AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Multiscale 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

N = 50

State
number
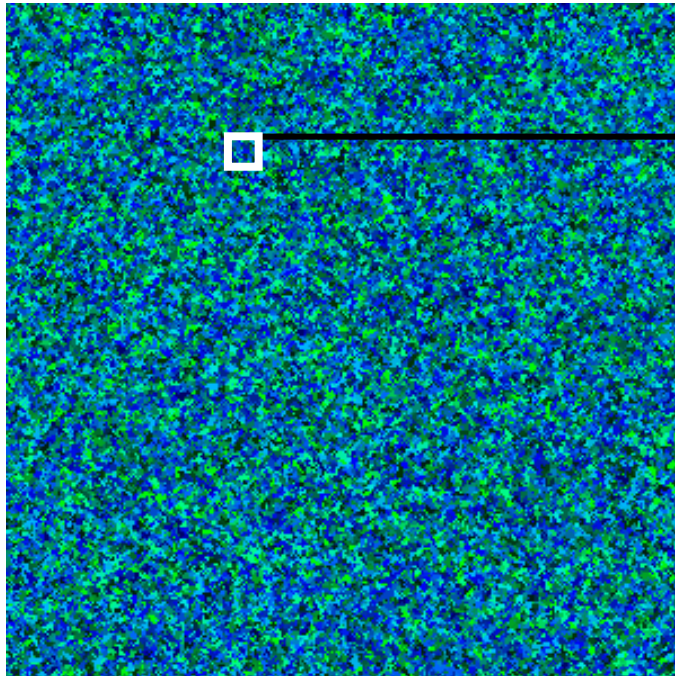
1 MCS

Cells in the same state represent particular grain

$$\Omega = \{Q_0, ..., Q_{n-1}\}$$
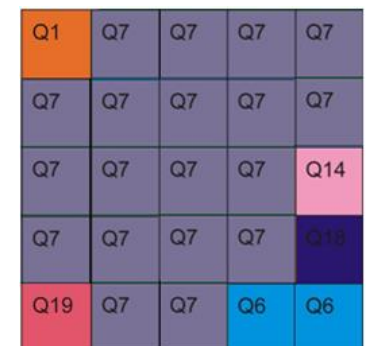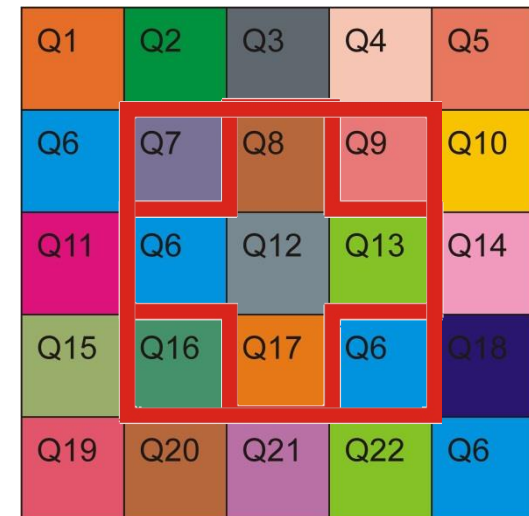
Grain Growth Algorithm steps:

Step 1: Random selection of element with specifically orientation.

Q1	Q1	Q2
Q3	Q3	Q2
Q3	Q2	Q2

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 $\sum_{<i,j>}\left(1 - \delta_{S_i S_j}\right) = 6$

Grain boundary Energy <0.1 – 1.0>

Surrounding neighbors points <Moore>

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.

$$\sum_{<i,j>}\left(1 - \delta_{S_i S_j}\right) = 8$$

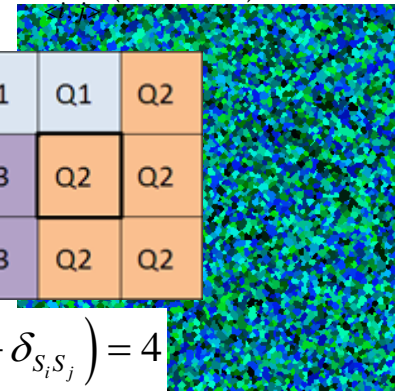**Step 4:** Calculate the change in energy Q_i caused by orientation changes

$$\Delta E = E_{after} - E_{before}$$

Q1	Q1	Q2
Q3	Q2	Q2
Q3	Q2	Q2

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

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

$$\sum_{<i,j>}\left(1 - \delta_{S_i S_j}\right) = 4$$
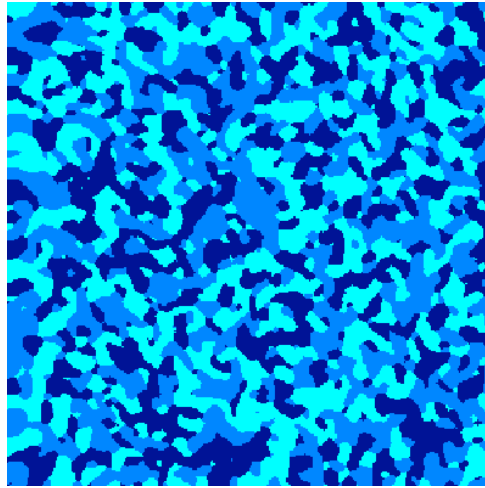
MC Grain Growth:
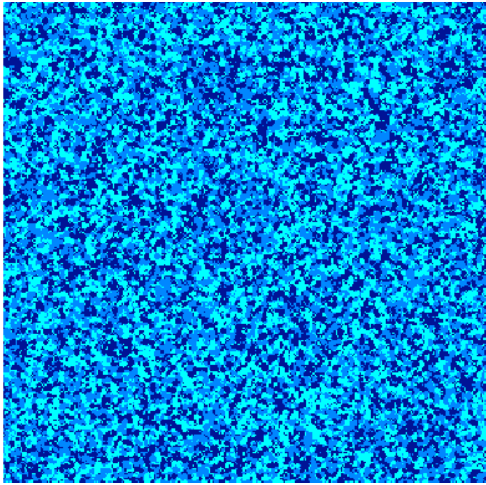
0 MCS

10 MCS
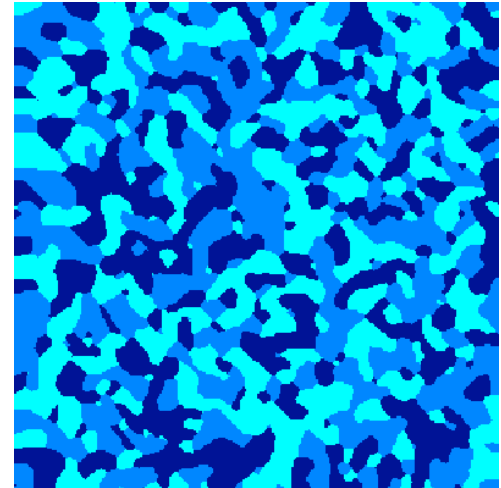
20 MCS

N = 3
Moore
MCS = 20

2nd project:

Advanced DP

Monte Carlo SRX

c2: Step 1: Simple grain growth MC/CA
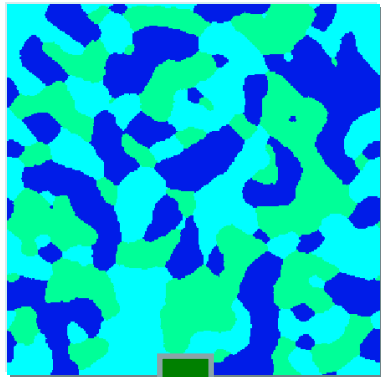
Mirco + Energy distribution

Step 3: Simple grain growth MC/CA
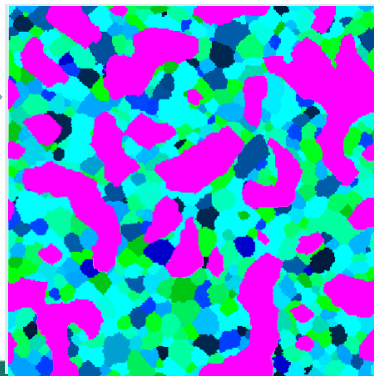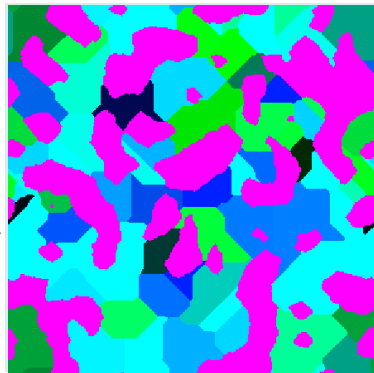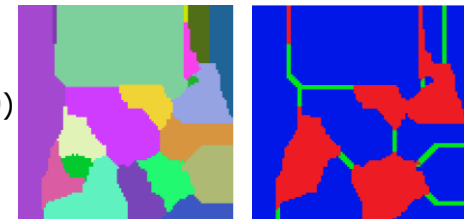
c3:
Distribution type:
Homogenous
Heterogenous

Visualisation
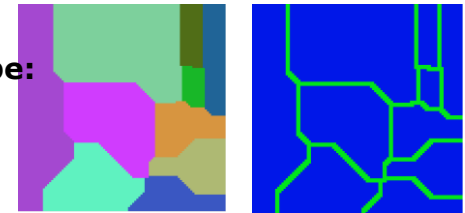
Nucleation and grain growth of recrystallized grains

c4:
Number of nucleons:
Constant (e.g. 10, 10, 10 ,10)
Increasing (e.g. 10, 20, 30 ,40)
At the begining of simulation
Location:
GB or Anywhere

c5: