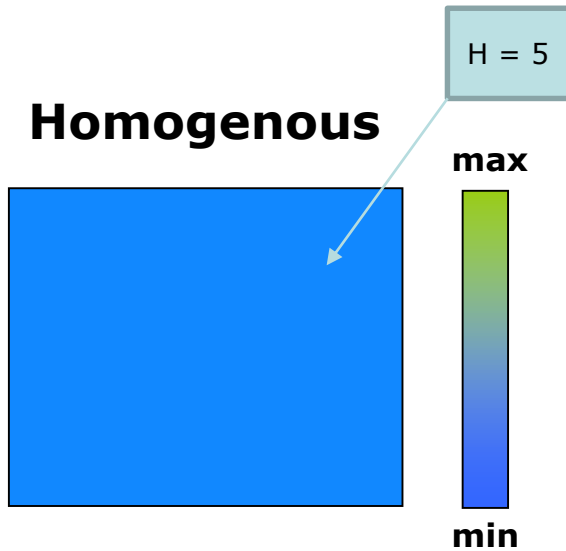


Nucleation and grain growth of recrystallized grains

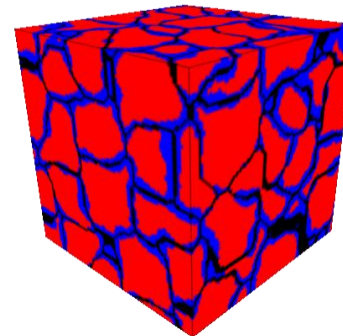
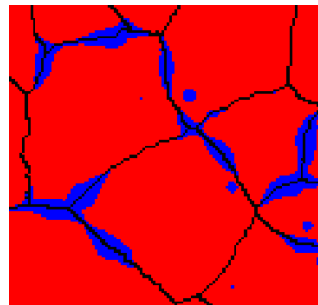
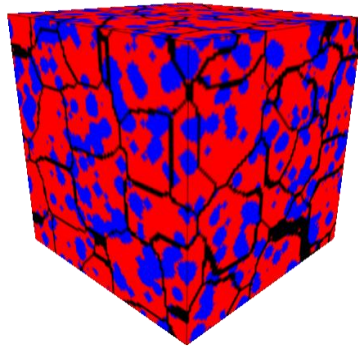
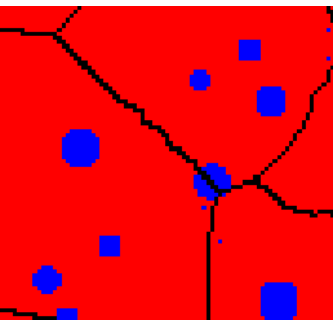
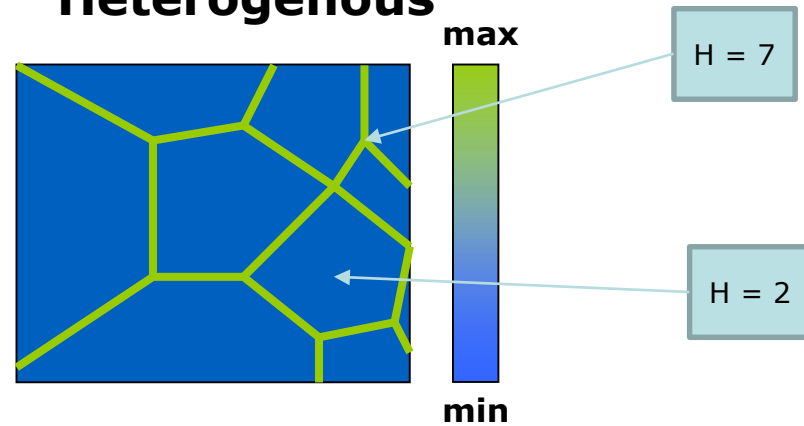


1st step of SRXMC - Energy distribution H

Homogenous



Heterogenous



SRXMC - Algorithm steps:

Number of nucleons:

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

Location:

GB or Anywhere

Driving force – Energy minimization

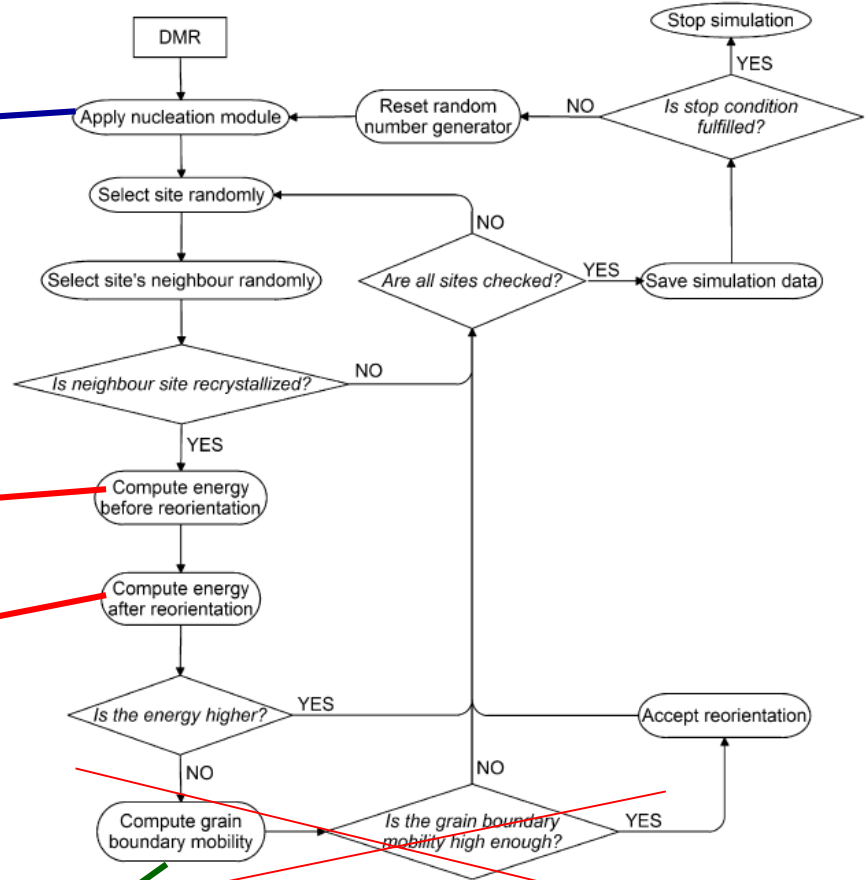
$$E_i^{beforeSRX} = J \sum_{j=1}^Z (1 - \delta_{S_i S_j}) + H_i$$

$$E_i^{afterSRX} = J \sum_{j=1}^Z (1 - \delta_{S_i S_j})$$

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

Driving force – grain boundary mobility

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

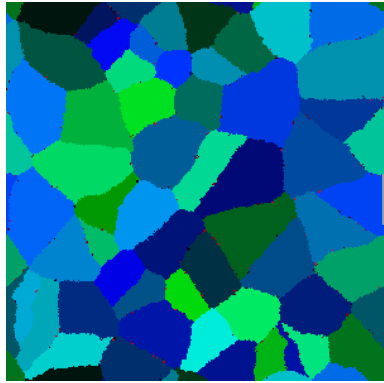




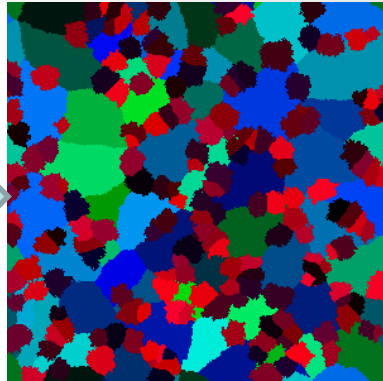
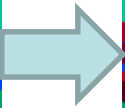
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Result obtain with different nucleation modules:

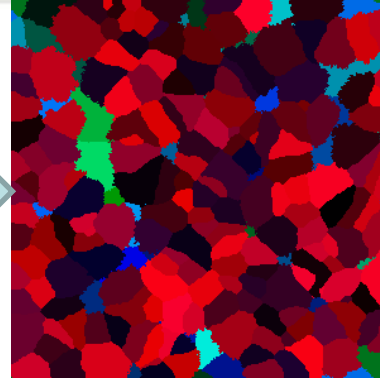
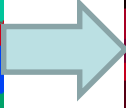
Site saturated nucleation



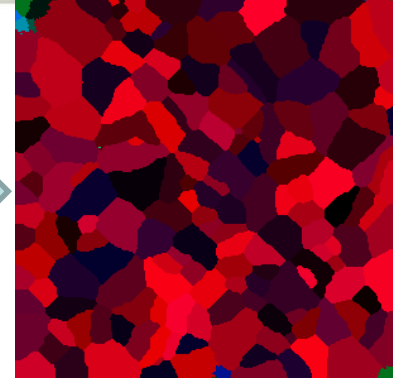
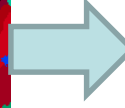
0MCS



20MCS

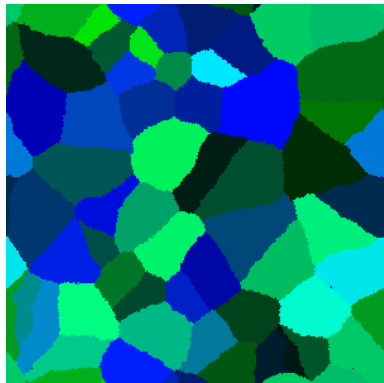


40MCS

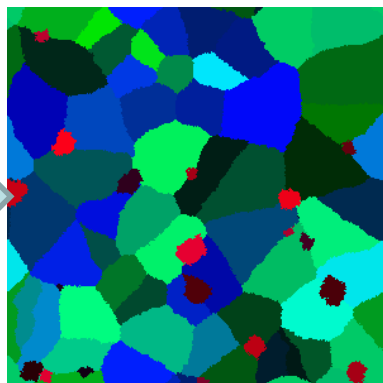
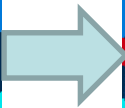


60MCS

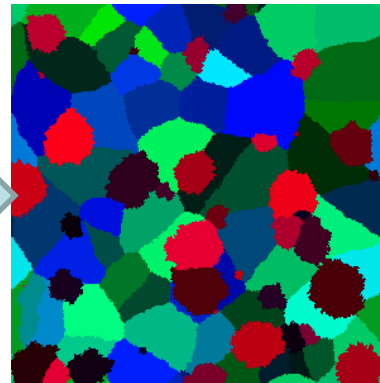
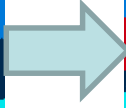
Constant



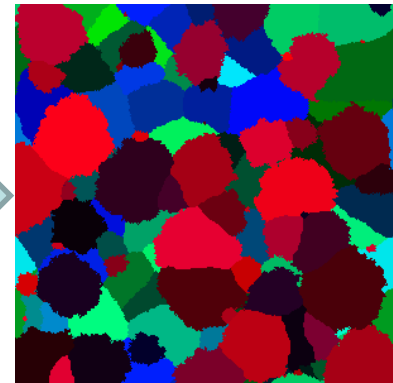
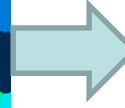
0MCS



20MCS



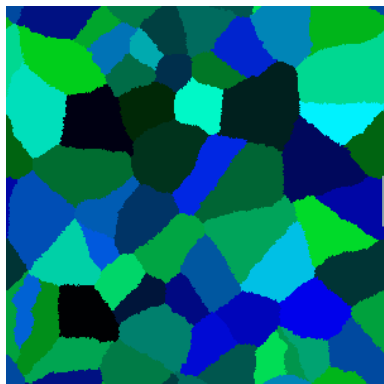
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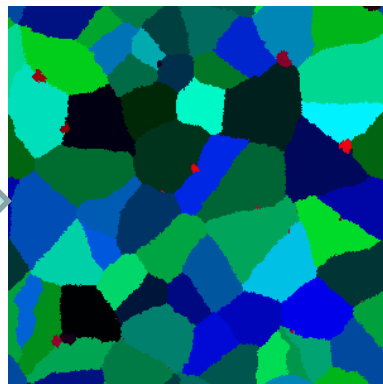
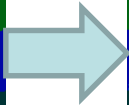
60MCS

Result obtain with different nucleation modules:

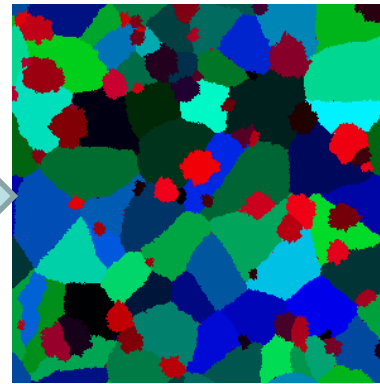
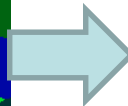
Increasing nucleation



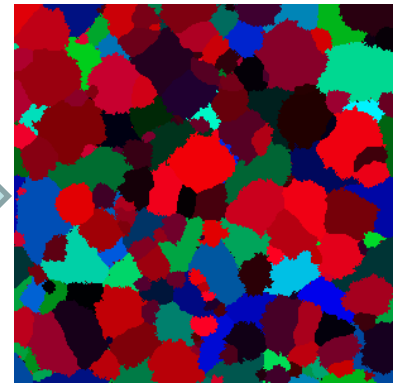
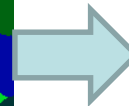
0MCS



20MCS



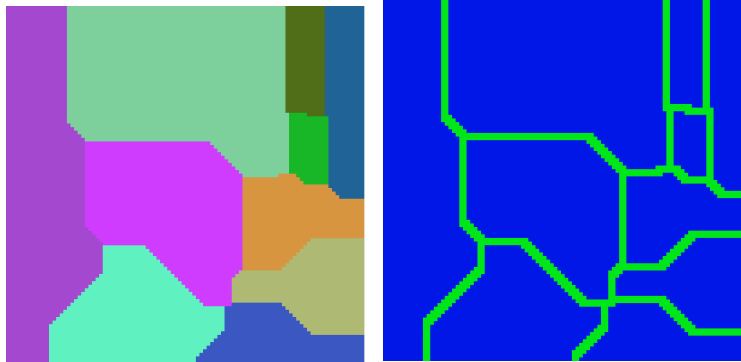
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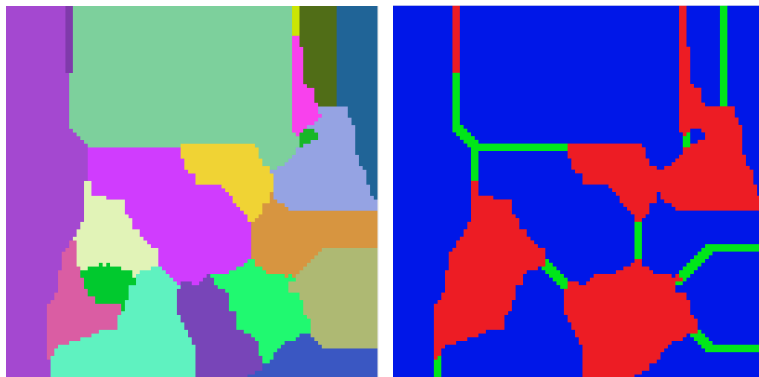
60MCS

Results:

Initial micro:



15 MSC:



Grain growth app

Matrix size: 300 300
 Number of grains: 30 ☐ Manually
 GENERATE SPACE

Amount of inclusions 5 Size 1
 Type of inclusion: Square
 ADD INCLUSION (BEFORE) ADD INCLUSION (AFTER)

Boundary condition: Absorbent
 Neighbourhood algorithm: Moore
 SIMULATE STEP BY STEP SIMULATE GRAIN GROWTH

☐ Delete grain/inclusion mode ☐ Lock phase mode

Amount of states 5
 Amount of MC steps 5
 GENERATE MONTE CARLO MONTE CARLO SIMULATION

MC Static recrystallization
 Energy distribution: Heterogenous
 Energy inside: 4 Energy on edges: 10
 Nucleation type: Constant Nucleons on start: 10 Iterations: 10
 START RECRYSTALLIZATION

SHOW FULL LOG
 SHOW ENERGY

10MSC:



100MSC:

