

# Multiscale Modelling

## Monte Carlo static recrystallization

Daniel Skimina

List of content:

1. Introduction
2. Application
3. Sample Simulation
4. Simulation on Grid
5. Results from Grid
6. Summary

# 1. Introduction

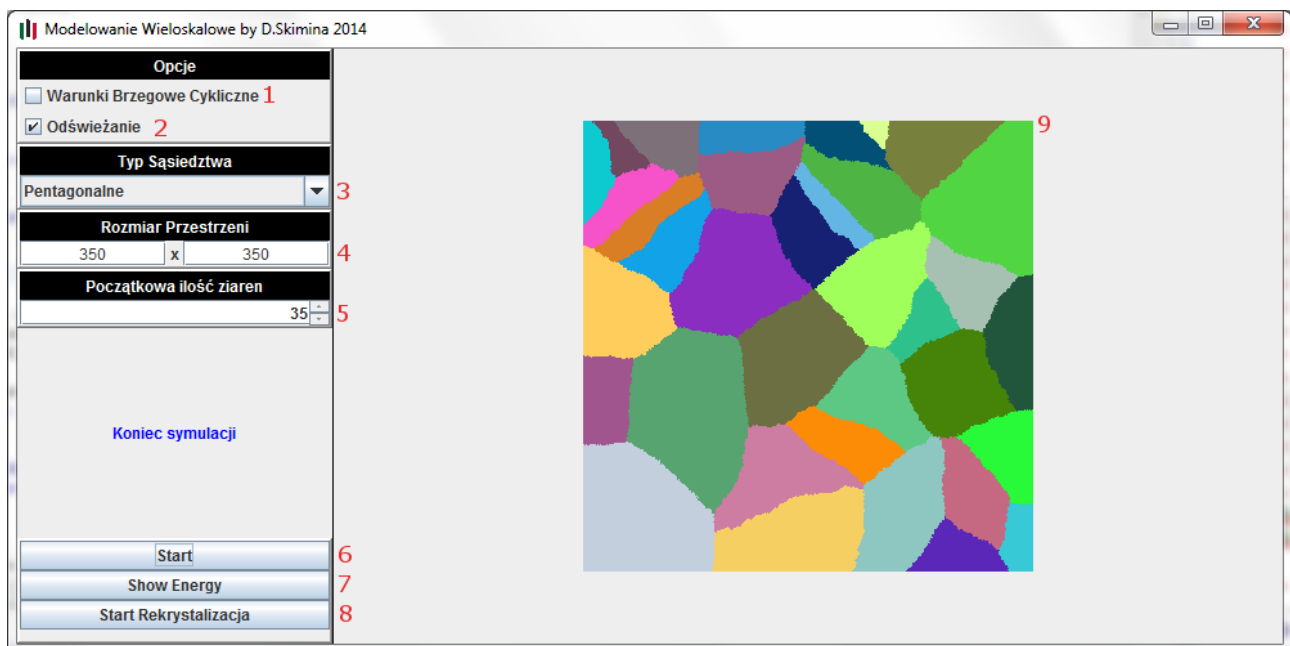
Main idea of Cellular Automata method is to divide part of the investigated material into 1,2,3 dimensional grid. Each cell of that grid is called Cellular Automaton. All of the cellular automata are known as Cellular Automata Space. Cellular Automata works in discrete time steps. After each time step the state of each cells in lattice is updated synchronically. CA algorithm base on states of cells from previous step and theirs neighbours.

## 2. Application

Application to simulate static recrystalization was written in JAVA. Whole sourcecode of my application is available on Github:

<https://github.com/danielsky/ModelowanieWieloskalowe/>

Main GUI of my program:



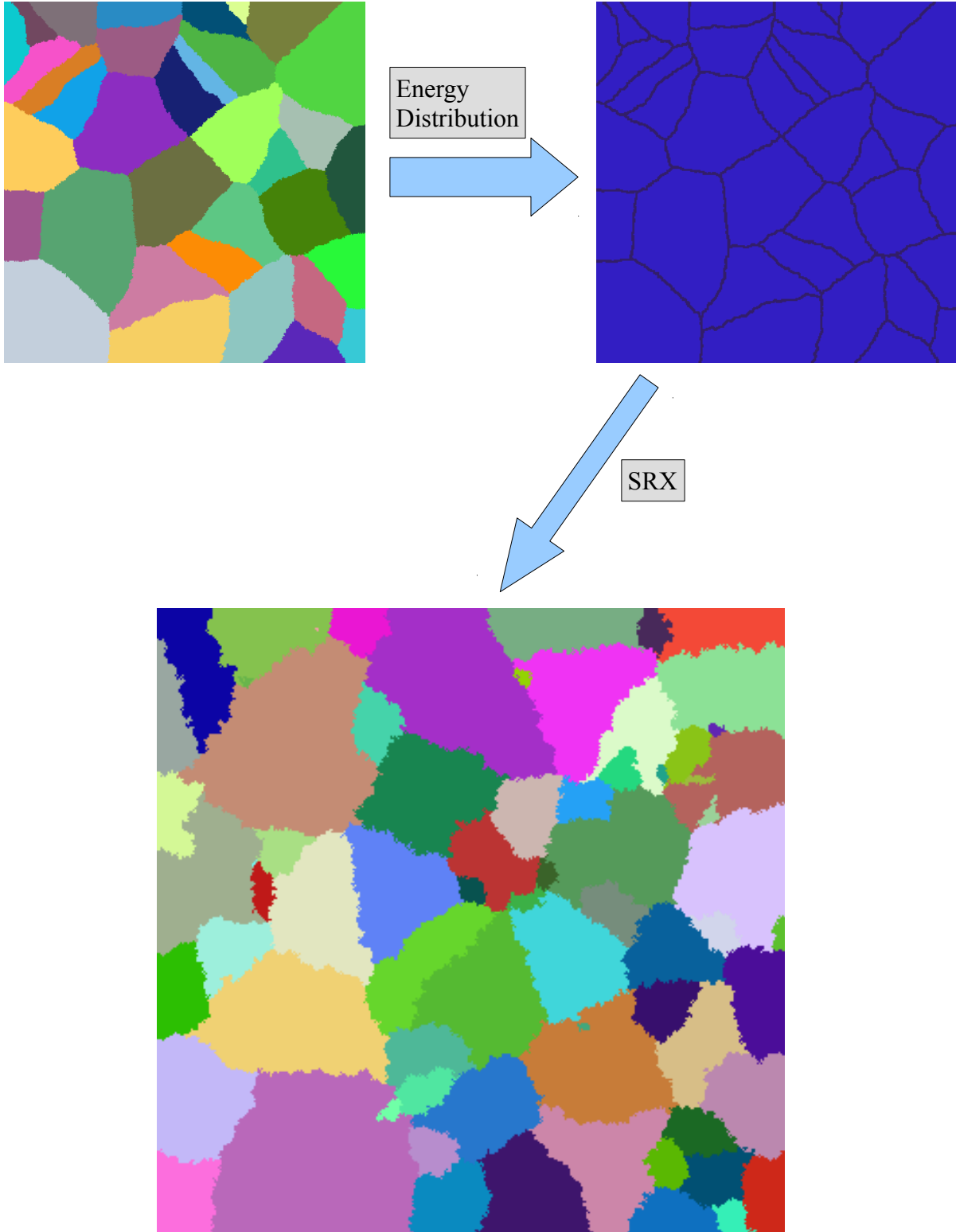
Description:

1. Boundary conditions (absorbing/periodic)
2. Refreshing structure during simulation
3. Type of neighborhood
4. Space size
5. Initial number of nuclees
6. Button for start simulation
7. Button for showing energy distribution after grain growth
8. Button for static recrystalization simulation
9. Preview of structure

### 3. Sample Simulation

Initial generated structure with parameters:

- **Absorbing** boundary conditions
- **Pentagonal** neighborhood
- Size of space **350 x 350** cells
- Initial number of nuclei **35**



## 4. Simulation on grid

Noticed problems during simulations:

- Middleware QCG\_Icon (version 1.4.8 for Windows) does not provide support for input files generated by MCMicro GUI
- Committed jobs for grid very often finished with errors. Most common exit code is 11 (Segmentation fault)
- MCMicroGUI have multiple problems with saving configuration files

Due to problem that QCG Icon doesn't provide method for committing jobs to MCMicro service, I must manually submit jobs via SSH using configuration files.

### Configuration files:

#### Configuration file for grain growth

```
#####APPLICATION OPTION
1 – Rodzaj symulacji (1 - rozrost ziaren, 2 – SRX, 3 – rozrost + SRX)
0 – Rodzaj zrównoleglenia OpenMP
0 – Rodzaj zrównoleglenia OpenMPI
#####GRAIN GROWTH
1200 – rozmiar przetrzeni X
1200 – rozmiar przetrzeni Y
1 – rozmiar przetrzeni Z
4 – sąsiedztwo (1 – neumann, 2 – moore, 3 – pent, 4 - hex)
0.6 - kbT
50 – liczba stanów
300 – liczba kroków MCS dla rozrostu ziaren
1 – warunki brzegowe (0 – nieperiodyczne, 1 - periodyczne)
#####SRX MC
```

## Configuration file for Grain growth + SRX

```
#####APPLICATION OPTION
1 – Rodzaj symulacji (1 - rozrost ziaren, 2 – SRX, 3 – rozrost + SRX)
0 – Rodzaj zrównoleglenia OpenMP
0 – Rodzaj zrównoleglenia OpenMPI
#####GRAIN GROWTH
1200 – rozmiar przestrzeni X
1200 – rozmiar przestrzeni Y
1 – rozmiar przestrzeni Z
4 – sąsiedztwo (1 – neumann, 2 – moore, 3 – pent, 4 - hex)
0.6 - kBT
50 – liczba stanów
300 – liczba kroków MCS dla rozrostu ziaren
1 – warunki brzegowe (0 – nieperiodyczne, 1 - periodyczne)
#####SRX MC
100 – liczba kroków dla SRX
1 – długość kroku SRX
1 – długość kroku po SRX
0 – zapis danych
2 – miejsce zarodkowania
3 – rodzaj zarodkowania
10 – interwał dodawania zarodków
100 – liczba dodawanych zarodków
1.0 – współczynnik skalujący
2 – podział energii zmagazynowanej
5.0 – energia przypadająca na pojedynczą komórkę
6.0 – średnia ilość energii zmagazynowanej
0.1 – prawdopodobieństwo przydzielenia pakietu energii wewnątrz ziarna
0.6 – prawdopodobieństwo przydzielenia pakietu energii na granicy ziarna
0.8 – prawdopodobieństwo przydzielenia pakietu energii na złączu potrójnym
1.0 – energia pomiędzy dwoma komórkami
0 – wpływ orientacji krystalograficznych
180 – górny zakres orientacji krystalograficznych
1 - sąsiedztwo
0 – warunki brzegowe
```

## Configuration file for job submission („runnable.sh”)

```
#PBS -l nodes=1:ppn=N
#PBS -M dskimina+grid@gmail.com
module add plgrid/apps/mcmicro/1.0
cd $PBS_O_WORKDIR
mpiexec MCMicro_MPI 1 simul.mcmicro
```

Where N is a number of cores per node.

Next step was adding job to grid queue. This could be done using command:

```
qsub runnable.sh
```

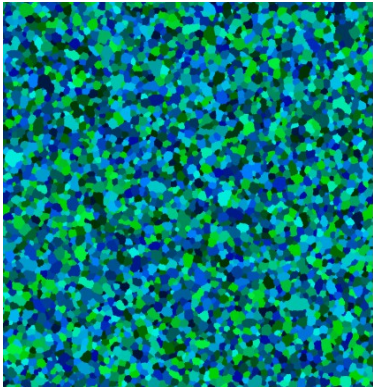
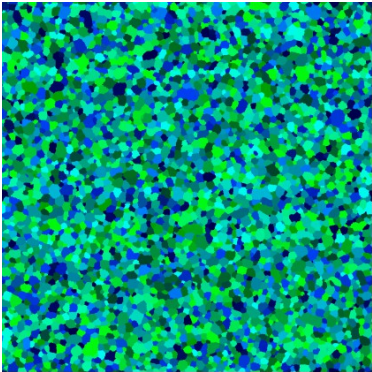
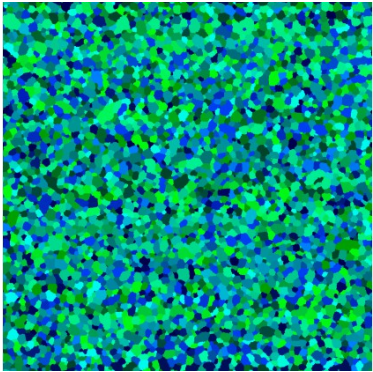
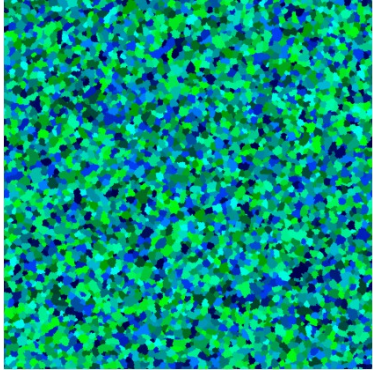
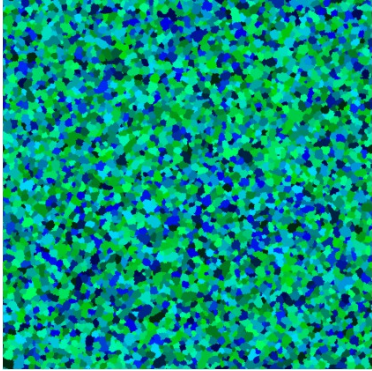
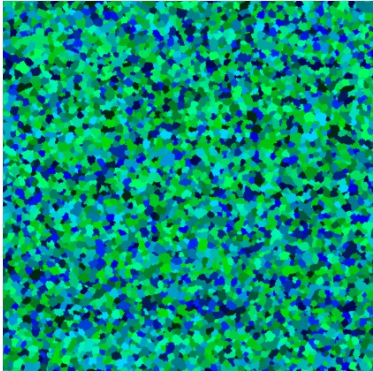
## 5. Results from Grid

Not all results are available because grid very often returned error code (segmentation fault).

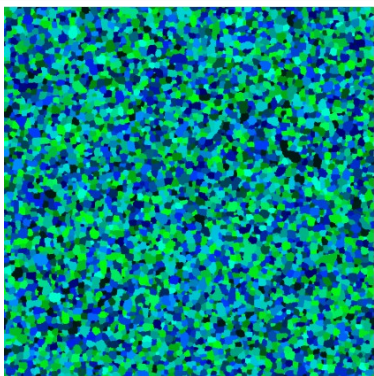
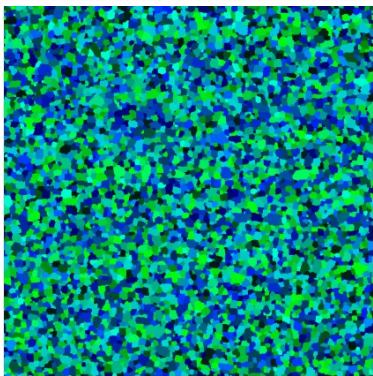
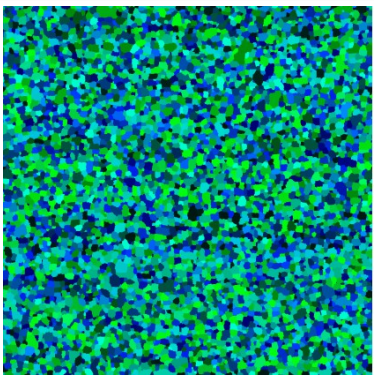
### Grain growth results:

	1	12	24
Hexagonal	Failed	Failed	Failed
Moore	OK	OK	OK
Pentagonal	OK	OK	OK
Von Neumann	OK	OK	OK

### Vizualized results of grain growth:

	1	12	24
Moore			
Pentagonal			

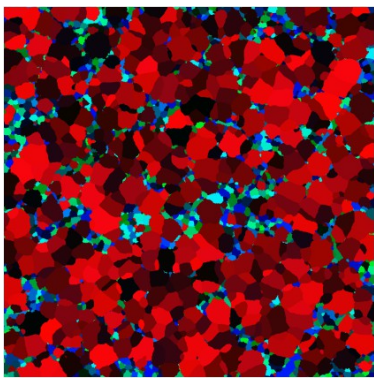
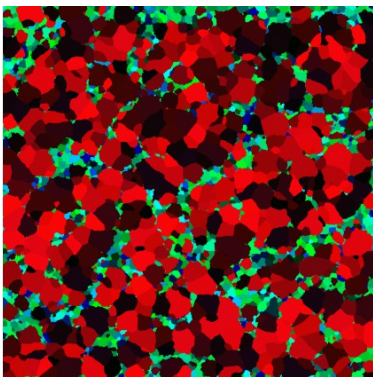
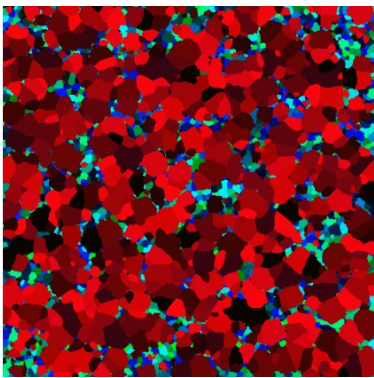
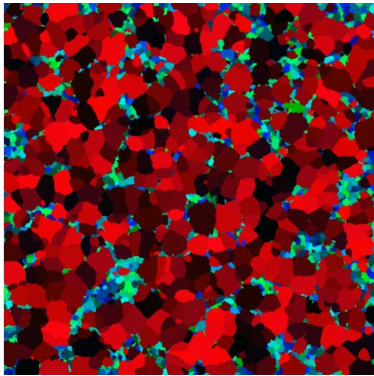
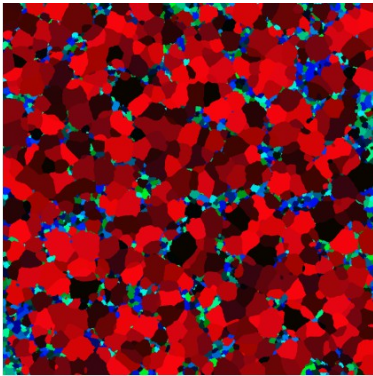
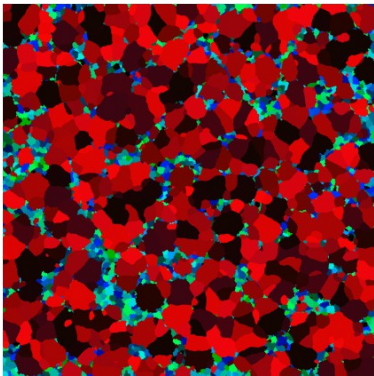


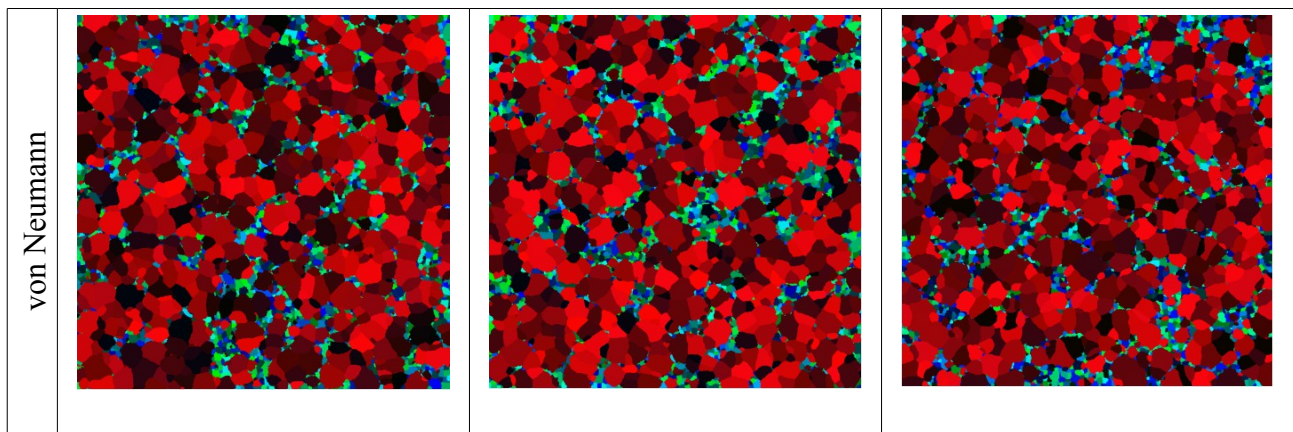
von Neumann			
-------------	---	--	---

### Grain growth + SRX results:

	1	12	24
Hexagonal	Failed	Failed	Failed
Moore	OK	OK	OK
Pentagonal	OK	OK	OK
Von Neumann	OK	OK	OK

### Vizualized results of grain growth + SRX:

	1	12	24
Moore			
Pentag			



## 6. Summary

- Services on grid should be more stable. Very often error: Segmentation Fault
- Problems while saving configuration files from MCMicro GUI
- QCQ Icon (version for windows) don't provide support for MCMicro