Multiscale modelling – report

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1. Technology

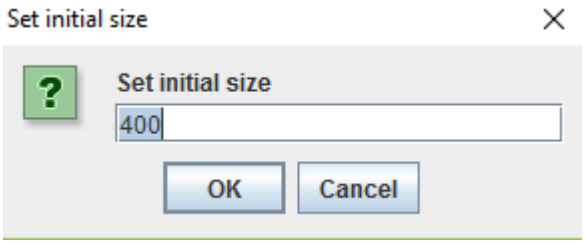
- Programming language: Java SE 8
- IDE: Intellij Community Edition 2016.3.4
- GUI implementation: JavaFX
- Applied design patterns: Strategy, MVC architecture
- Multithreading processing used

Explanation:
Currently, Java is one of the most popular programming languages and is widely used as a modern development technology. Apart of the popularity itself, I prefer this language among the others because of the portability and predefined set of high level libraries. It is also a kind of personal choice, considering my former experience with this technology.

2. GUI

a) Size input window

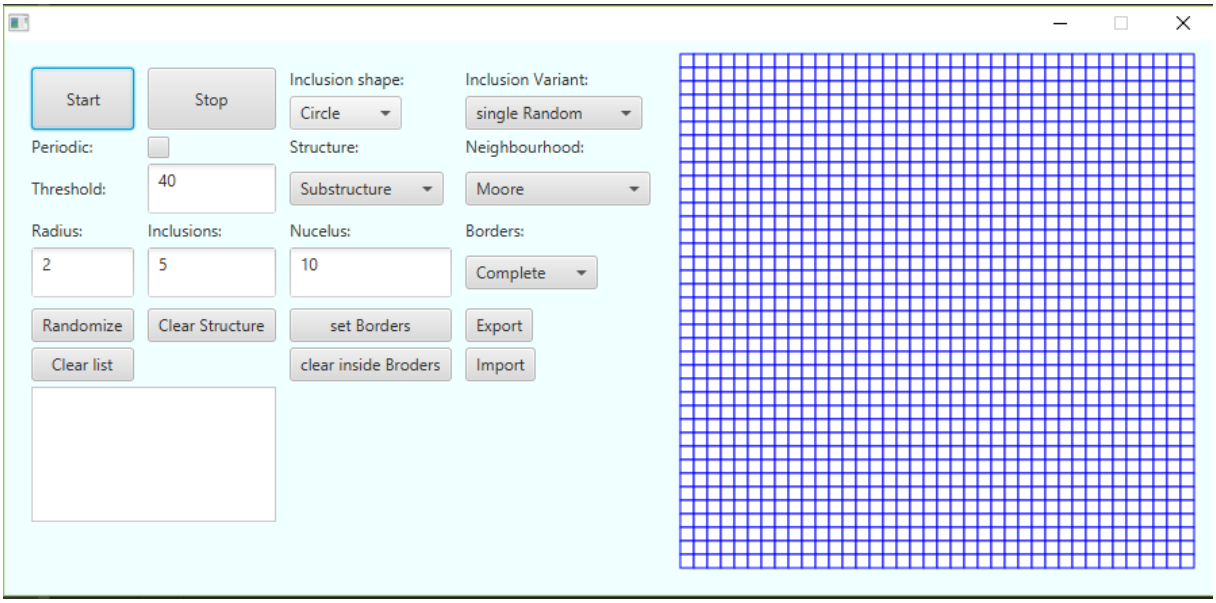
Graphical user interface consist of the main frame (2.2) and the initial size input window (2.1)



2.1 Initial size input window

Initial size should be set on the beginning of each application initialization, but this setting is not permanent across the application lifecycle, as the size of a frame could be also changed by importing the different schema. The size is configured by one dimension, determining the cell matrix in a form of a square.

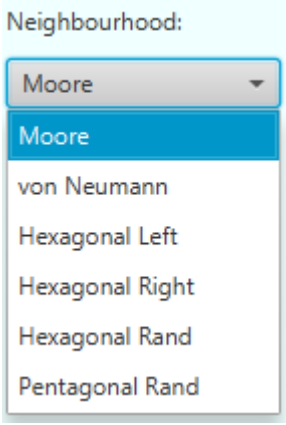
b) Main Frame



2.2 Main application frame

Components accessible on a frame could be grouped in a set of features:

- Lab 1: Simple grain growth:
    - Neighborhood ComboBox:
      This component is a list of choice of accessible neighborhood types (2.2)



2.2 Neighborhood

    - Randomize Button
      This button verifies the value of Nucelus EditBox and generating the appropriate amount of nucleuses randomizing their initial position between all the free cells

    - Nucleus EditBox
      This Edit Box determines the amount of initial nucleuses to be randomly allocated

- Start Button
  This button starts the multithreaded nucleus growing process, or start the process again after stopping it manually

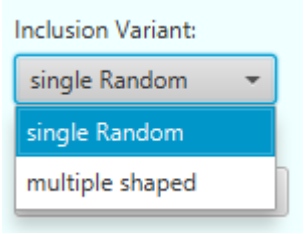
- Stop Button
  This button has been implemented to stop the nucleating operation on demand

- Export Button
  Export button has been created to save the workspace state to BMP or TXT formats. It activates the choice window, which make us able to specify the direct path of the exported file. If the target extension will be different than BMP or TXY, validation will fail and exception will occur.

- Import Button
  Importing is similar to the exporting process, as it also consider the extension validation. Additionally, if the target artifact contains a different matrix size, the main frame will automatically rescale accordingly to the imported BMP or TXT file.

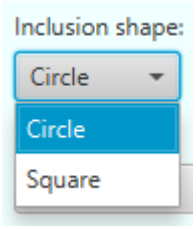
- Periodic CheckBox
  This checkbox is responsible for activating/disabling the periodic grain grow feature. If the checkbox is active, grains will grow independently of the borders, and will be reflected across the cells scope when crossing outside the matrix dimension

- Lab 2: Inclusions
  - Inclusion Variant ComboBox
    This combo box is responsible for specifying the appropriate variant of inclusion, choosing between “single random” and “multiple shaped” (2.3). “Single random” strategy is initializing the desired amount of inclusions as a single inclusion cells, without the ability to grow or being overridden. From the other hand, “Multiple shaped” is dedicated to create inclusions of desired shape (2.4), which could be chosen between the square and a circle.



2.3 Inclusion variant

- Inclusion Shape ComboBox
  This ComboBox make us possible to choose the desired shape of inclusion, which could be chosen between the circle and a square. This component work only with “multiple shaped” strategy of Inclusion Variant.



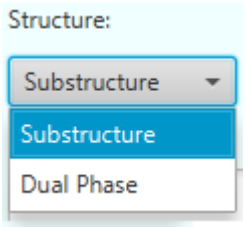
2.4 Inclusion Shape

- Radius EditBox
  Basing on this EditBox we are able to specify the radius of a Multiple Shaped inclusion.

- Inclusion EditBox
  EditBox dedicated to choose the amount of generated inclusions. It affects both of the strategy types.

- Lab 3: Moore neighborhood extension
  - Threshold EditBox
    According to this EditBox, we are able to specify the threshold used for 4^{th} grain grow rule purposes. In other words, the number placed under this component determinates a probability for cell to be changed when the last grow rule will be applied.

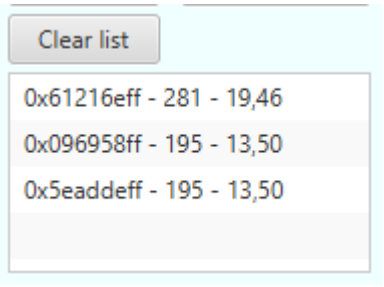
- Lab 4: Different microstructure types
  - Structure ComboBox
    ComboBox dedicated for the choice of the structure (2.5). By specifying the “Substructure” option we are able to simply exclude the chosen colors of grains and leave the rest untouched. The second option, named “Dual Phase”, is designed to additionally set the color of untouched structures to the specified one.



2.5 Structure

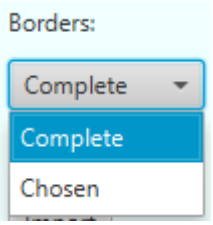
- Clear Structure Button
  Using this button we are able to clear all previously selected colors, leaving the rest of a grains without any impact, which make us possible to customize the grain grow

- Clear List Button
  This button is responsible for clearing the list of colors (2.6) specified to be removed. All such colors are collected in a list component, providing the information about the color id, and the amount & percentage of cells usage from the whole matrix perspective



2.6 List of selected colors

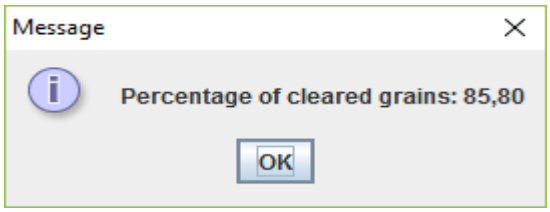
- Lab 5: Grain boundaries selection
  - Borders ComboBox
    The Borders ComboBox is a way of choosing the borders creation strategy (2.7); if the “Complete” variant will be chosen, the border will be created across all the grains. From the other hand, the “Chosen” option will be specified, border will surround only the manually pointed colors.



2.7 Borders

  - Set Borders Button
    This button is responsible for creating the borders. Could be used always after the nucleation process will be finished. It will create the borders according to the strategy specified in a Borders ComboBox

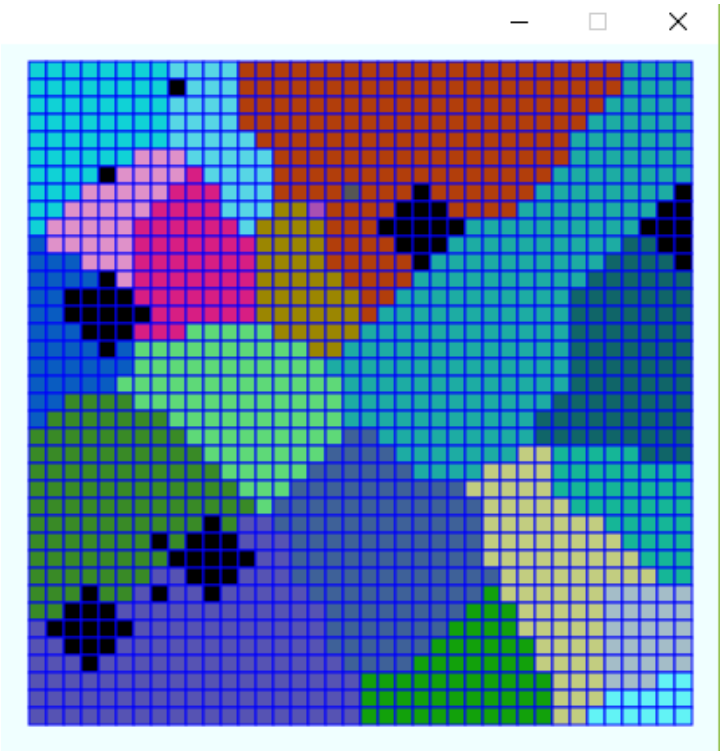
- Clear Inside Borders Button
  Is an additional feature clearing the space inside the created borders, and displaying the percentage of released space (2.8)



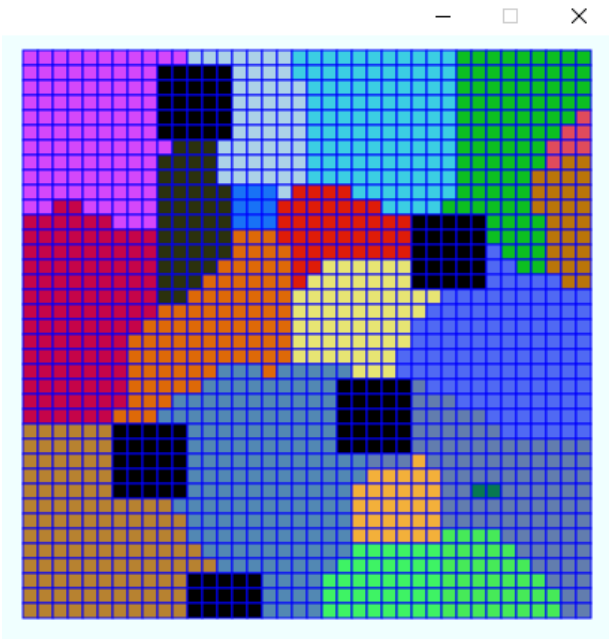
2.8 Alert containing the percentage of a cleared space

3. Example results

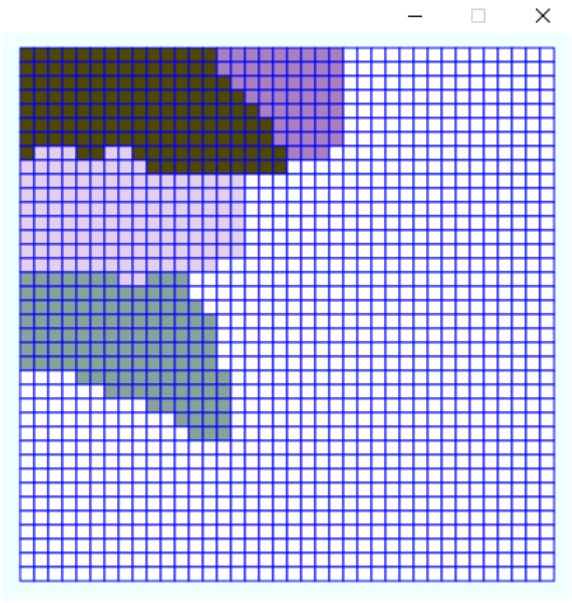
- Circle Inclusions
  This example consist of the simulation including the both types of inclusions, which means the single inclusions and the “multiple shaped” with the shape of circle. Initial amount of the inclusions has been set to 5, and it refer to both of the types independently. Inclusion radius is set to 2.



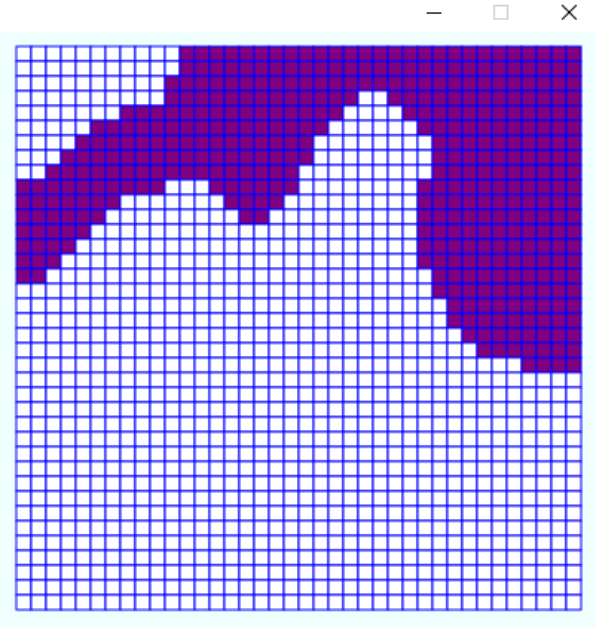
- Square Inclusions
  This screenshot contains the example of generating square-shaped “multiple shaped” inclusions, with the radius equal 2. Initial number of inclusion has been set to 5.



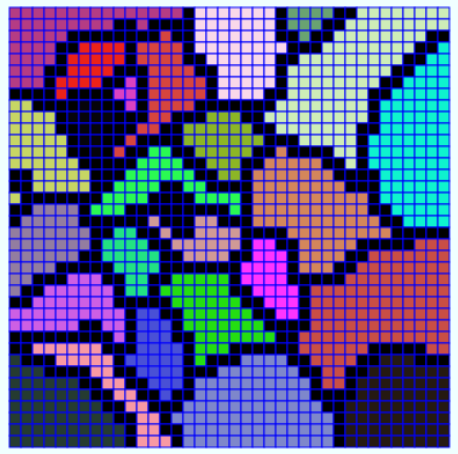
- Substructure
  This example presenting the usage of Substructure feature usage. After generating the grains, the specified amount of colors has been pointed manually, and cleared from the matrix by clicking the “Clear Structure” button. The chosen colors are listed in a list of colors.



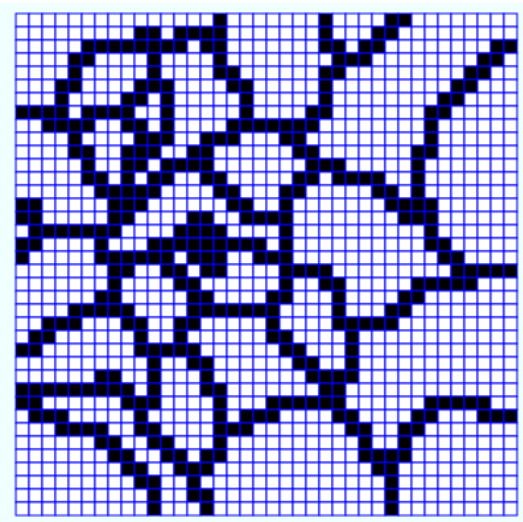
- Dual Phase
  This is the example of using “Dual Phase” structure variant. After generating the grains the specified colors has been indicated manually and listed under the list of colors to be cleared. After selecting the “Dual Phase” structure option and clicking “Clear Structure” button, all not cleared grains has been set as one purple structure.



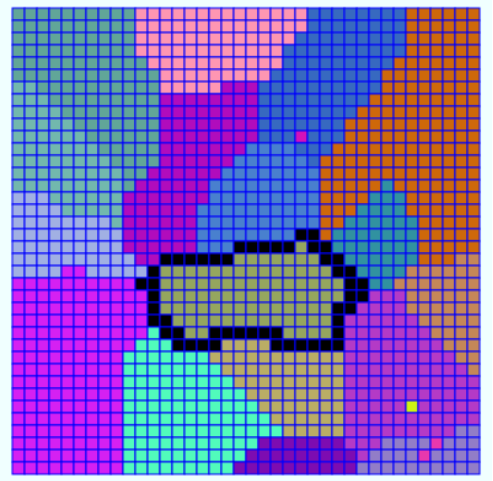
- Full Borders
  In this example I would like to present the usage of Complete borders generation variant. After generating the grains, choosing “Complete” from the Borders ComboBox and confirming by clicking “set Borders” button, all cells whose neighborhoods contains the different colors has been transformed into black.



- Empty Borders
  This screenshot contains a modification of previous full borders generation mode, but in this example all grains have been cleared and only the borders left intact. After removing the core of a grains, we would be able to regenerate the grains and continue the grain grow simulation within specified limitations



- Partial Borders
  This example is an presentation of “Chosen” variant of Borders specification. By choosing this type of borders, manually indicating the colors and confirming the operation via “set Borders” button after generating the grains, we would achieve the result of one grain surrounded by the black-painted border

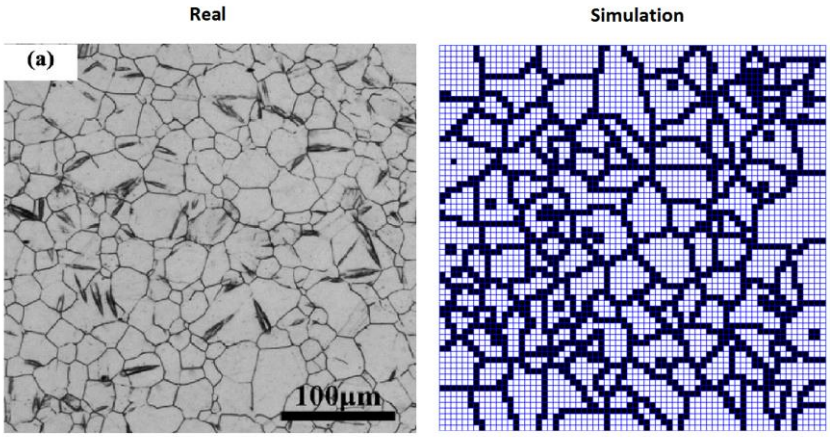


- Exported Matrix

  This example demonstrating the output of the matrix export process. Left part contains the snapshot of the matrix exported to the txt file, and the right one is a screenshot of newly exported bmp.

```
38
0-0-0x543f7eff
0-1-0x543f7eff
0-2-0x543f7eff
0-3-0x543f7eff
0-4-0x543f7eff
0-5-0x543f7eff
0-6-0x543f7eff
0-7-0x543f7eff
0-8-0x543f7eff
0-9-0x543f7eff
0-10-0x543f7eff
0-11-0x543f7eff
0-12-0x543f7eff
0-13-0xe2649aff
0-14-0xe2649aff
0-15-0xe2649aff
0-16-0xe2649aff
```

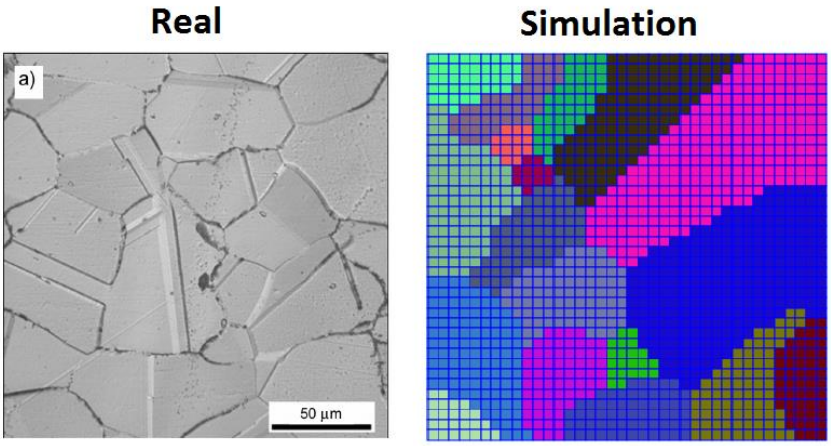
4. Comparison with the real structures



3.1 Austenite microstructure #1

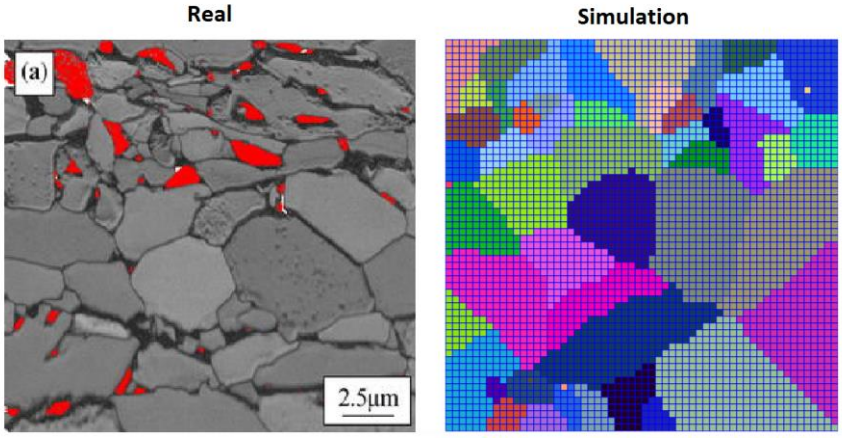
Comment:
The Nano/ultrafine-grained (Nano/UFG) structure was obtained in Fe-17Cr-6Ni austenitic steel using a combination of severe cold deformation and reverse-transformation annealing.

Ref: https://www.researchgate.net/figure/The-microstructure-of-the-solution-treated-as-received-austenitic-stainless-steel_fig1_305922578



3.2 Austenite microstructure #2
Comment:
standard austenitic stainless steel (1.4841, Böhler H525)

Ref: https://www.researchgate.net/figure/Microstructure-of-the-materials-investigated-a-austenite-b-Fe-Cr-C-B-complex-alloy_fig1_233812884



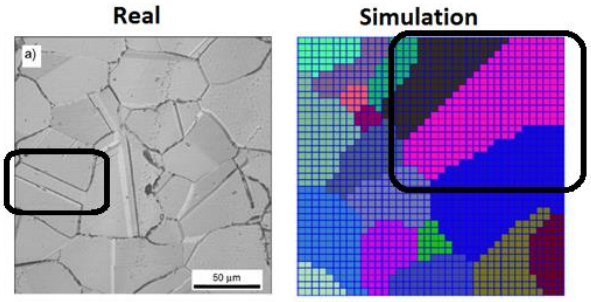
3.3 Austenite microstructure #3
Comment:
EBSD analysis of retained austenite distribution in the experimental steel before tensile deformation

Ref: http://www.amse.org.cn/article/2014/1006-7191-27-3-389.html

5. Conclusions

According to the comparison, we are able to draw the following conclusions:

- Application could be used to simulate grain grow from the various perspectives (100,50 or 2.5 um)
- We could simulate various sizes of a grains, f.e. small grains (3.1), big and medium grains (3.2) and also the mixed-sized microstructures(3.3)
- We are able to simulate grains with the one dominating dimension, according to 3.3



- In some cases the grains didn't nucleated, as these were too close to the neighborhoods which were showing the greater tendencies to grow.

Basing on the mentioned conclusions it can be stated that the application meets the requirements of a project and could be used to successfully simulate the grow of a grains