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Report 2 – Monte Carlo method

Intro

This project is a continuation / extension of already existing one which contains only Cellular Automata grains growth method.

Program presents new Monte Carlo grain growth method with additional features:

- Static grain recrystallization with various type and position of creation
- Visualization of energy distribution
- Creating substructures, Dual Phase, boundaries of grains
- Save / Load bitmap to file

Main interface

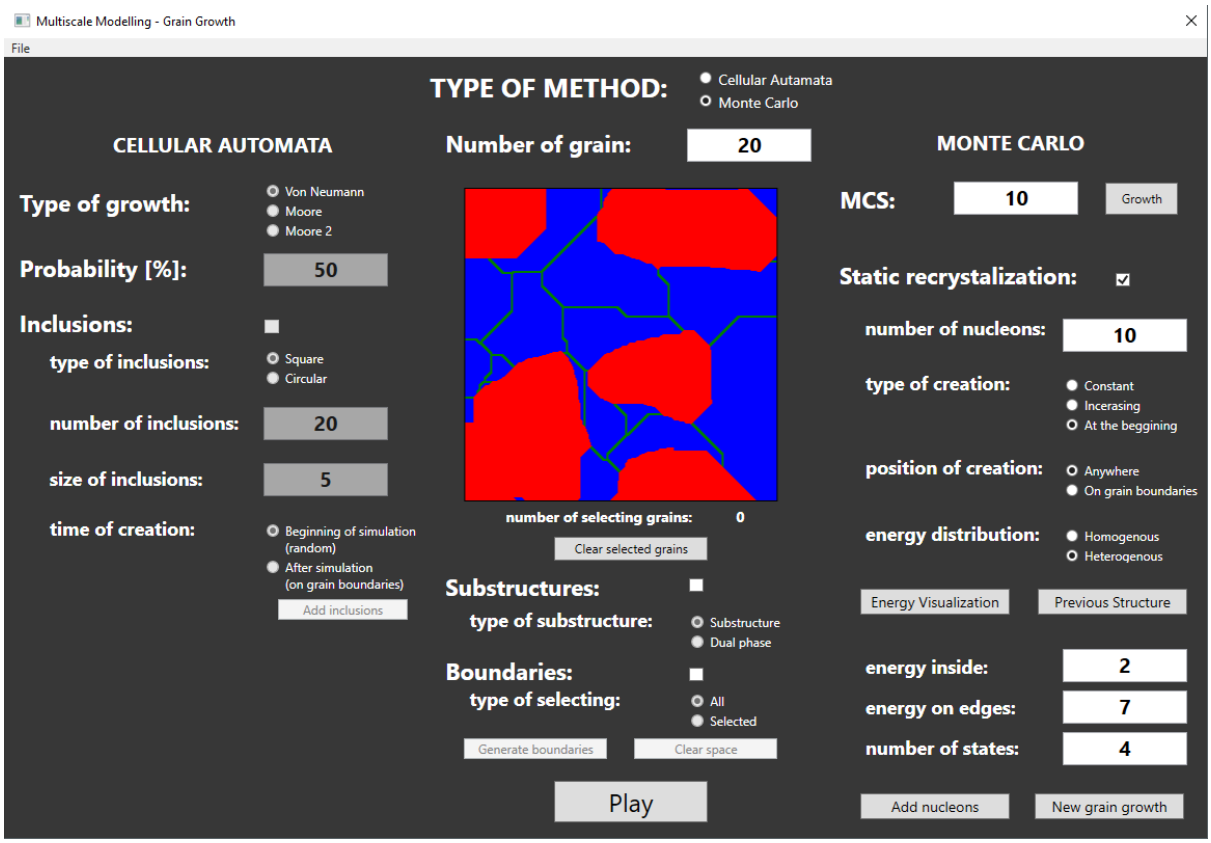

Figure 1 - main interface with presented all features that contains, visualization of energy and nucleation's

To start the process of grains growing user can setting necessary parameters and pressing the “Play” button presented above on Figure 1. The resulting structures obtained after each step are displayed in the middle of GUI so the user can see how the whole process is performed. After that, by pressing “Add nucleons” button user can start the process of static recrystallization. After nucleons growth by pressing “New grain growth” possible to create new grains growth in place old nucleons.

Additional parameters:

1. Number of Monte Carlo Steps (MCS) – it’s a basic parameter that user have to provide. Determines how much grains will growth - Figure 2.
2. Number of nucleons – it’s a number of nucleons which are recrystallized grains visualized in gradient of red color to make it easier to differ them from the non-recrystallized ones.
3. Type of creation – user can choose three types of creation
    a. Constant (e. g. 10, 10, 10 …for each MCS step)
    b. Increasing (e. g. 10, 20, 30, …)
    c. At the beginning
4. Position of creation – user can choose two types of creation
    a. Anywhere
    b. On grain boundaries
5. Energy distribution
    a. Homogenous
    b. Heterogeneous
6. Energy inside – energy distributed not on grains boundaries
7. Energy on edges – energy distributed not on grains boundaries
8. Number of states – number of nucleon colors

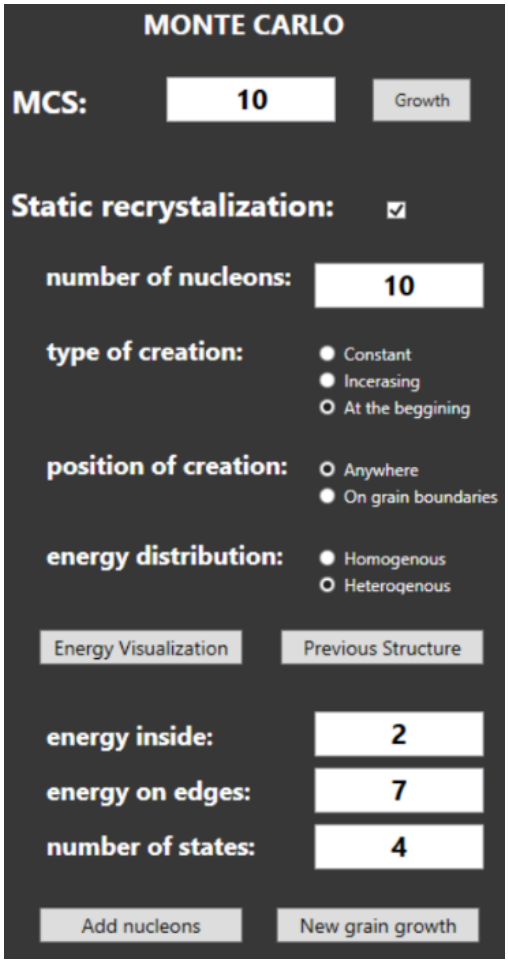

Figure 2 - additional parameters

Basic MC structures

Process of generation 20 Monte Carlo Steps with Dual Phase (DP) (Figure 3 - 6):

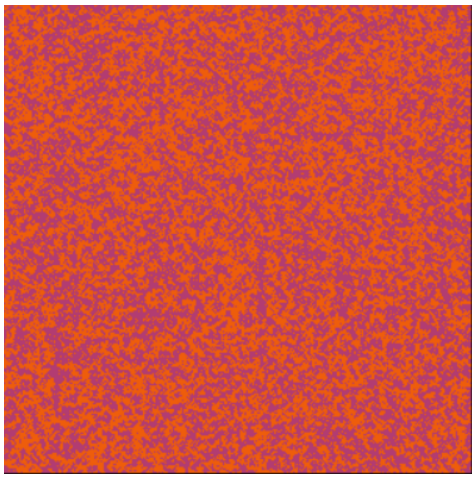

Figure 3 - MCS: 1, grains: 2, method: MC

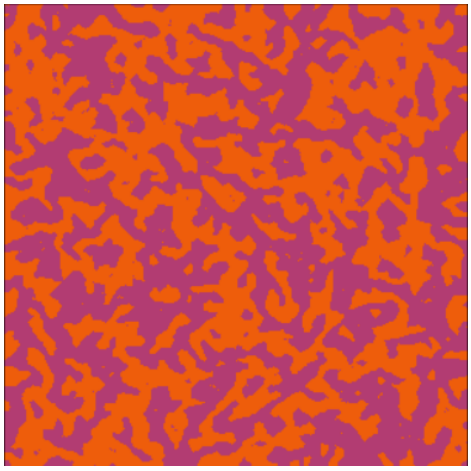

Figure 4 – MCS: 10, grains: 2, method: MC

Figure 5 – MCS: 20, grains: 2, method: MC

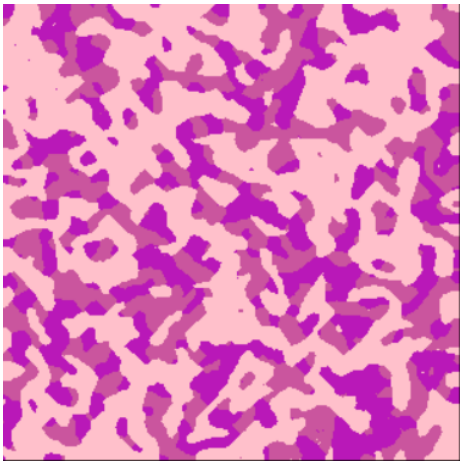

Figure 6 - after 20 MCS dual phase, grains: 2, MCS: 20 method MC

Advanced MC structures

Process of generation combined structures Cellular Automata to Monte Carlo with Dual Phase (Figure 7 – 8):

Figure 7 - grains: 20, growth: Moore 2, method: CA

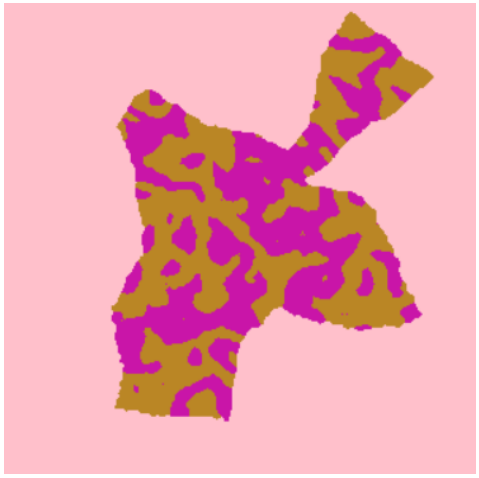

Figure 8 - after Dual Phase, MCS: 20, grains: 2, method: MC

Process of generation combined structures Monte Carlo to Cellular Automata with Dual Phase (Figure 9-10):

Figure 9 - MCS: 100, grains 2, method: MC

Figure 10 - after 100 MCS with Dual Phase, grains: 50, growth: von Neuman, method: CA

SRX – static recrystallization

Recrystallization is a process by which deformed grains are replaced by a new set of defect-free grains that nucleate and grow until the original grains have been entirely consumed. The following bitmaps shows resulted SRX processed accordingly to the specify parameters configuration. At first user should distributed energy and then is possible to visualization of energy. To present energy three color where used (Figure 18):

Blue – energy inside grain

Green – energy on boundaries

Red – nucleons

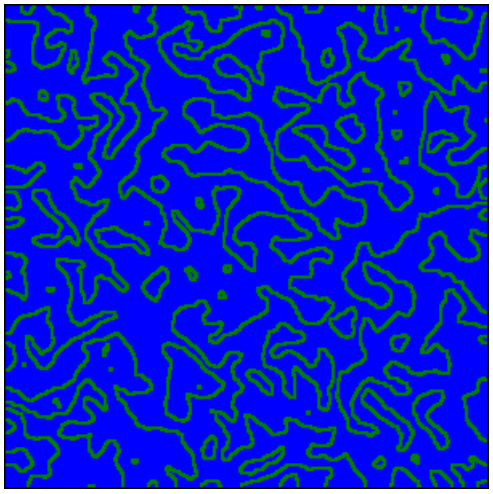

Figure 11 - MCS: 20 , grains: 2, method: MC

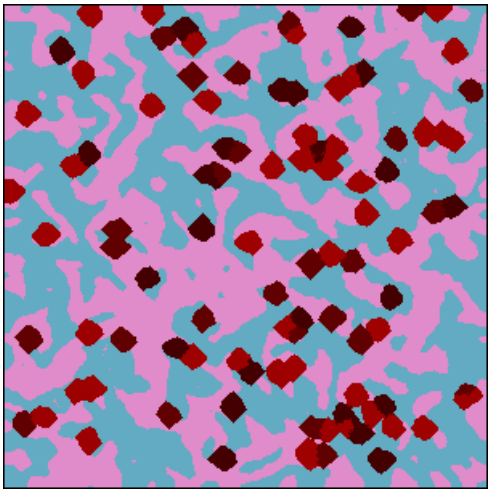

Figure 12 - MCS: 10, nucleons: 100, type of creation: at the beginning, position: on grain boundaries, energy distribution: homogenous

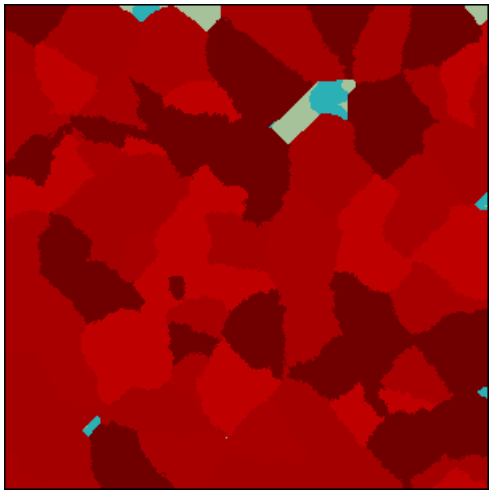

Figure 13 - MCS: 50, nucleons 100, type of creation: at the beginning, position: on grain boundaries, energy distribution: homogenous

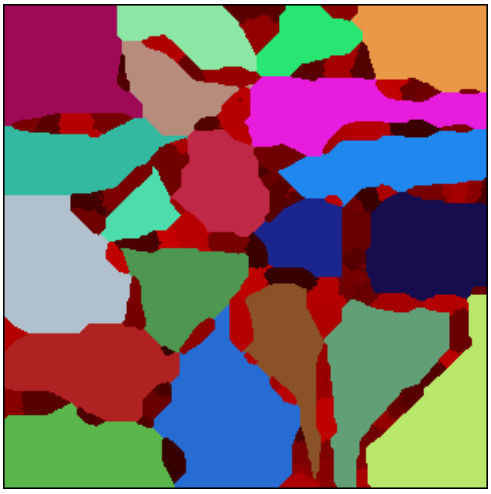

Figure 14 - I. grains: 20, growth: von Neumann, method CA; II. MCS: 15, Nucleons: 10, type of creating: constant, energy: heterogeneous, method MC

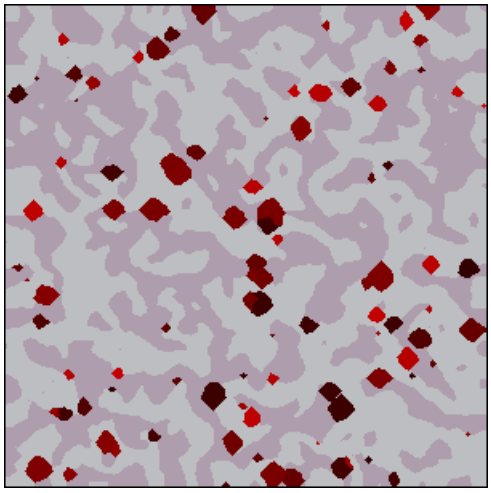

Figure 15 - MCS: 10, nucleons 10, type of creation: constant, position: on grain boundaries, energy distribution: heterogeneous

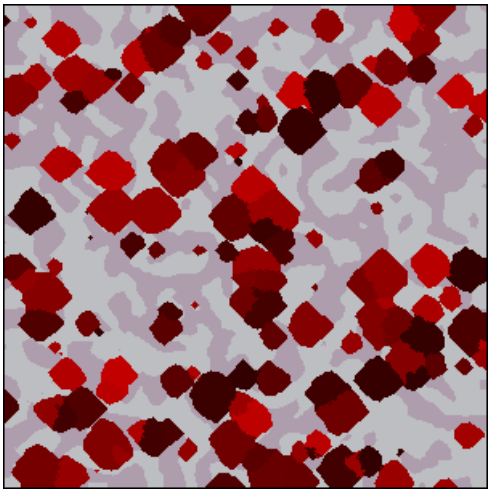

Figure 16 - MCS: 20, nucleons: 10, type of creation: constant, position: on grain boundaries, energy distribution: heterogeneous

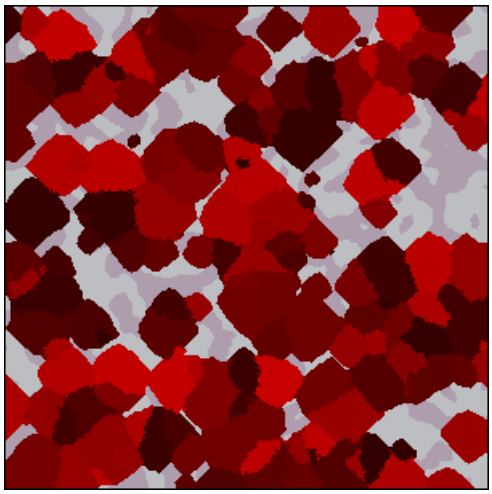

Figure 17 - MCS: 30, nucleons: 10, type of creation: constant, position: on grain boundaries, energy distribution: heterogeneous

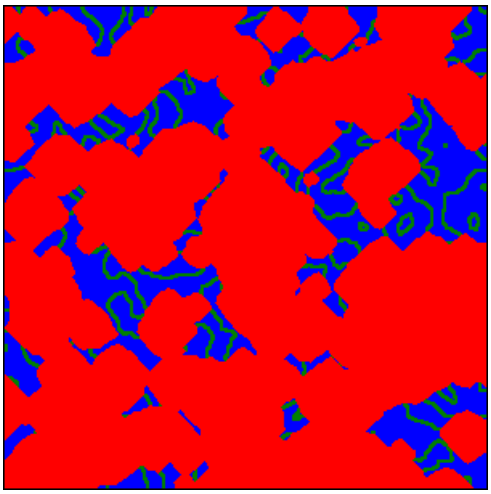

Figure 18 - MCS: 30, nucleons: 10, type of creation: constant, position: on grain boundaries, energy distribution: heterogeneous, energy visualization

After nucleons growth user can create new grain growth:

Figure 19 - I. grains: 20, growth: von Neuman, method: CA; II. MCS: 110, nucleons: 10, type of creation: at the beggining, position: on grain boundaries, energy distribution: heterogeneous

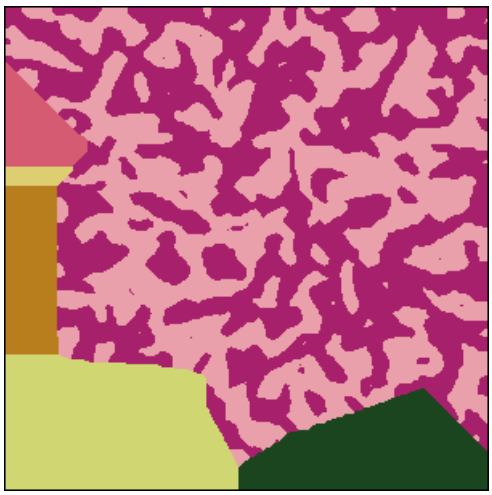

Figure 20 - III. MSC: 20, grains: 2, method: MC

Technology

For the purpose of building this application was used the C# programming language with WPF framework what resulted easier way to creating a GUI and efficient program.

Comparing with real structures:

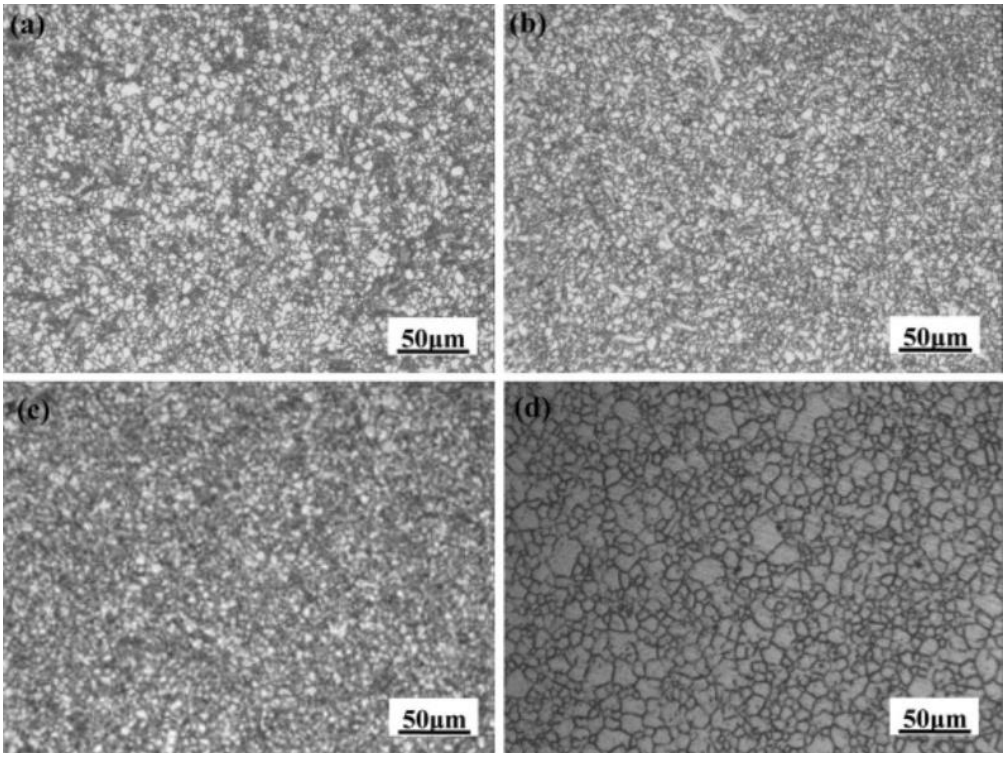

Figure 21 - [1]Optical microstructures annealed at a) 250 °C, b) 300 °C, c) 350 °C, and d) 400 °C for Mg–1.5Zn–0.6Zr–4Er alloy extruded at 420 °C.

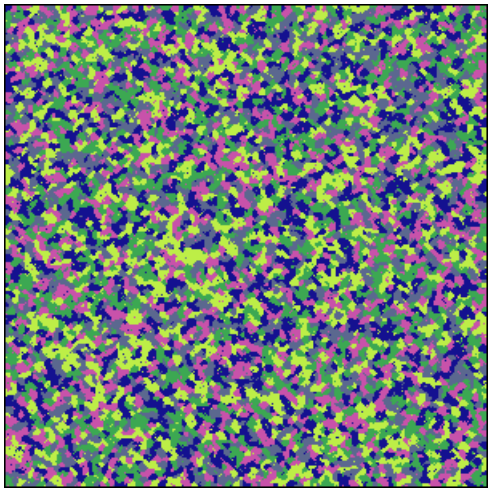

Figure 22 - MCS: 10, grains: 5, method: MC

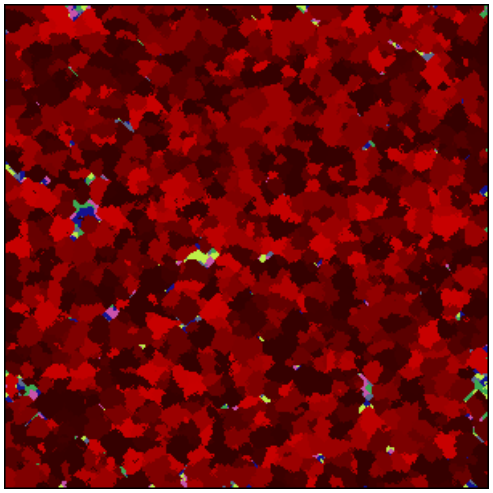

Figure 23 - I. MCS: 10, grains: 5, method: MC; II. MCS: 15, nucleons: 100, type of creating: increasing; position: on boundaries, energy: heterogenous

[1] https://www.sciencedirect.com/science/article/pii/S2213956713000133, 10.01.2019

Conclusion

The program allows for the free creation of various metallurgical structures along with the simulation of recrystallization that may be close to the real ones.

The algorithm of the Monte Carlo method differs significantly from the Cellular Automata. MC handle better with a small amount of grains, generates completely different structures.

During SRX, increasing energy on the boundaries made it more likely that the nucleon would grow along the boundaries.

In case of “increasing” type of creation, too much MCS and the number of nucleons at once made too many operations and the inability to complete the program in the right way.

If all nucleons are distributed at the beginning of simulation, on the resulted structure we can see that recrystallized grains have similar size. In case of adding new nucleons during the next steps, the size of recrystallized grains is significantly different.

Repository with source code is available on GitHub[2].

[2] https://github.com/pawelbrzoza/multiscale-modelling, 10.01.2019