AGH University of Science and Technology

Multiscale Modelling

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

Project

- Application (c++, java, c#..) (wa = 0.8):
  - Grain growth algorithm modifications (Cellular automata)
- Report (wr = 0.2):
  - Interface + results + comparison with real microstructures + conclusions/discussion

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

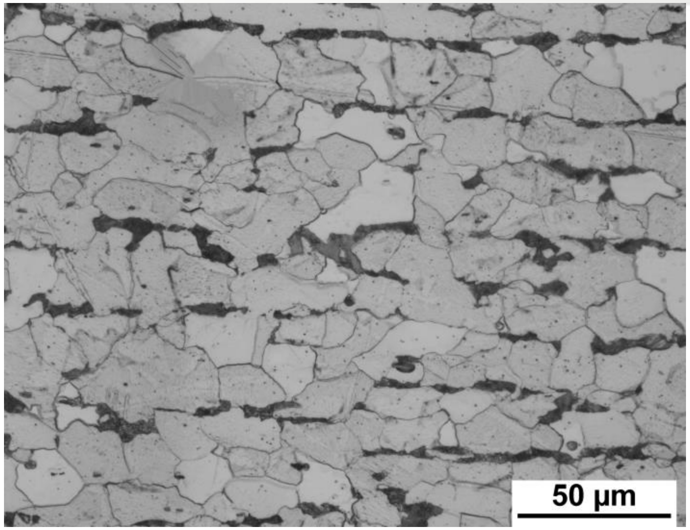
- **Git**

- 1 unexcused absences (**remainder – medical leave**)
- 1 short test - optional
- Exam „0” – final degree min 4.5/5.0 (in 1st term)

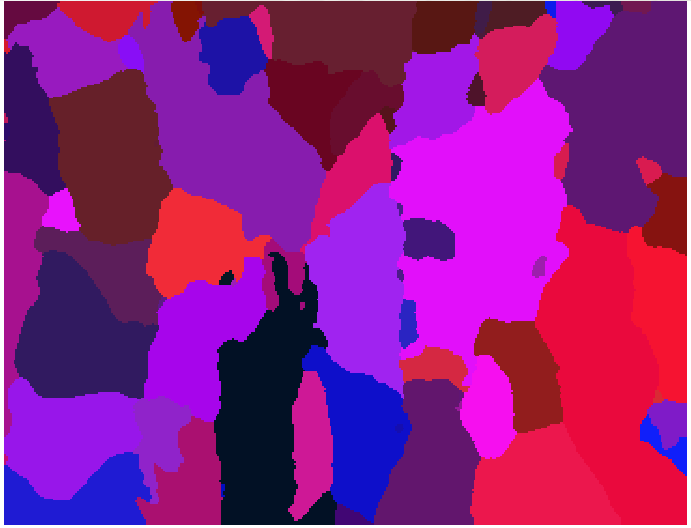
Classes calendar

	group: 1	group: 2	Tasks
1	25.10	25.10	Organizational class - simple grain growth CA + visualization + Microstructures export/import to/from txt files, pictures. Modification of cellular automata grain growth algorithm- inclusions (at the beginning/end of the simulation)
2	19.12	20.12	Modification of CA grain growth algorithm - influence of grain curvature
3	19.12	20.12	Modification of CA grain growth algorithm – dual-phase + substructures CA,
4	19.12	20.12	Modification of CA grain growth algorithm - boundaries coloring
5	30.01	30.01	**Reports – final grade – for 0 term exam**
6	31.01	31.01	**Reports and other issues**

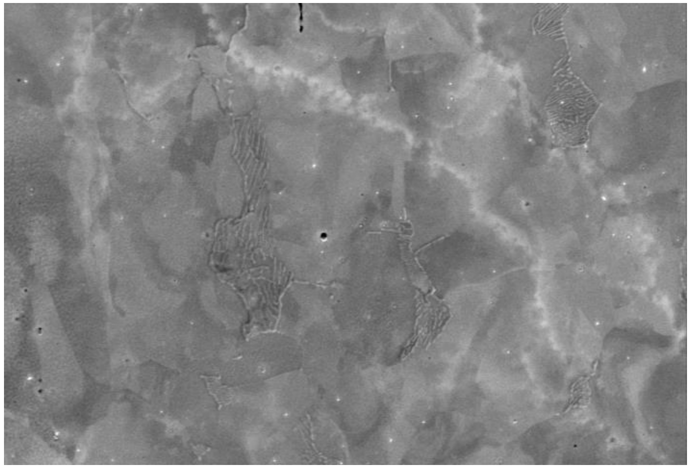
Material morphology



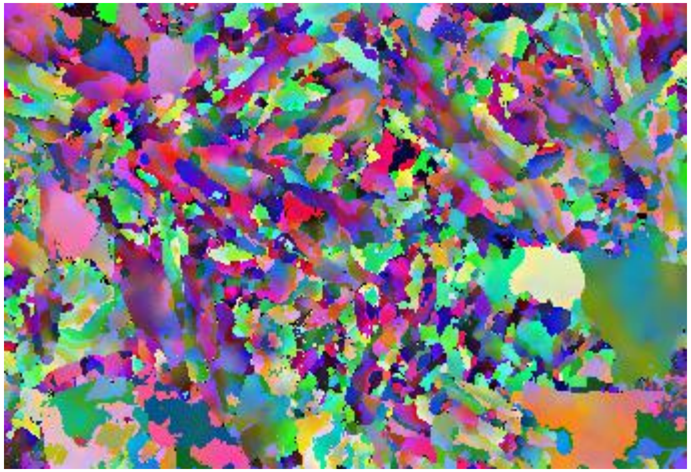
OPTI



EBSD



SEM



EBSD

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.

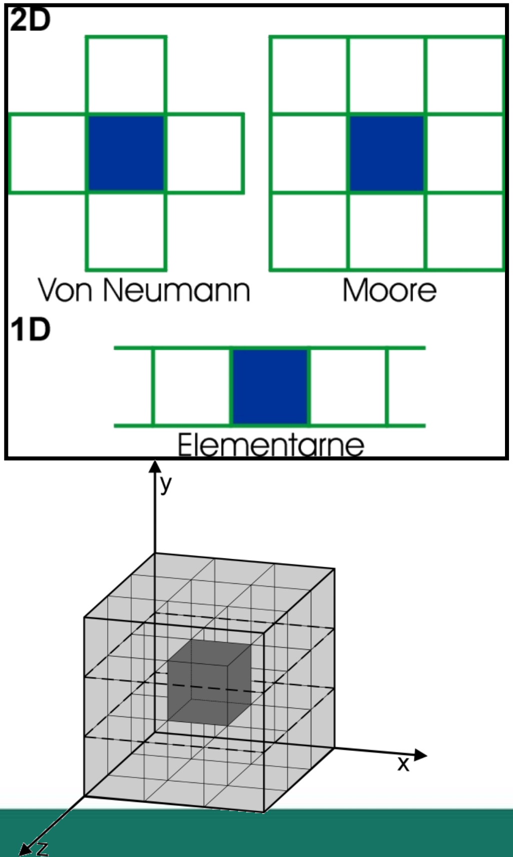
- CA space - finite set of cells, where each cell is described by a set of internal variables describing the state of a cell.

- 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

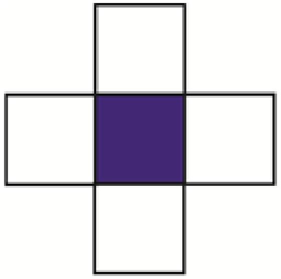
$$\boxed{\gamma_i^{t+1} = f\left(\gamma_j^t\right)} \quad \text{where} \quad \boxed{j \in N\left(i\right)}$$

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

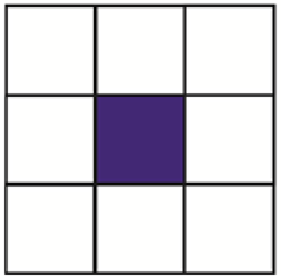


Neighbourhoods types

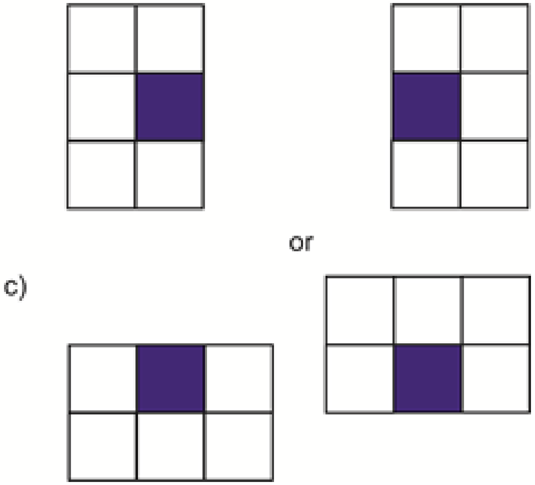
- Von Neumann



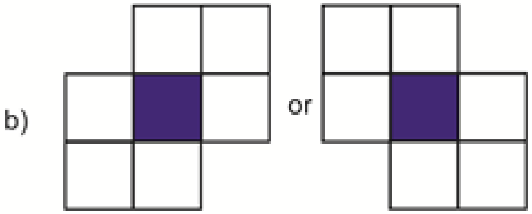
- Moore

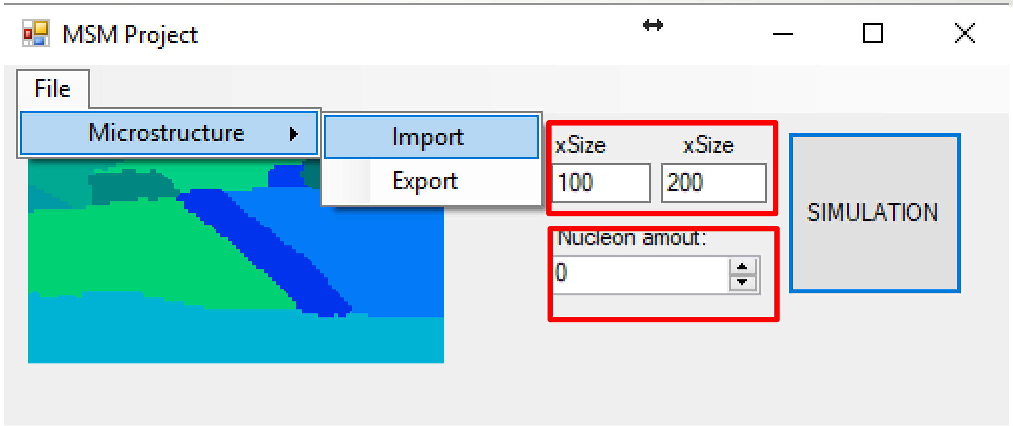


- Pentagonal random



- Hexagonal random





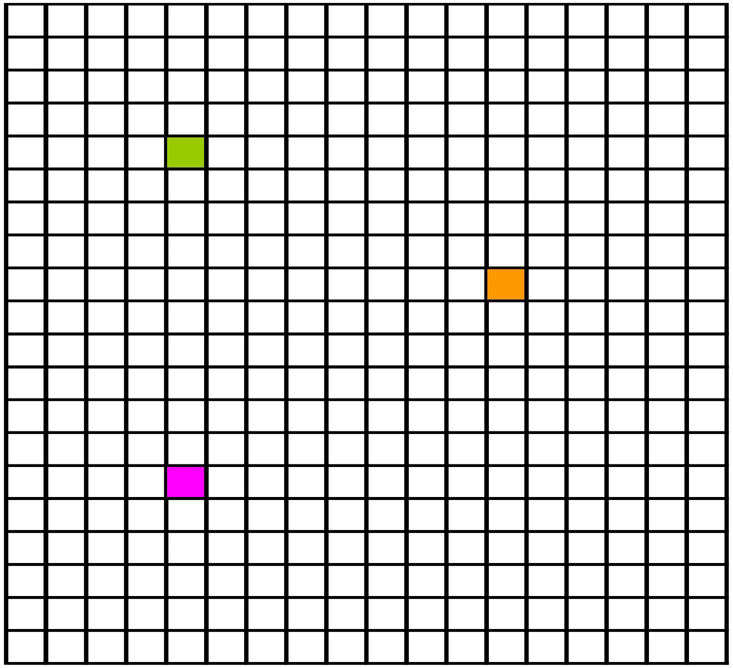
xSize 100

xSize 200

Nucleon amout: 0

1. Define the space size and the space (all CA cells are empty)
2. Define numer of new grains
3. Nucleation – randomly select cells that will represent the nuclei (centers) of new grains.
4. **In a loop Grain Growth – several iterations (one iteration of a loop involves checking each CA cell in the space (0,0), (0,1), (0,2), ……. (n-1, n-1)).**
5. The algorithm stops if is there are no more empty CA cells in the space.

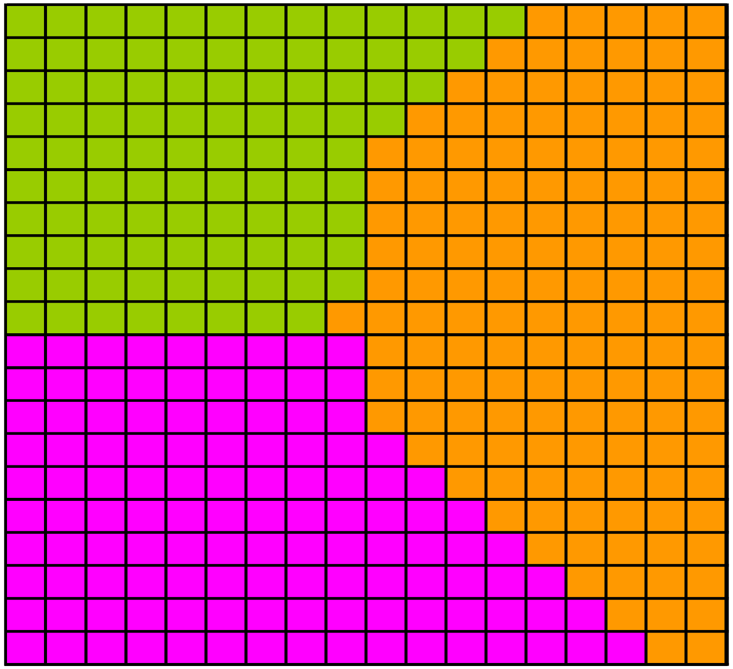
Nucleation (Zarodkowanie) – only one time at the bagining



Losowy wybór komórek i zmiana stanu na komórka, przypisanie wartości zmiennym wewnętrznym: numer ziarna, orientacja krystalograficzna

🟩 Ziarno nr 1 🟧 Ziarno nr 2 🟪 Ziarno nr 3

Grain Growth (Rozrost) – in each iteration



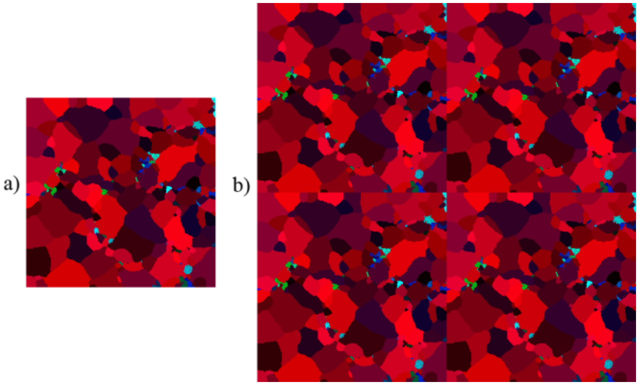
Jeżeli sąsiad danej komórki w poprzednim kroku był w stanie ziarno to komórka również zmienia stan na „ziarno”. Zmienne wewnętrzne przejmuje takie jakie posiada większość jej sąsiadów w stanie „ziarno”.

W przypadku takiej samej liczby sąsiadów o różnych własnościach, wprowadza się losowość wyboru.

Boundary conditions

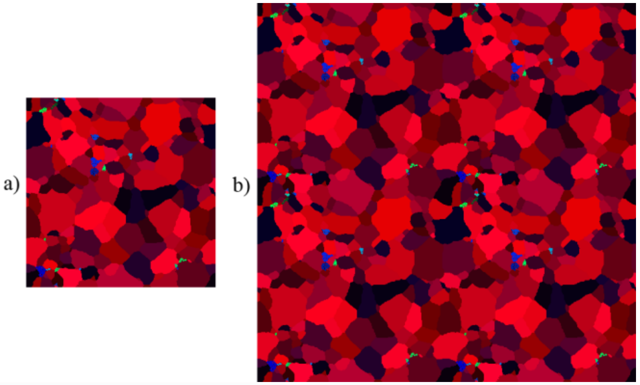
- **absorbing boundary conditions** – the state of cells located on the edges of the CA space are properly fixed with a specific state to absorb moving quantities.

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

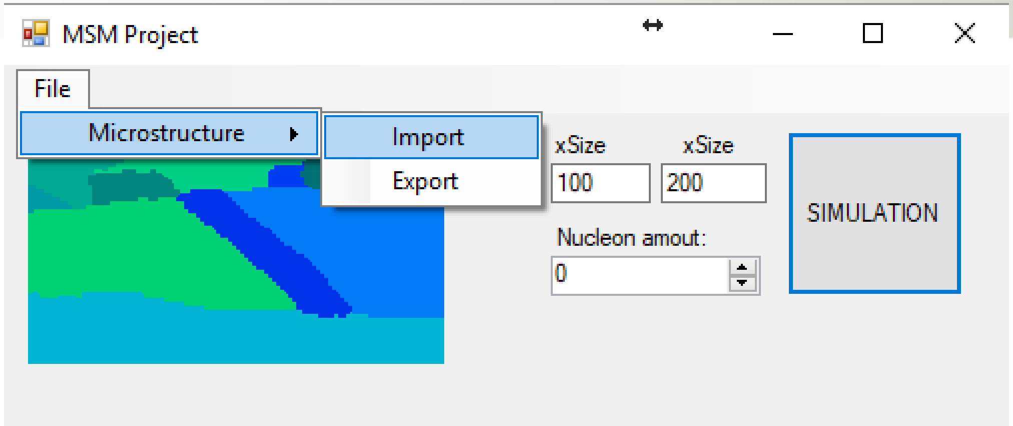


- **periodic boundary conditions** – the CA neighborhood is properly defined and take into account cells located on subsequent edges of the CA space.

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



Microstructures export/import to/from txt files, pictures

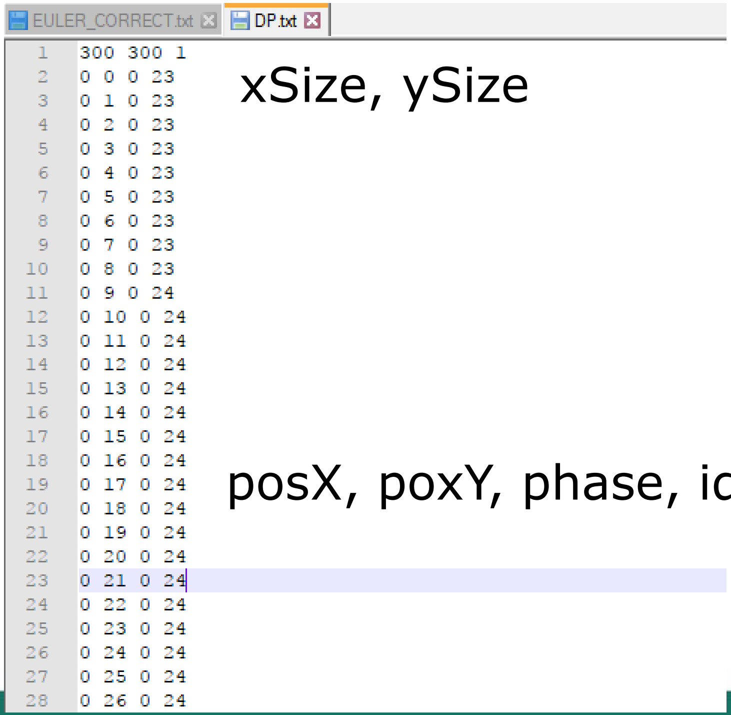


xSize 100

xSize 200

Nucleon amout: 0

TXT:

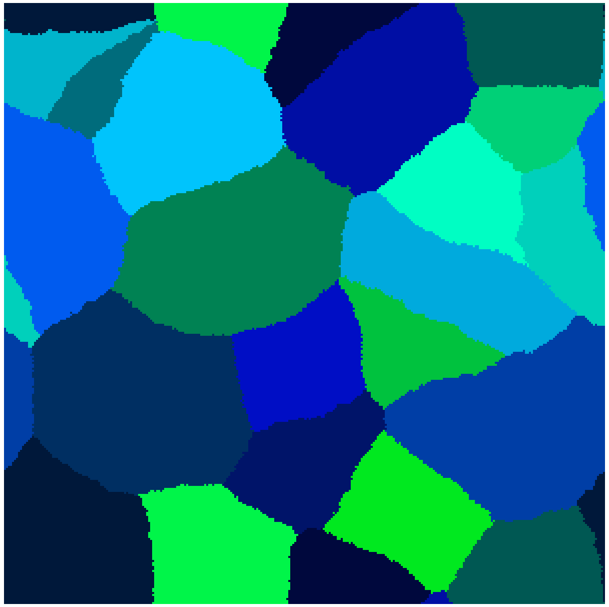


```
300 300 1
0 0 0 23
0 1 0 23
0 2 0 23
0 3 0 23
0 4 0 23
0 5 0 23
0 6 0 23
0 7 0 23
0 8 0 23
0 9 0 24
0 10 0 24
0 11 0 24
0 12 0 24
0 13 0 24
0 14 0 24
0 15 0 24
0 16 0 24
0 17 0 24
0 18 0 24
0 19 0 24
0 20 0 24
0 21 0 24
0 22 0 24
0 23 0 24
0 24 0 24
0 25 0 24
0 26 0 24
```

xSize, ySize

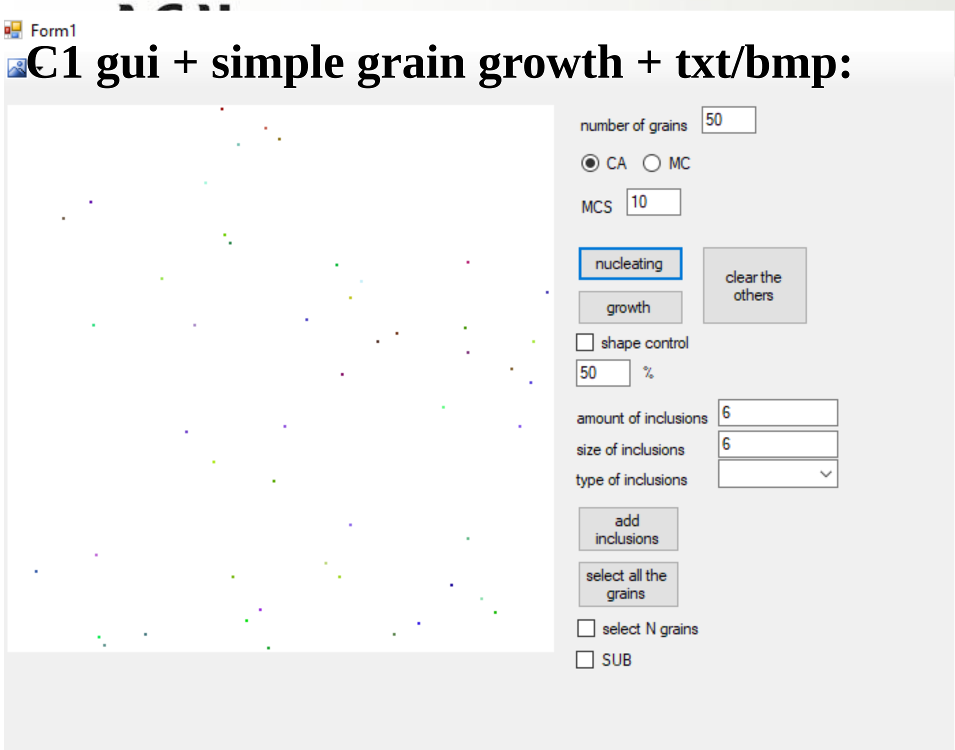
posX, poxY, phase, id

BMP:



projects

C1 gui + simple grain growth + txt/bmp:



number of grains 50

● CA ○ MC

MCS 10

nucleating

clear the others

growth

□ shape control

50 %

amount of inclusions 6

size of inclusions 6

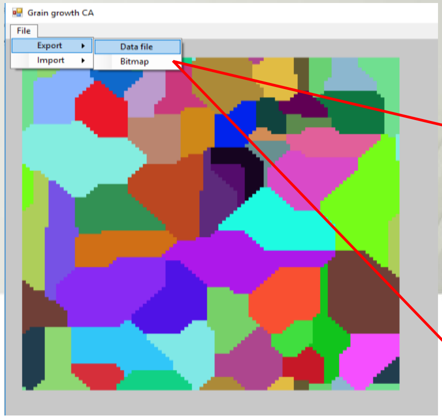
type of inclusions

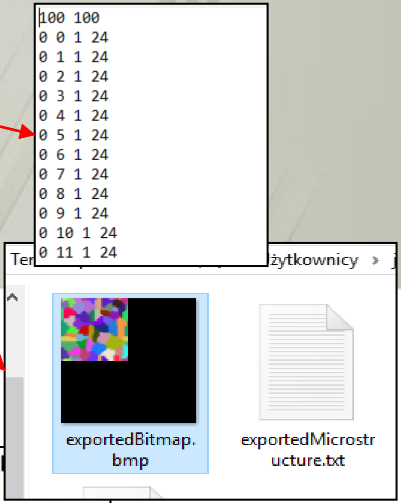
add inclusions

select all the grains

□ select N grains

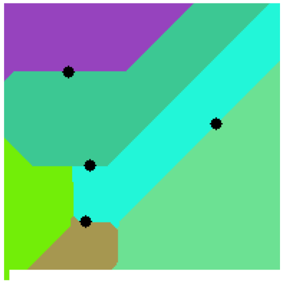
□ SUB

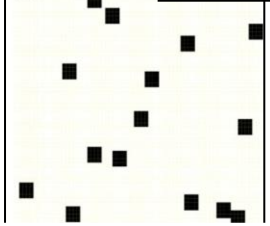




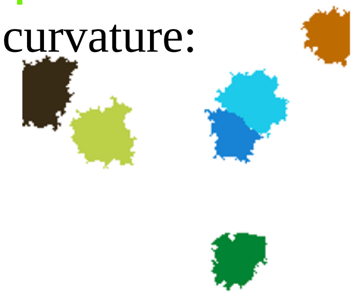
```
100 100
0 0 1 24
0 1 1 24
0 2 1 24
0 3 1 24
0 4 1 24
0 5 1 24
0 6 1 24
0 7 1 24
0 8 1 24
0 9 1 24
0 10 1 24
0 11 1 24
```

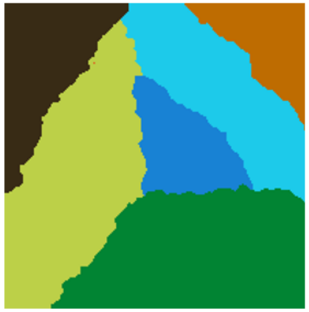
C2 inclusions:



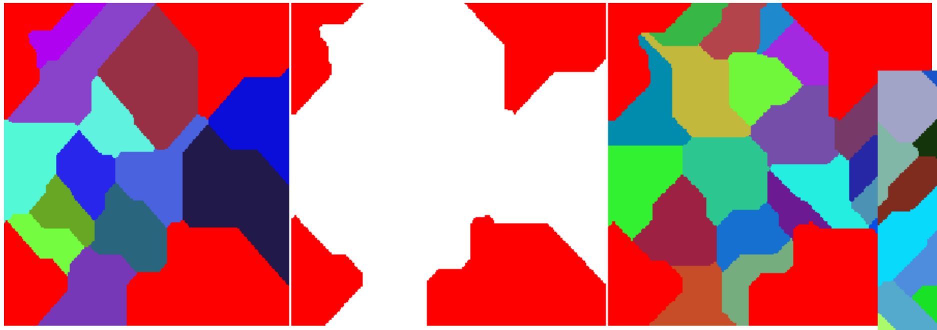


C3 curvature:





C4 dual phase:



C5 grain boundaries:

10% probability for rule 4