

Report for multiscale modeling projects 2020/2021

GUI Explanation

The screenshot shows a Tkinter window titled 'tk' with a light gray background. It contains several sections of controls:

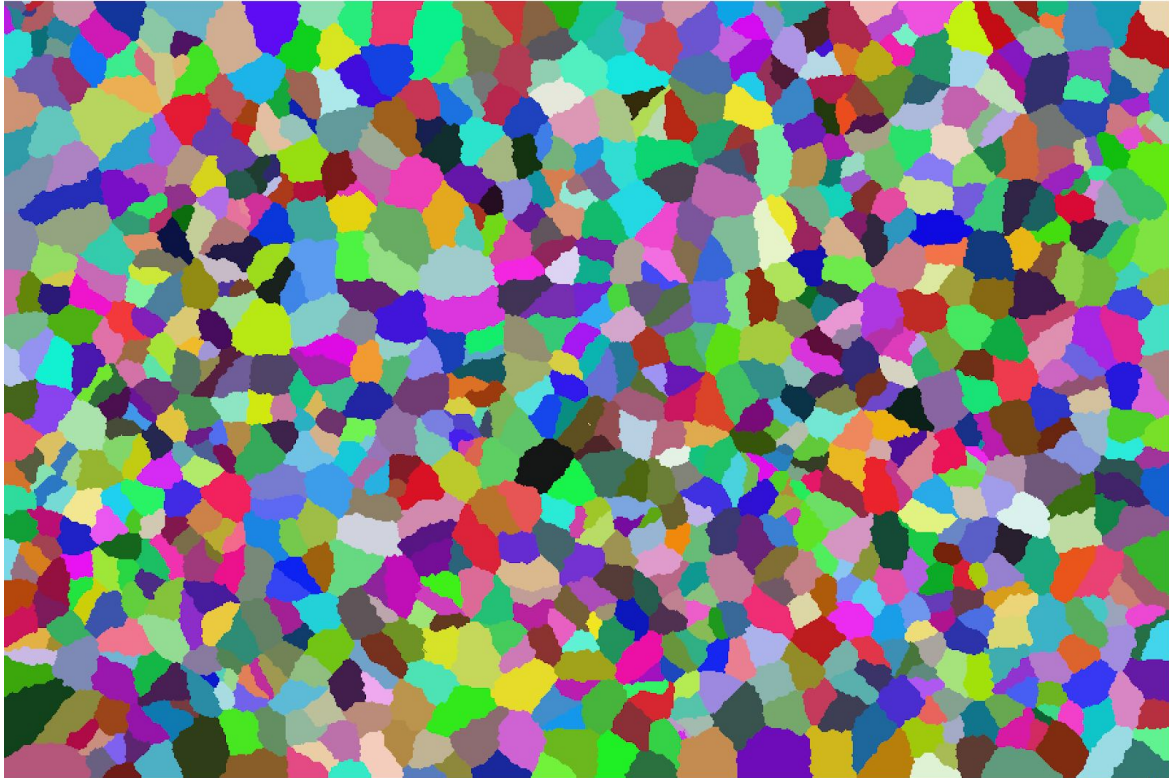
- Pick CA space size**: A text input field with '100' entered and a small '100' label below it.
- Number of nucleons**: A text input field with '100' entered.
- Number of inclusions**: A text input field with '0' entered.
- Size of inclusions**: A text input field with '0' entered.
- Inclusion insertion time**: A dropdown menu with 'before growth' selected.
- Inclusion shape**: A dropdown menu with 'circular' selected.
- choose boundary condition**: A dropdown menu with 'Absorbing' selected.
- choose grain curvature type**: A dropdown menu with 'curvature' selected.
- probability**: A text input field with '30' entered.
- select option**: A button labeled 'START'.
- Buttons**: Two buttons labeled 'save to txt file' and 'load from txt file'.
- Legend**: A section at the bottom with text: 'I - add inclusions', 'SPACE - start animation', 'B - show borders', and 'D - dualPhase'.

From the top:

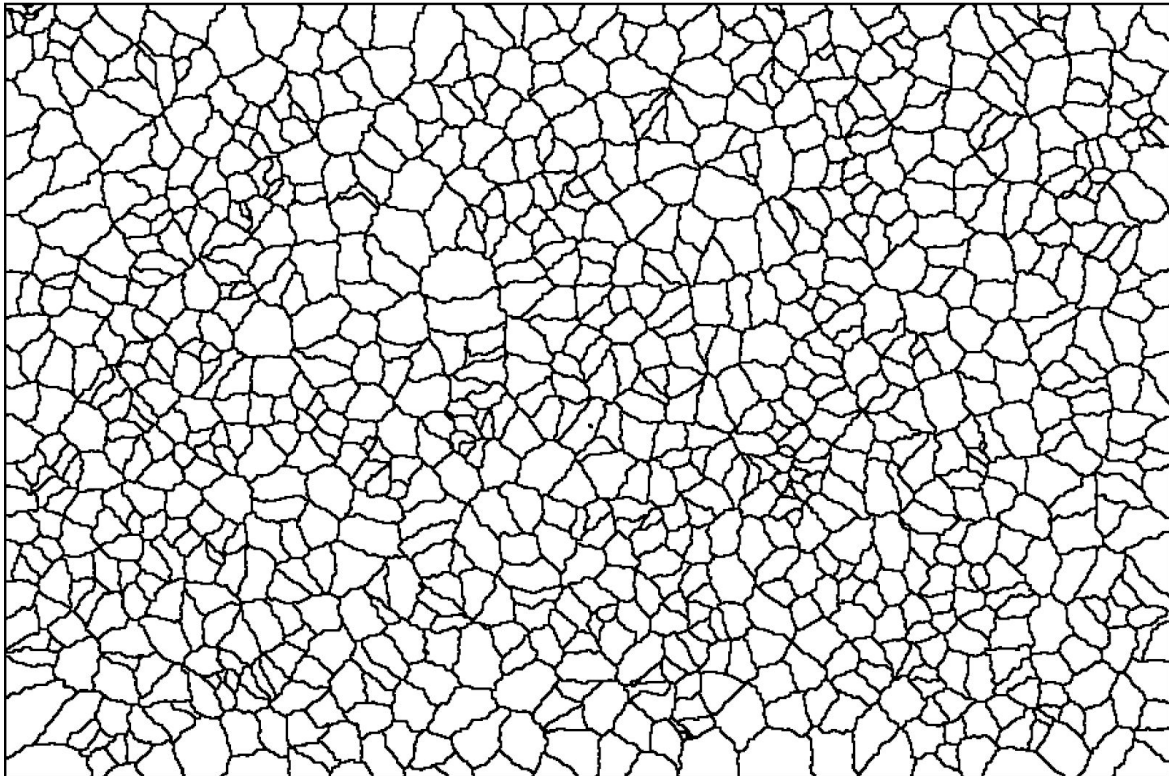
- Size x and size y of the CA space, these values will determine number of squares in the simulation(each square has 4x4px size for better visibility)
 - Number of randomly placed nucleons during the start of simulation
 - Number of inclusions to put in the simulation(before or after, circular or square), optional
 - Size of a single inclusion, diameter for circle, edge length for square
 - Selection of the moment when the inclusions are placed. Before growth, inclusion are placed randomly, before the nucleons grow, after growth, they are placed on the grain borders
 - inclusion shape determines whether they are squared or circular
- Boundary condition determines whether borders of the ca space are absorbing or if they let the grains pass through and appear on the other edge
 - grain curvature chooses between simple moore neighbourhood growth or the 4 rule growth with probability to better show grain curvature
 - Probability option allows to set probability for the 4 rule algorithm used for curvature option
- Start the simulation and save/import to file options
- Buttons to press to control the simulatio

Results

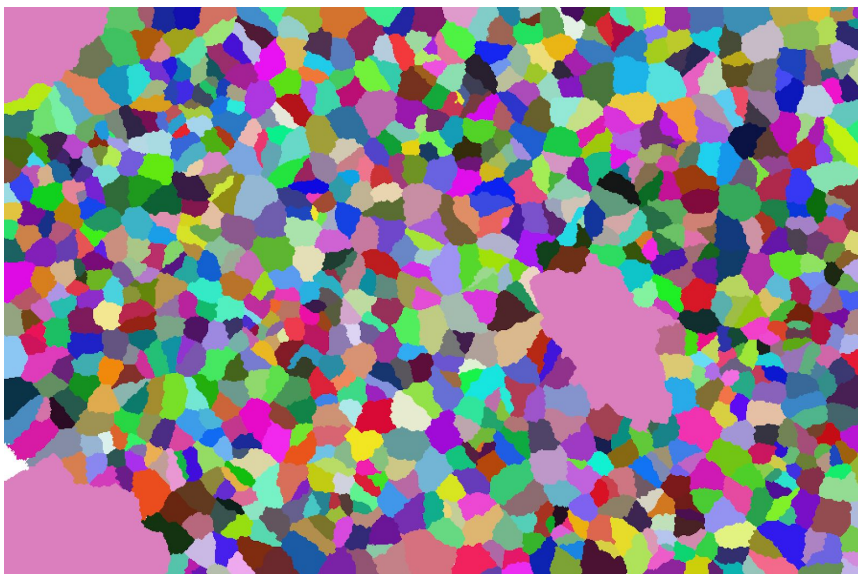
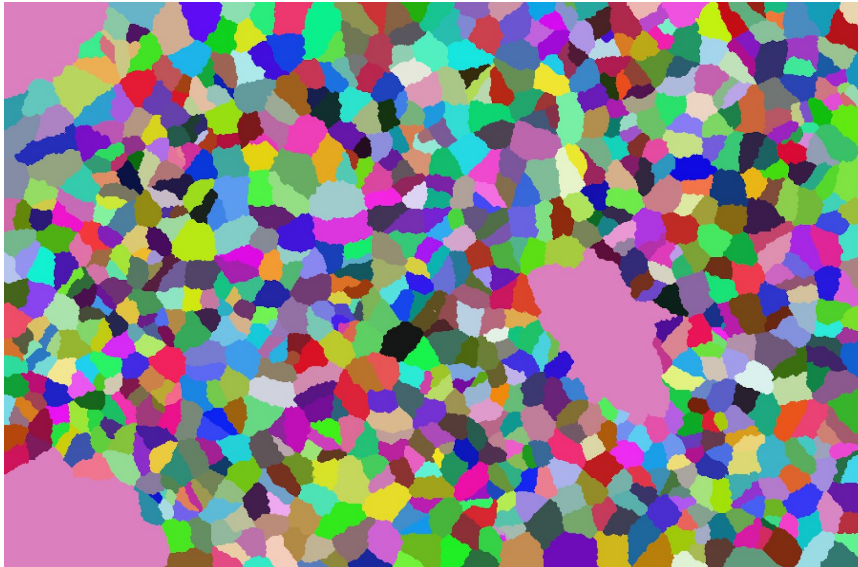
CA space 900x600, 1000 nucleons, curved grain boundaries



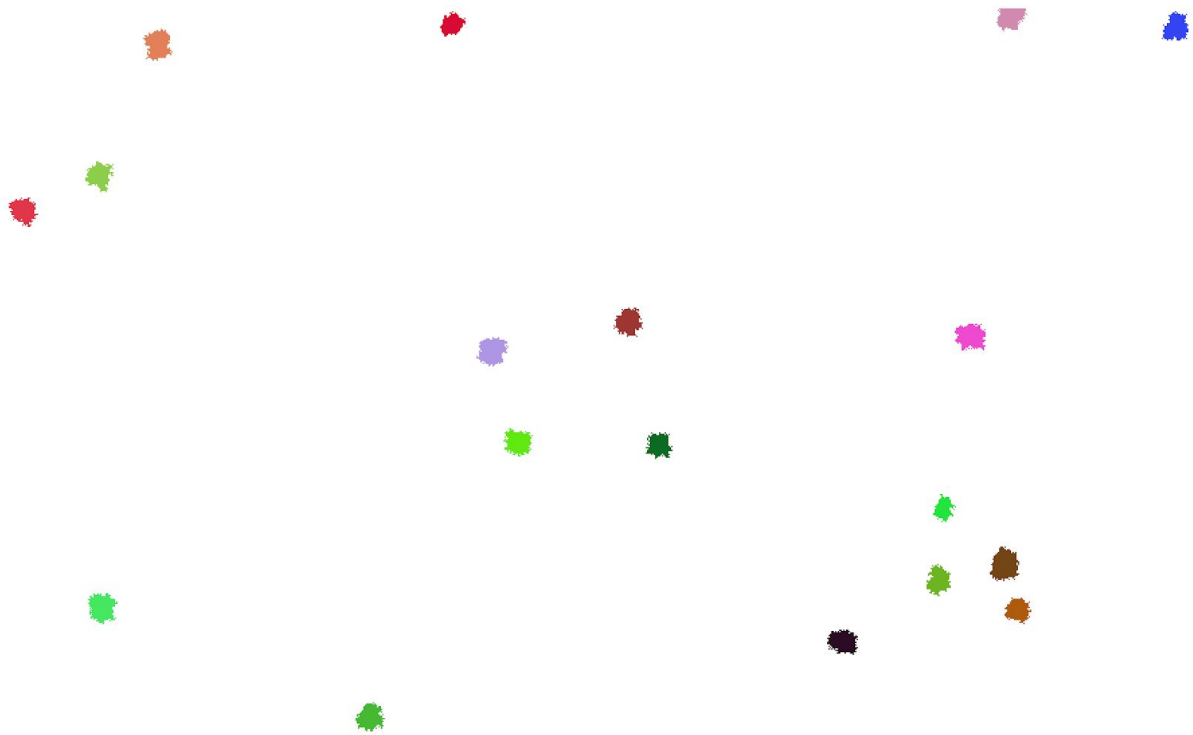
Boundries of the microstructure



Dual Phase Example on Above microstructure



Grain curvature growth



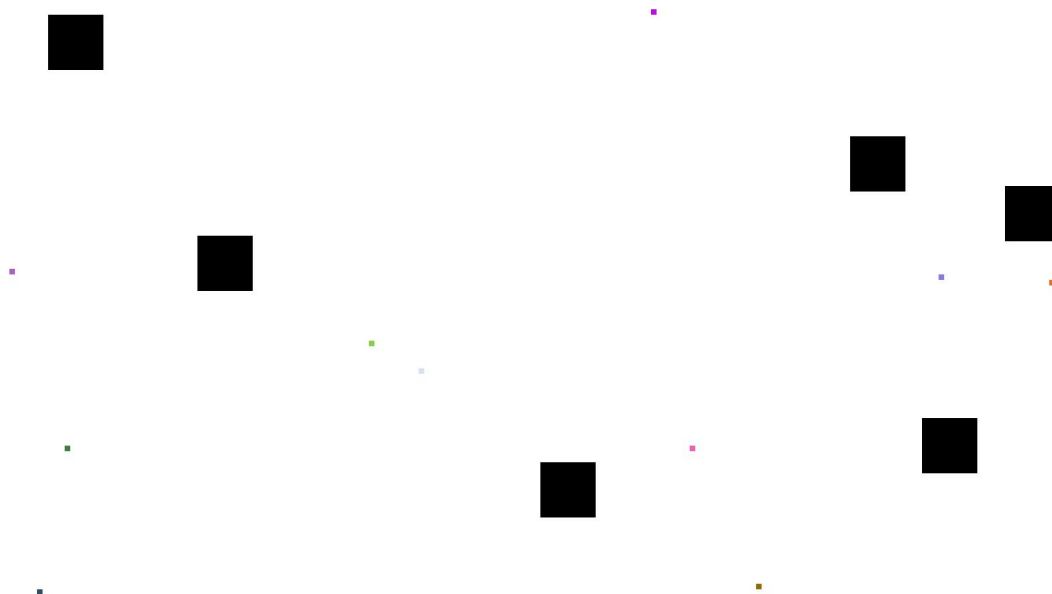
Fully grown



Inclusions on grain boundaries, smaller space, magnified pixel for better visibility
Circular after grain growth



Squared before before grain growth



Conclusion

Results are close to real microstructures, the output is similar to EBSD microstructures. Algorithm performance is good for the 300x300 CA space. It can also calculate bigger structures(900x600 in report) but it takes few minutes to compute. To achieve higher performance, some code would need to be rewritten to e. g. c++ to support multithreading.