AGH University of Science and Technology

Multiscale Modelling

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Office hours:
Monday 09:30 – 10:30

- 1 application (c++, java, c#..) (wa = 0.8):
  - 1st – Grain growth algorithm modifications (Cellular automata)
  - 2nd – Monte Carlo grain growth + MC static recrystallization algorithm
- 2 reports (wr = 0.2):
  - 1st application part
  - 2nd application part

  - Final degree will be positive if each part gets **min 3.0** and average is **above 3.0**

- 2 unexcused absences (**remainder – medical leave**)

- 1 short test?

??????

- Exam „0” – final degree min 4.0 (in 1st term)

??????

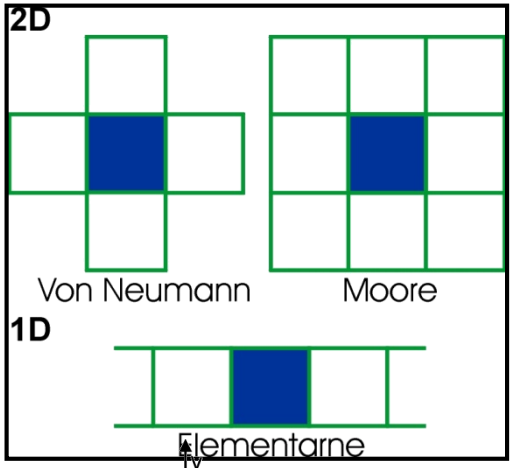
Classes calendar

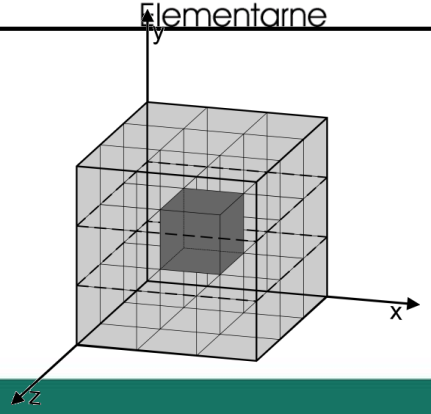
	groups: 1,2	groups: 3,4	**Issues**
1	3-10	**4-10**	Organizational class - simple grain growth CA + visualization
2	10-10	11-10	Microstructures export/import to/from txt files, pictures.
3	17-10	18-10	Modification of cellular automata grain growth algorithm- inclusions (at the beginning/end of the simulation)
4	24-10	25-10	Modification of CA grain growth algorithm - influence of grain curvature
5	31-10	08-11	Modification of CA grain growth algorithm - substructures CA
6	07-11	15-11	Modification of CA grain growth algorithm - boundaries coloring
7	14-11	22-11	**Reports 1st part**
8	21-11	29-11	Monte Carlo grain growth algorithm
9	28-11	06-12	Modification of MC grain growth algorithm - substructures CA, MC
10	05-12	13-12	MC static recrystallization algorithm - energy distribution
11	12-12	20-12	MC static recrystallization algorithm - nucleation
12	19-12	03-01	MC static recrystallization algorithm - growth
13	09-01	10-01	**Reports 2nd part**
14	16-01	17-01	Final degree

CA method

The main idea of the cellular automata technique is to divide a specific part of the material into one-, two-, or three-dimensional lattices of finite cells, where cells have clearly defined interaction rules between each other. Each cell in this space is called a cellular automaton, while the lattice of the cells is known as cellular automata space.

- CA space - finite set of cells, where each cell is described by a set of internal variables describing the state of a cell.
- Neighborhood – describes the closest neighbors of a particular cell. It can be in 1D, 2D and 3D space.
- Transition rules - f, the state of each cell in the lattice is determined by the previous states of its neighbors and the cell itself by the f function



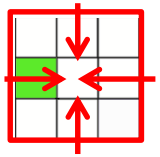


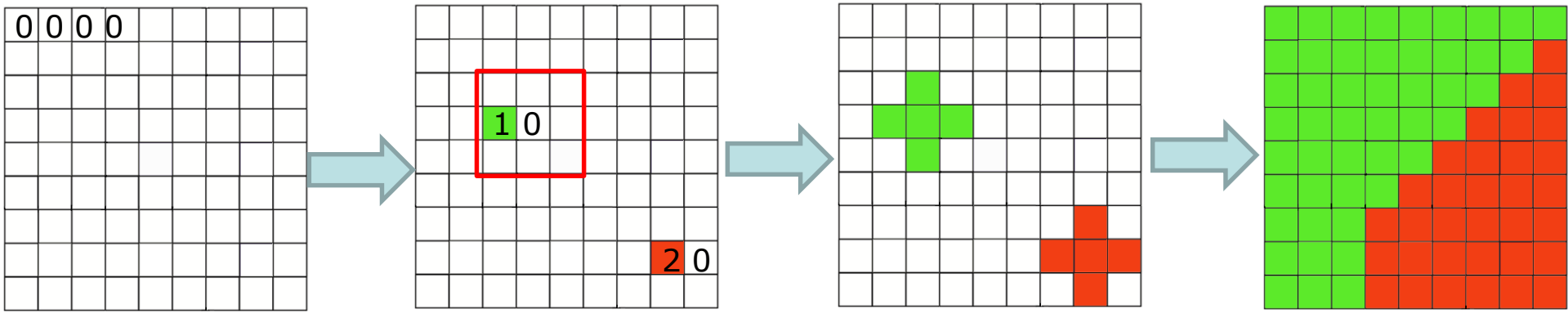
$$\gamma_i^{t+1} = f\left(\gamma_j^t\right) \quad \text{where} \quad j \in N(i)$$

N(i) – neighbours of the *i*th cell, γ_i – state of the *i*th cell

Simple Grain Growth CA algorithm

2 grains
Von Neumann neighborhood





Initial space

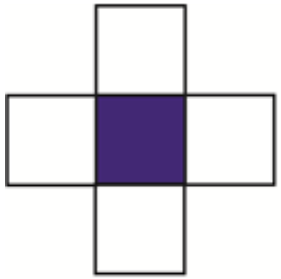
1st step

2nd step

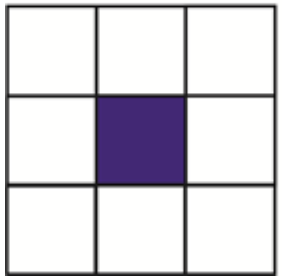
last step

Neighbourhoods types

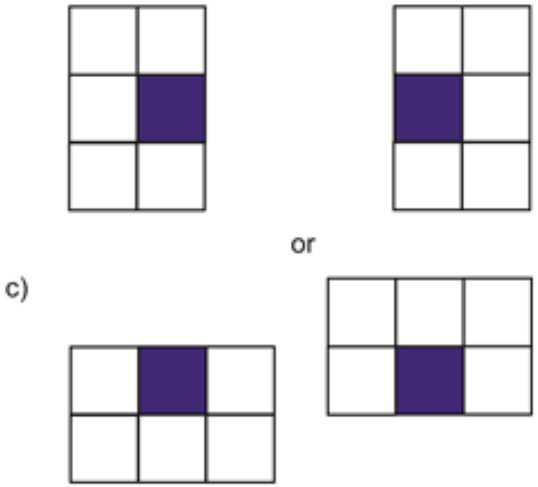
- **Von Neumann**



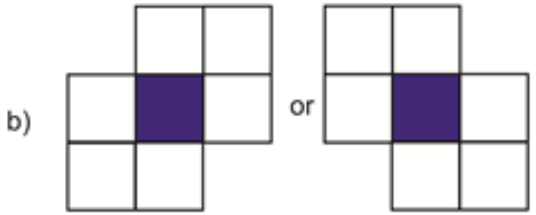
- **Moore**



- **Pentagonal random**



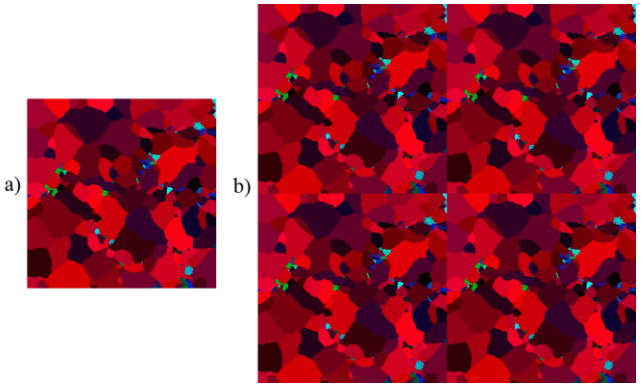
- **Hexagonal random**



Boundary conditions

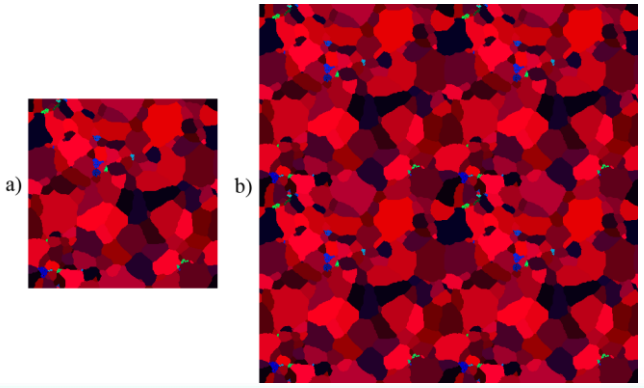
- **absorbing boundary conditions** – the state of cells located on the edges of the CA space are properly fixed with a specific state to absorb moving quantities.

0	0	0	0	0
0	1	4	7	0
0	2	5	8	0
0	3	6	9	0
0	0	0	0	0



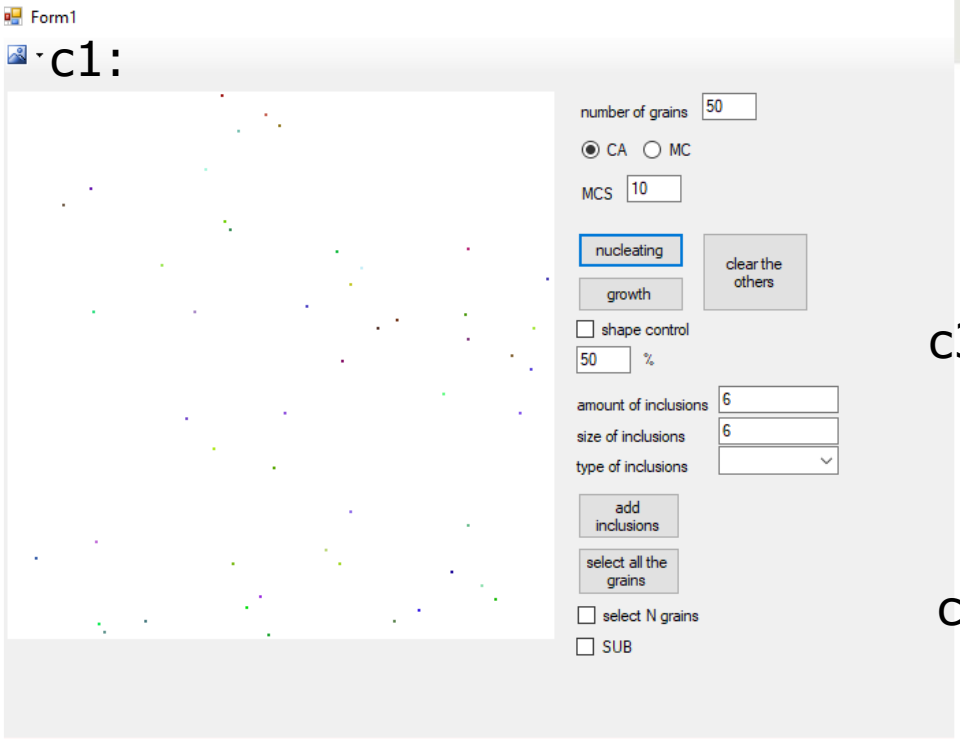
- **periodic boundary conditions** – the CA neighborhood is properly defined and take into account cells located on subsequent edges of the CA space.

9	3	6	9	3
7	1	4	7	1
8	2	5	8	2
9	3	6	9	3
7	1	4	7	1

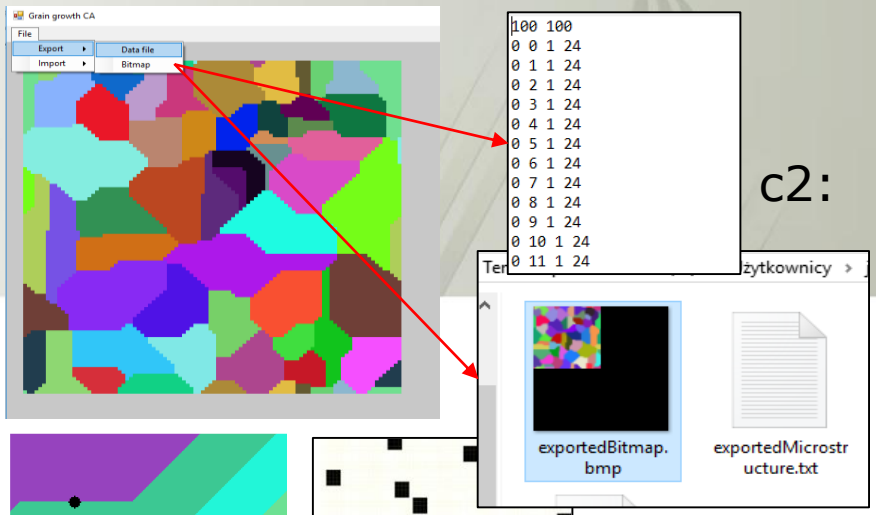


1st project

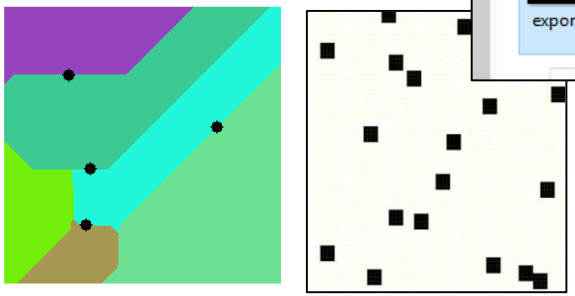
c1:



c2:



c3:



c4:

c5:

c6: