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

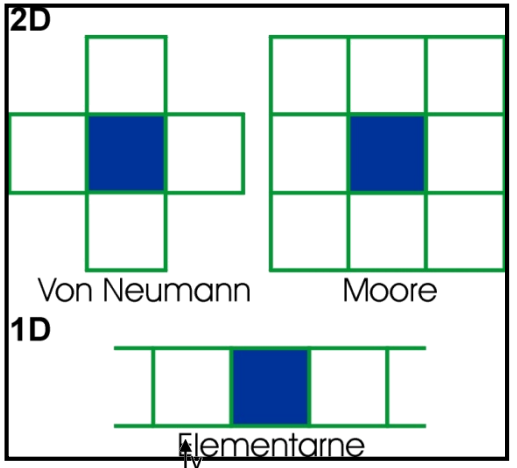
Classes calendar

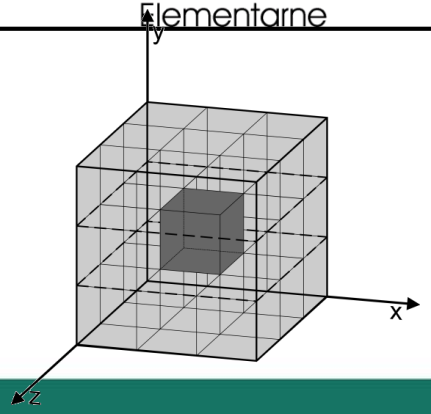
	Issues
1	Organizational class - simple grain growth CA + visualization
2	**Microstructures export/import to/from txt files, pictures.**
3	Modification of cellular automata grain growth algorithm- inclusions (at the beginning/end of the simulation)
4	Modification of CA grain growth algorithm - influence 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

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



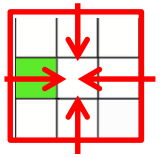


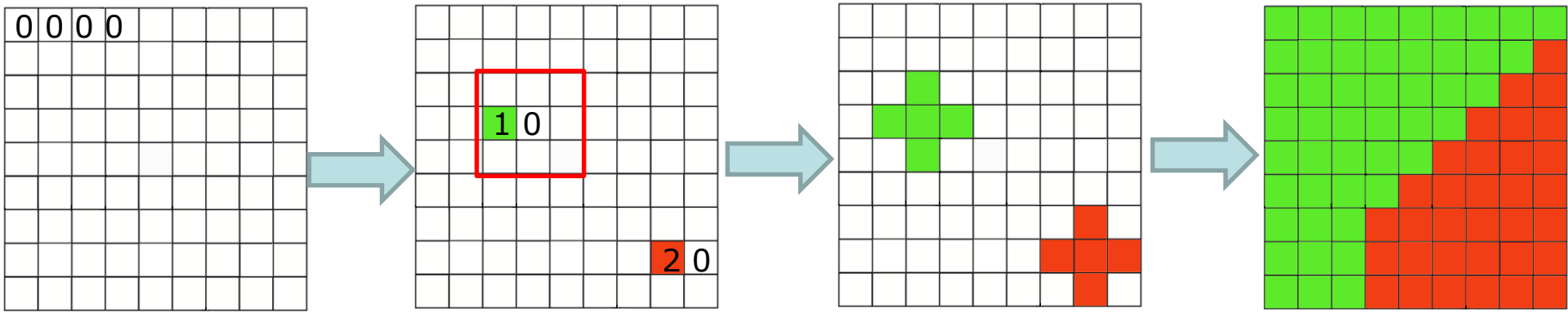
$$\gamma_i^{t+1} = f\left(\gamma_j^t\right) \quad \text{where} \quad j \in N(i)$$

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





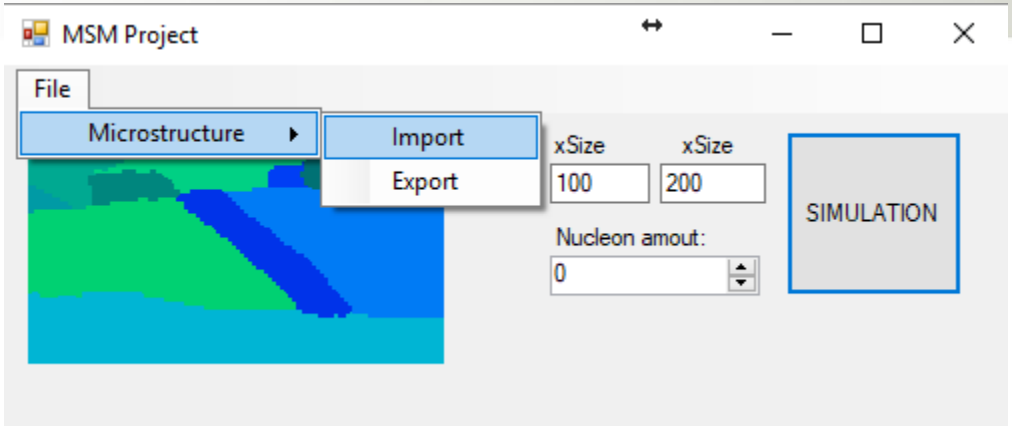
Initial space

1st step

2nd step

last step

Microstructures export/import to/from txt files, pictures



TXT:

EULER_CORRECT.txt | DP.txt

```
300 300 1
0 0 0 23
0 1 0 23
0 2 0 23
0 3 0 23
0 4 0 23
0 5 0 23
0 6 0 23
0 7 0 23
0 8 0 23
0 9 0 24
0 10 0 24
0 11 0 24
0 12 0 24
0 13 0 24
0 14 0 24
0 15 0 24
0 16 0 24
0 17 0 24
0 18 0 24
0 19 0 24
0 20 0 24
0 21 0 24
0 22 0 24
0 23 0 24
0 24 0 24
0 25 0 24
0 26 0 24
```

xSize, ySize

posX, poxY, phase, id

BMP: