



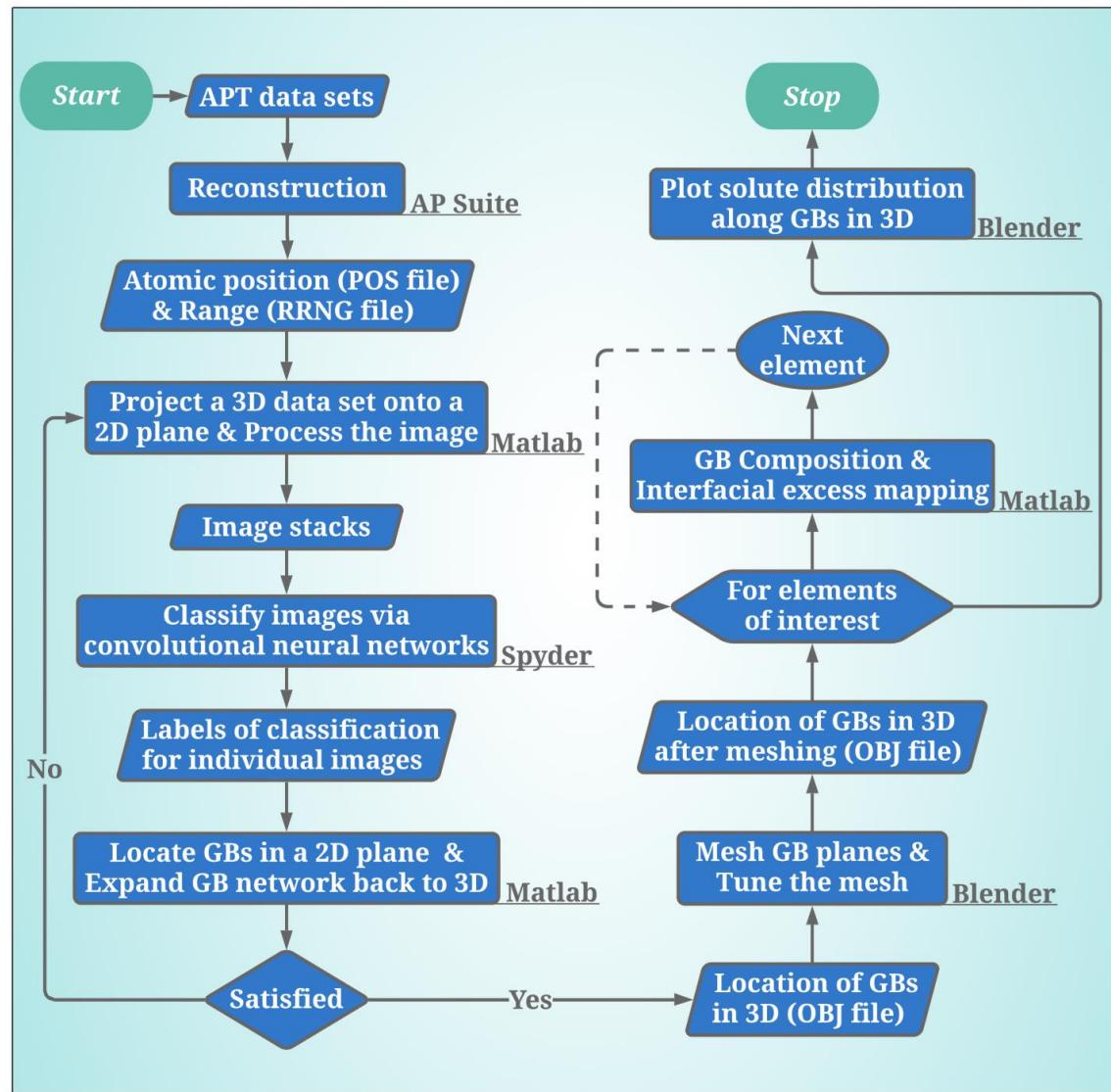
0. Introduction

0. 1. Atom probe tomography _ grain boundary (APT_GB)



- Grain boundaries (GBs) are planar lattice defects that govern the properties of many types of polycrystalline materials. Hence, their structures have been investigated in great detail. However, much less is known about their chemical features, owing to the experimental difficulties to probe these features at the atomic length scale inside bulk material specimens. Atom probe tomography (APT) is a tool capable of accomplishing this task, with an ability to quantify chemical characteristics at a near-atomic scale. Using APT data sets, we present here a machine-learning-based approach for the automated quantification of chemical features of GBs. We trained a convolutional neural network (CNN) using twenty thousand synthesized images of grain interiors, GBs, or triple junctions. Such a trained CNN automatically detected the location of the GBs from APT data. Those GBs are then subjected to compositional mapping and analysis, including revealing in-plane chemical patterns.
- The whole process has been interpreted in this software package. We provide graphical interfaces for all analysis procedures. The details for each step are documented in the following slides with an synthetic data set as an example. The software package “APT_GB” is available via the GitHub link: https://github.com/RhettZhou/APT_GB.
- Please use, edit and distribute it freely! Please do not use it for commercial purposes!

0. 2. Workflow for the in-plane grain boundary composition analysis approach



Flow chart summarizes the steps of machine learning - enhanced mapping of GB composition and interfacial excess from APT data sets. 'AP Suite' refers to the atom prober's toolkit for data analysis workstations. Matlab is a numerical computing environment developed by MathWorks, Inc. Spyder is an open-source integrated development environment (IDE) for scientific programming in Python. Blender is an open-source computer graphics software. POS is an APT file format for the atomic positions and their respective mass-to-charge-state ratios. RRNG is a range file format identifying the chemical information of each ion species in APT data by associating an element with its mass-to-charge-state ratios. OBJ is a geometry definition file format. 2D and 3D refer to two- and three dimensions, respectively.

Xuyang Zhou, Ye Wei, Markus Kühbach, Huan Zhao, Florian Vogel, Reza Darvishi Kamachali, Gregory B. Thompson, Dierk Raabe, Baptiste Gault, Revealing in-plane grain boundary composition features through machine learning from atom probe tomography data, Preprint arXiv (2021)



1. Installation

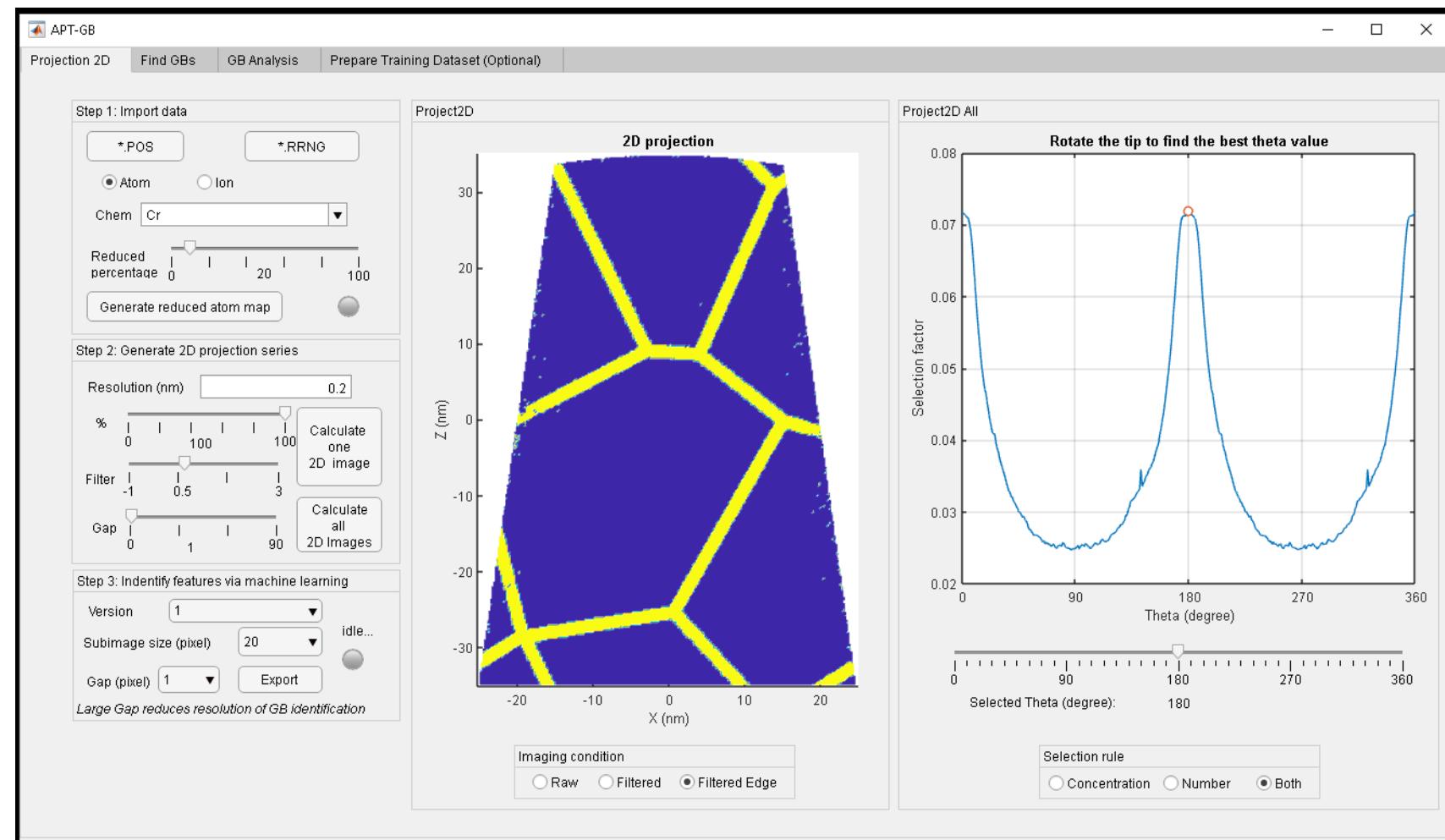
-- Installation and application applies to Windows 10 computer system

1. 1. Installation - Matlab



Version: Matlab 2018a

- The program was developed in Matlab **2018a**. But users do not need to have Matlab installed on their computer.
- It works by installing the program ("..\APT_GB.exe") on the local computer.
- The right image shows the interface of the installed program "APT_GB". Details on the individual control panels can be found in section 2.



1. 2. Installation - Blender



Version: Blender 2.92.0

A. Download (version 2.92.0): link: <https://download.blender.org/release/>

Blender2.90/	23-Sep-2020 09:13	-
Blender2.91/	01-Feb-2021 19:47	-
Blender2.92/	25-Feb-2021 12:03	-
Blender2.93/	02-Jun-2021 14:22	-
BlenderBenchmark1.0/	17-Aug-2018 12:31	-
BlenderBenchmark2.0/	20-Jan-2020 14:19	-
Publisher2.25/	20-Aug-2003 11:13	-
plugin/	23-Nov-2004 12:56	-
yafray.0.0.6/	03-Feb-2004 22:31	-
yafray.0.0.7/	05-Aug-2004 10:33	-
GPL-license.txt	19-Aug-2013 11:54	17997
GPL3-license.txt	19-Aug-2013 11:54	35147
blender2.04-ipaq.zip	20-Aug-2003 11:14	2048262

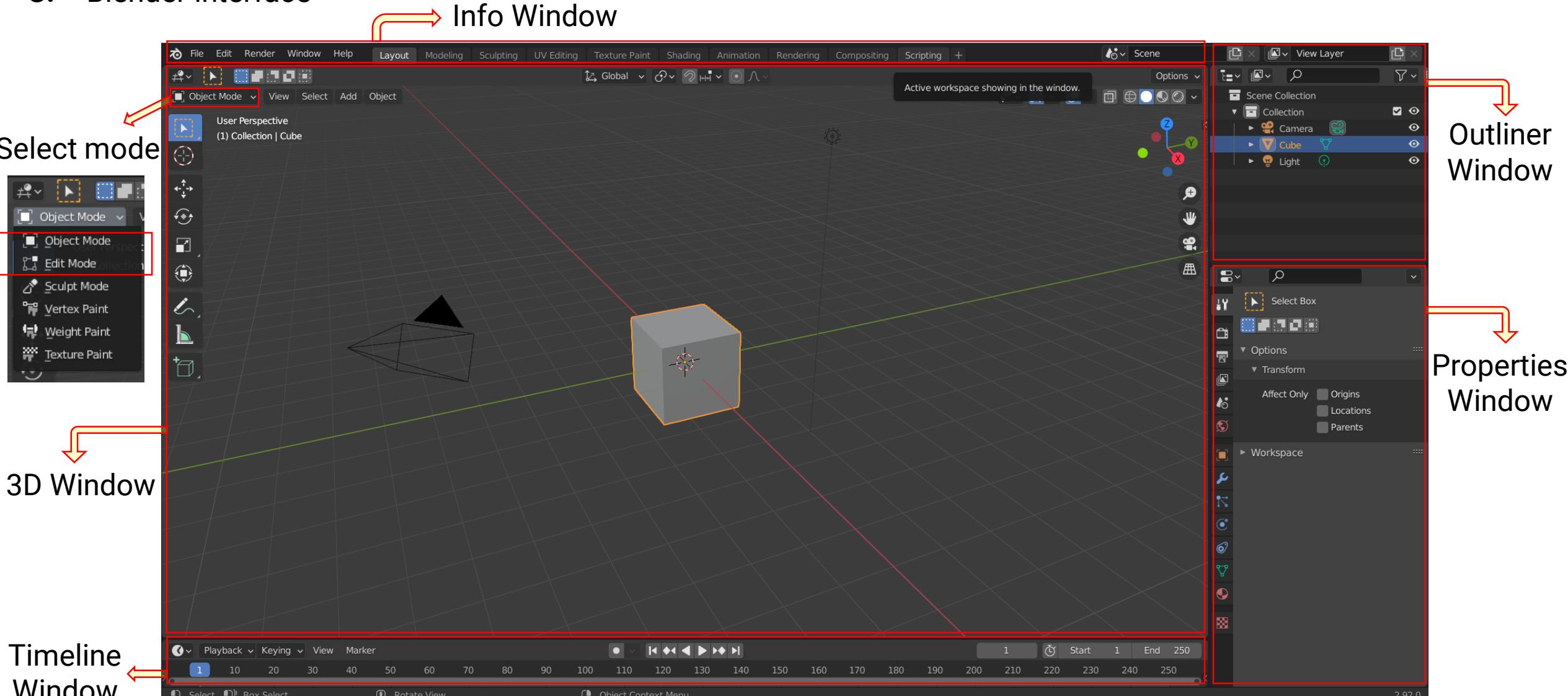
B. Installation:

- Default path: C:\Program Files\Blender Foundation\Blender 2.92\
(!Please do not change the path for installing Blender!)



1. 2. Installation – Blender (continue 1)

C. Blender interface





1. 2. Installation – Blender (continue 2)

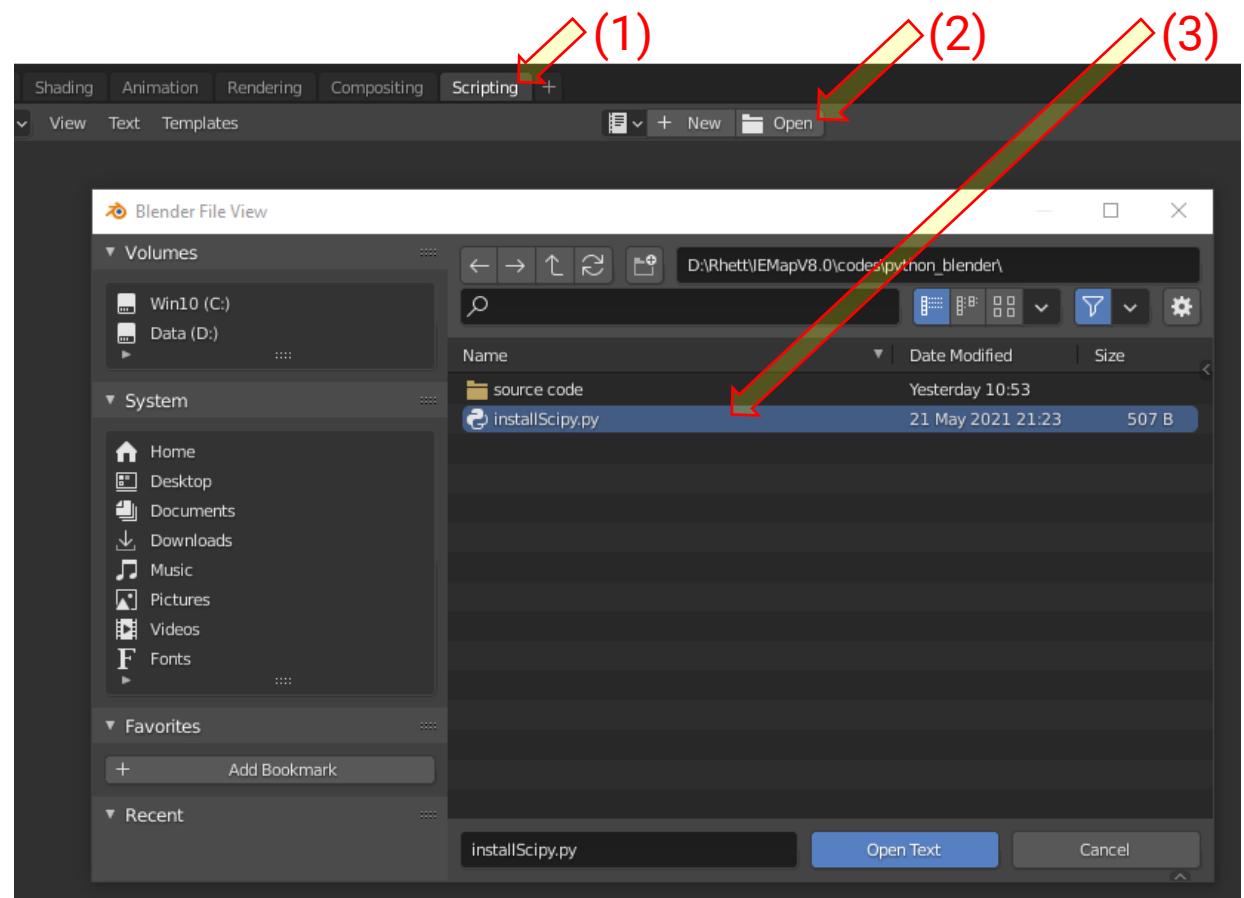
D. Install “Scipy” library

- Run Blender as administrator
- Info Window -> Click Scripting (1)
- Click Open (2)
- Select “installScipy.py” (3)

The location of this file is

(“..\\installScipy.py”)

- Click ► Button (4)
- Wait and Done (The color of ►Button will change once the process is done. ~1 min.)



```
1 import sys
2 import subprocess
3
4 py_exec = sys.executable
5 py_prefix = sys.exec_prefix
6 # ensure pip is installed & update
7 subprocess.call([str(py_exec), "-m", "ensurepip", "--user"])
```

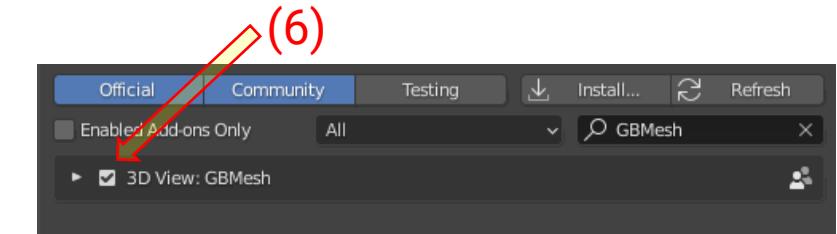
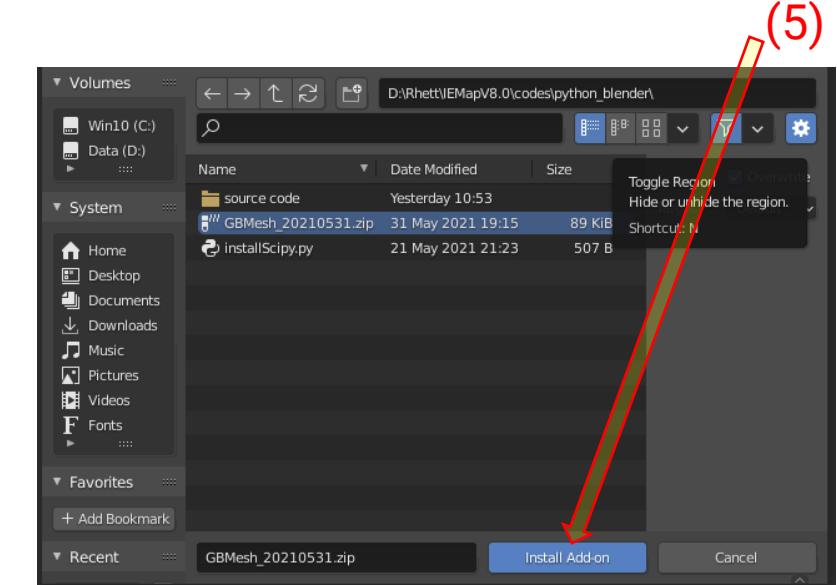
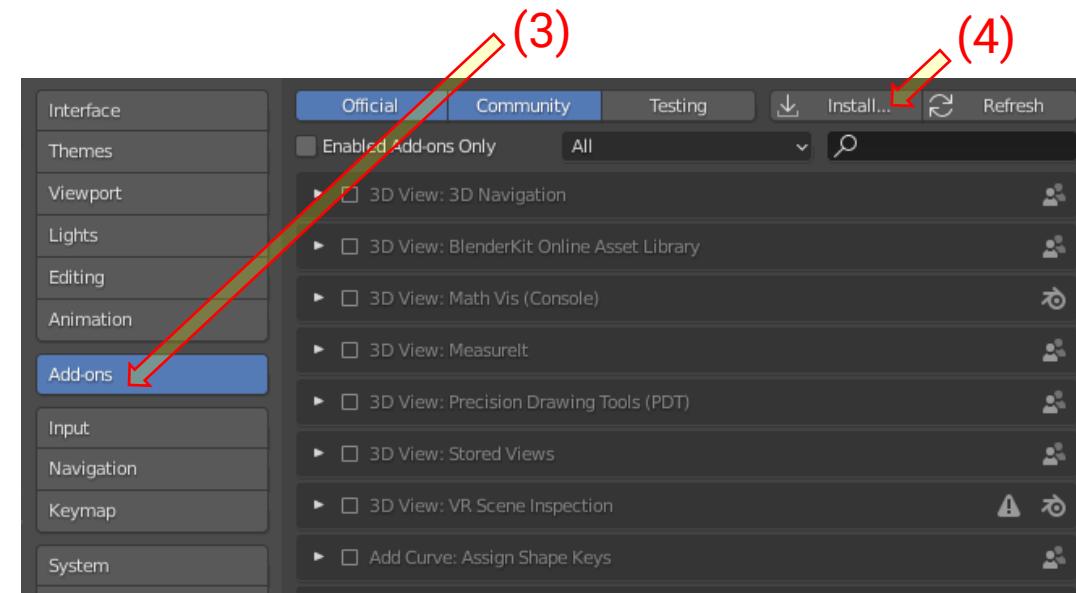
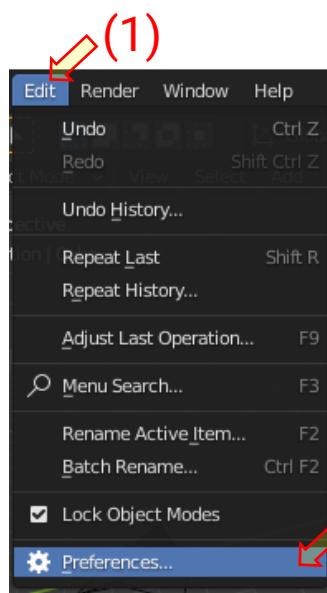


1. 2. Installation – Blender (continue 3)

E. Install “GBMesh” add-on

- Info Window -> Edit (1)
- Select Preferences (2)
- Select Add-ons (3)
- Click Install... (4)

- Select “GBMesh_20210531.zip” and click “Install Add-on” (5)
(..\GBMesh_20210606.zip)
- Check the box “3D View: GBMesh” (6)





2. How to use?

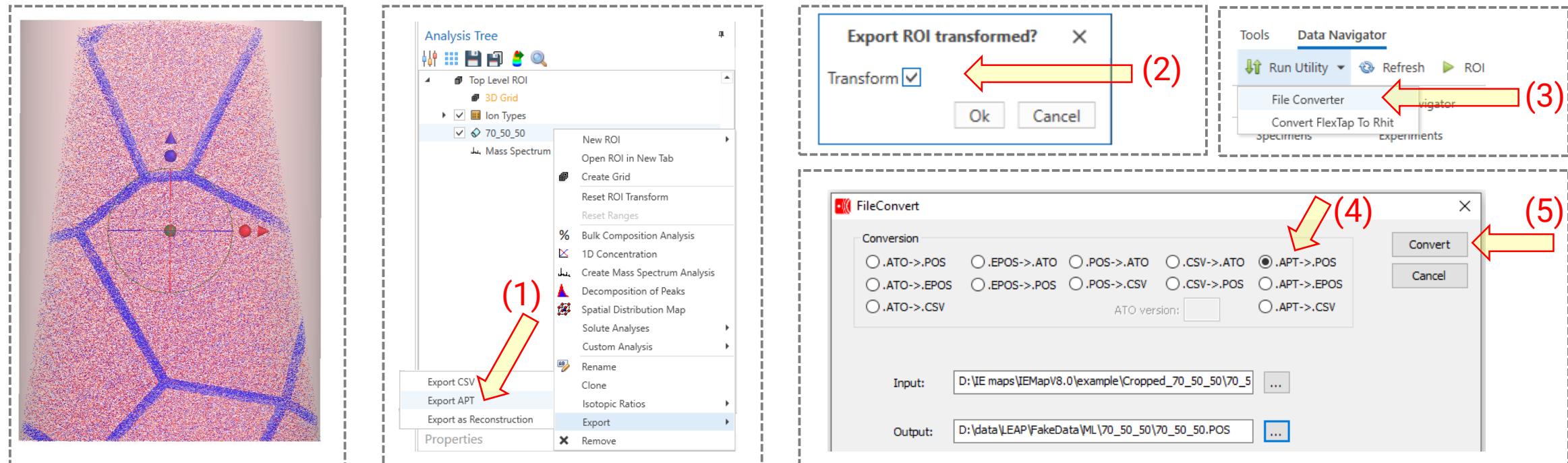
2. 1. Have an atom probe data set (AP Suite 6.1)

A. Import the synthetic data set to AP Suite 6.1

- POS file ("..\example\Synthetic_500_500_700_4\700_500_500_4.POS")
- RRNG file ("..\example\Synthetic_500_500_700_4\AB.RRNG")

B. Cut a cylinder region (with orientation like bottom left. The data must be columnar with the columnar grains normal to the Z-axis of the cylinder)

C. Export a “*.APT” file, as shown by red arrow (1), check Transform (2)



- APT file ("..\example\Crop ped_70_50_50\70_50_50.apt")
- Convert the APT file to a POS file, red arrows (3-5)
- POS file ("..\example\Crop ped_70_50_50\70_50_50.POS")

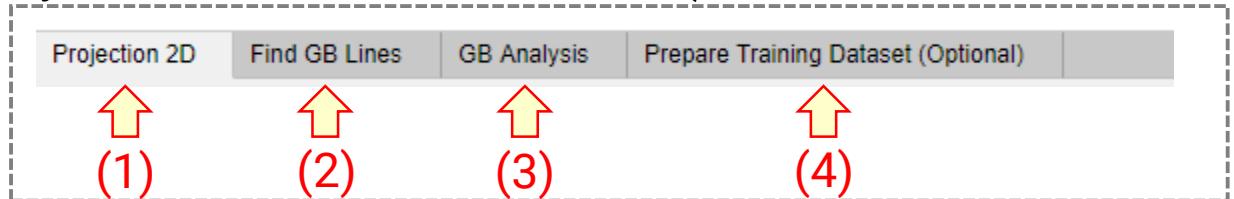
2. 2. Program interface for atom probe tomography – grain boundary (APT_GB) analysis (Matlab 2018a)



Open the installed program "APT_GB" from Desktop Shortcut or Windows Menu

This program is structured in a task-oriented way. Six steps are required to perform the analysis, which are distributed over the panels "Projection 2D" (1), "Find GBs" (2), and "GB Analysis" (3). The hidden step(s) will appear once the required previous step is done. Here, we briefly present the steps in each panels.

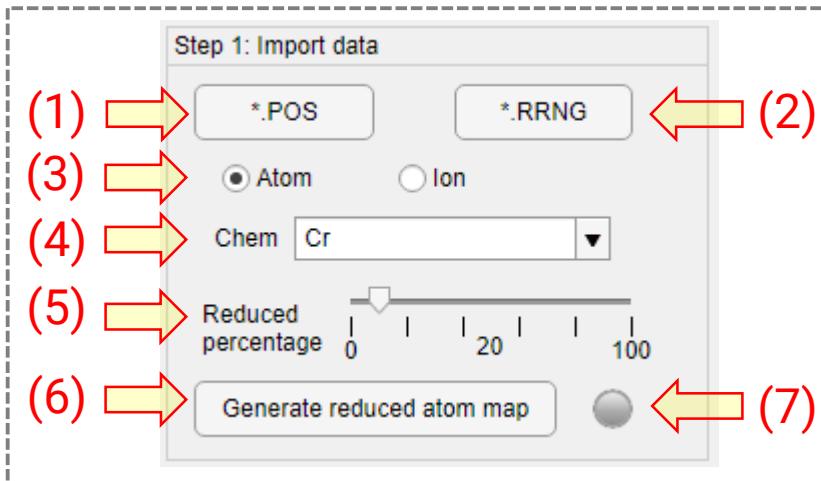
- Panel "Projection 2D" (1): This panel includes three steps: 1. import atom probe data; 2. generate an individual 2D projection and projection series; 3. Image segmentation and feature identification via machine learning.
- Panel "Find GBs" (2): This panel has two steps: 1. display GB/Triple junctions after machine learning; 2. generate GB Meshes.
- Panel "GB Analysis" (3): The step in this panel is the GB analysis, which generates the composition and interfacial excess maps, as well as the visualization of the results.
- Panel "Prepare Training Dataset (Optional)" (4): In this panel, a new training dataset is created. This function in this panel is a optional as the software package already contains the trained dataset ("..\codes\matlab\source code\cnn\model.h5").



2. 3. Step 1 – Import data

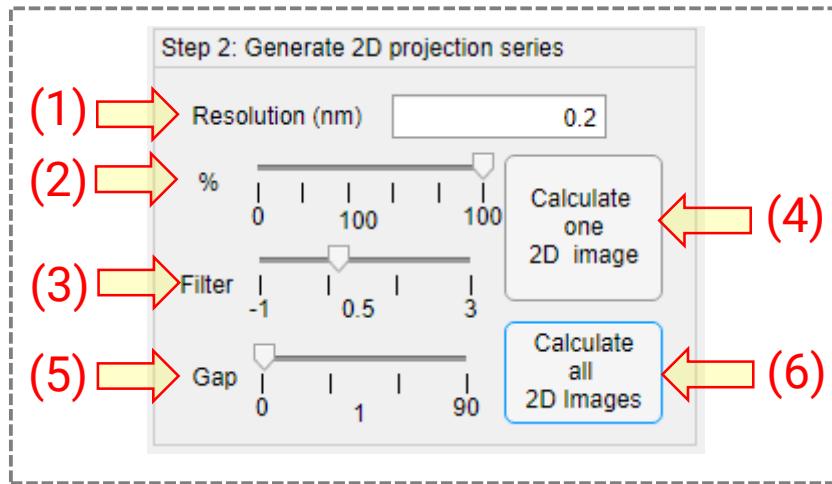


- Button “*.POS” (1): Click it to import an APT dataset for the atomic positions and their respective mass-to-charge-state ratios.
 (“..\\example\\Cropped_70_50_50\\70_50_50.POS”)
- Button “*.RRNG” (2): Click it to import a range file for identifying the chemical information of each atom/ion species in APT data by associating an element with its mass-to-charge-state ratios.
 (“..\\example\\Synthetic_500_500_700_4\\AB.RRNG”)



- After this step, an RNG file is automatically created. (“..\\example\\Cropped_70_50_50\\AB.rng”)
- Ratio Button group “Atom/Ion” (3): Click one of the two options to determine the preferred calculation.
- Drop Down “Chem” (4): Click the down-arrow to select the atom/ion specie for the following calculation.
- Slider “Reduced percentage” (5): Click to choose the percentage of atoms/ions to export for display in Blender. The number in the middle indicates the selected value (The same applies to the following Sliders).
- Button “Generate reduced atom map” (6): Click to execute. The purpose of this step is to generate a less dense point cloud for 3D imaging. (“..\\example\\Cropped_70_50_50\\blenderImaging\\70_50_50_atom_Cr_10%.pos”)
- “Lamp” (7): The lamp lights up green when the calculation is in progress. As soon as it is finished, it returns grey.

2. 4. Step 2 – Generate 2D projection series



- Edit Field “Resolution (nm)” (1): Enter the resolution for the projected 2D image. The unit is nm.
- Slider “%” (2): Click to select the percentage of atoms/ions used to generate the 2D projection image.
- Slider “Filter” (3): Click to select the image filter factor. We binarized the composition map by filtering the non-random distribution of solutes over a threshold T defined as

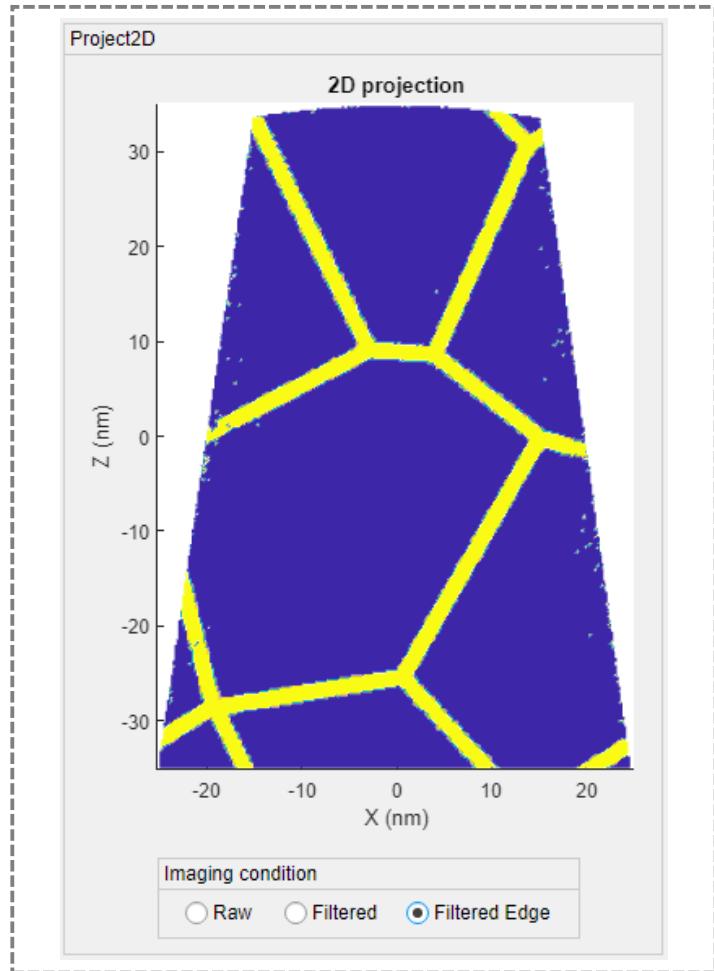
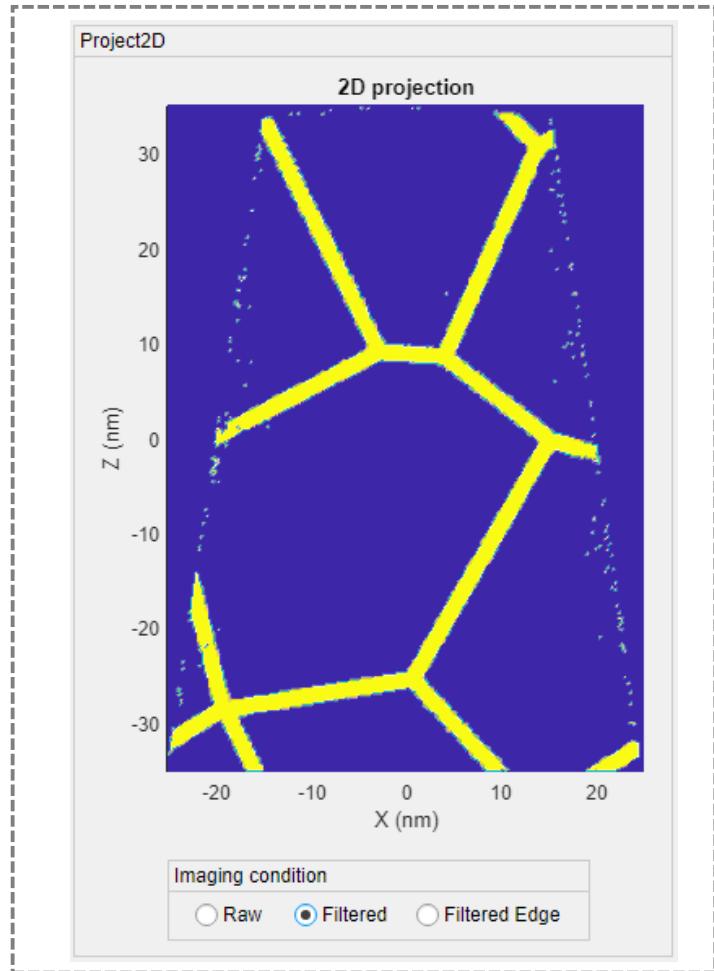
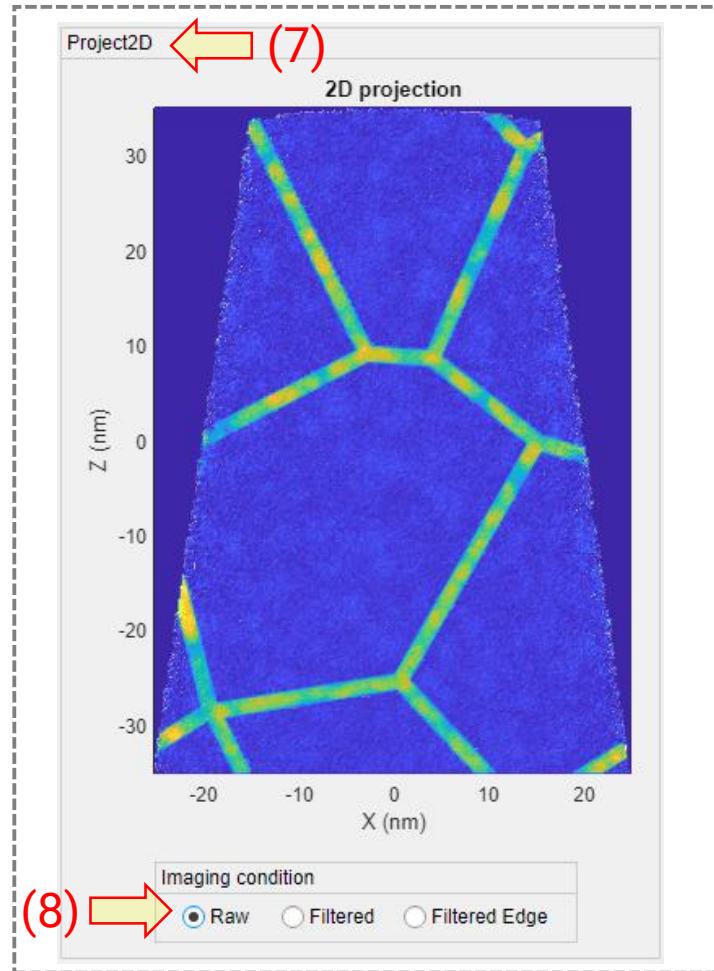
$T = \mu + k \times \sigma$, where μ corresponds to the mean composition for all pixels in the projected composition map, σ is the standard deviation among all pixels, and k is an adjustable number, here as the value of Filter.

- Button “Calculate one 2D image” (4): Click it to execute the calculation. Next page shows the result.
- Slider “Gap” (5): Click to choose the gap (degree) between each 2D projected image. The smaller the value is selected, the more 2D projection images will be created. The user could get a more accurate projection direction where GB edge-on configuration applies. However, more computing time is needed.
- Button “Calculate all 2D images” (6): Click it to perform the calculation. The two pages after next page shows the results.



2. 4. Step 2 – Generate 2D projection series (continue 1)

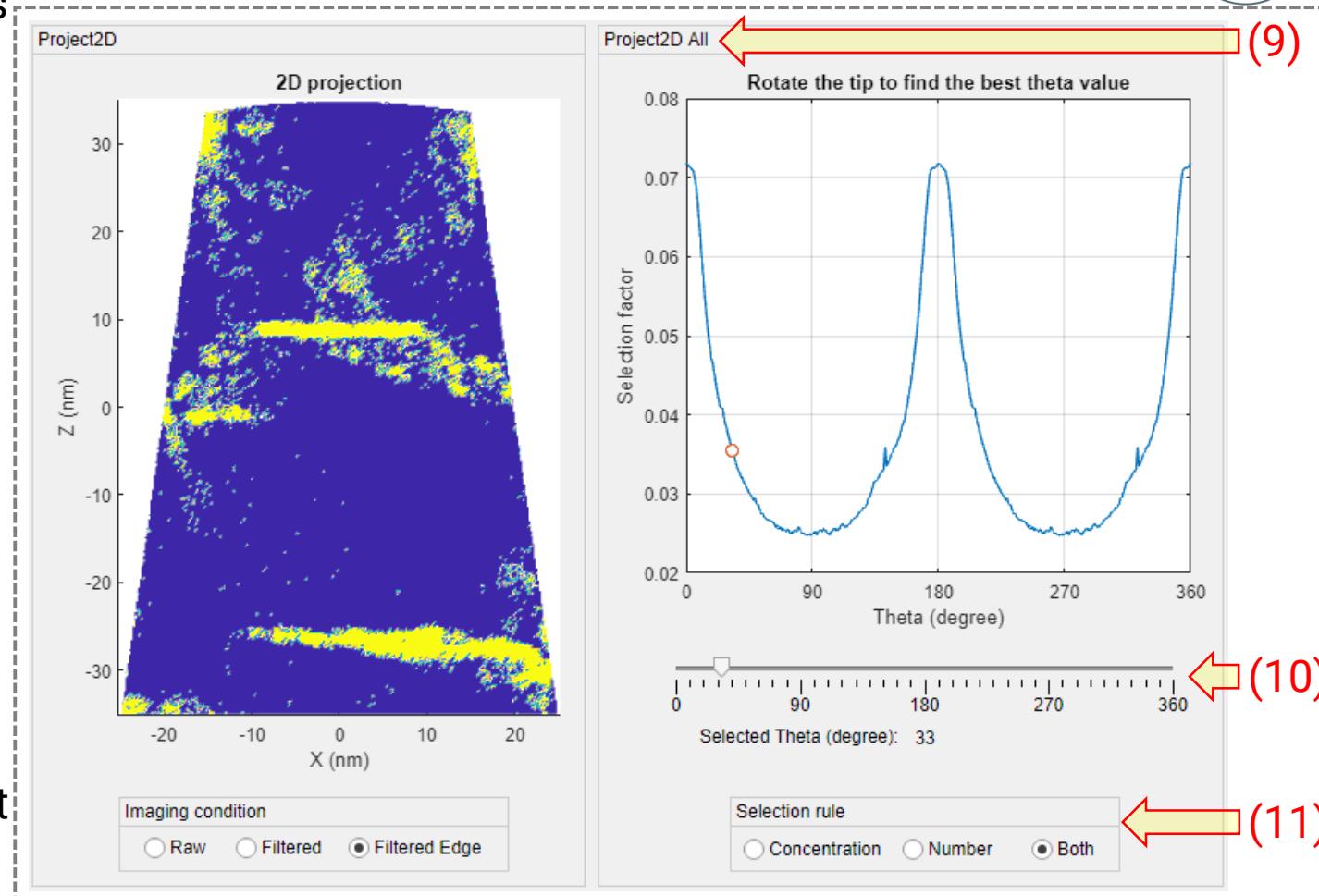
- Axis “Project2D” (7): The figure for this axis shows a projected 2D image.
- Ratio Button group “Imaging condition” (8): Option 1 – “Raw” is the raw composition map. Option 2 – “Filtered” shows the filtered image. Option 3 – “Filtered Edge” presents the filtered image with the blank areas removed.





2. 4. Step 2 – Generate 2D projection series (continue 2)

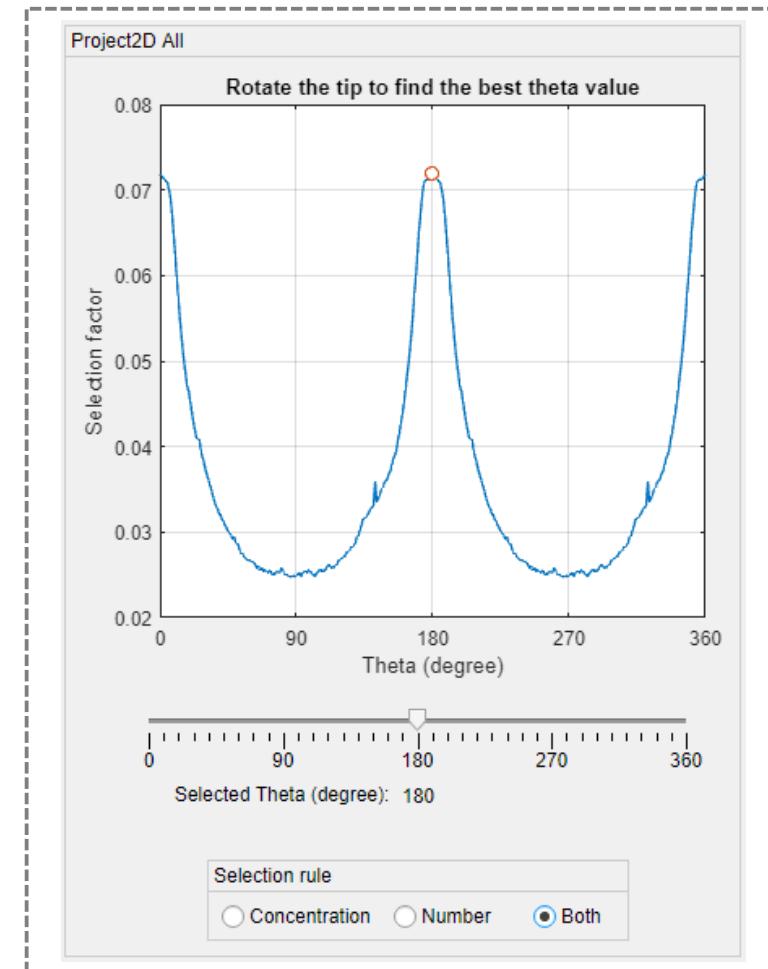
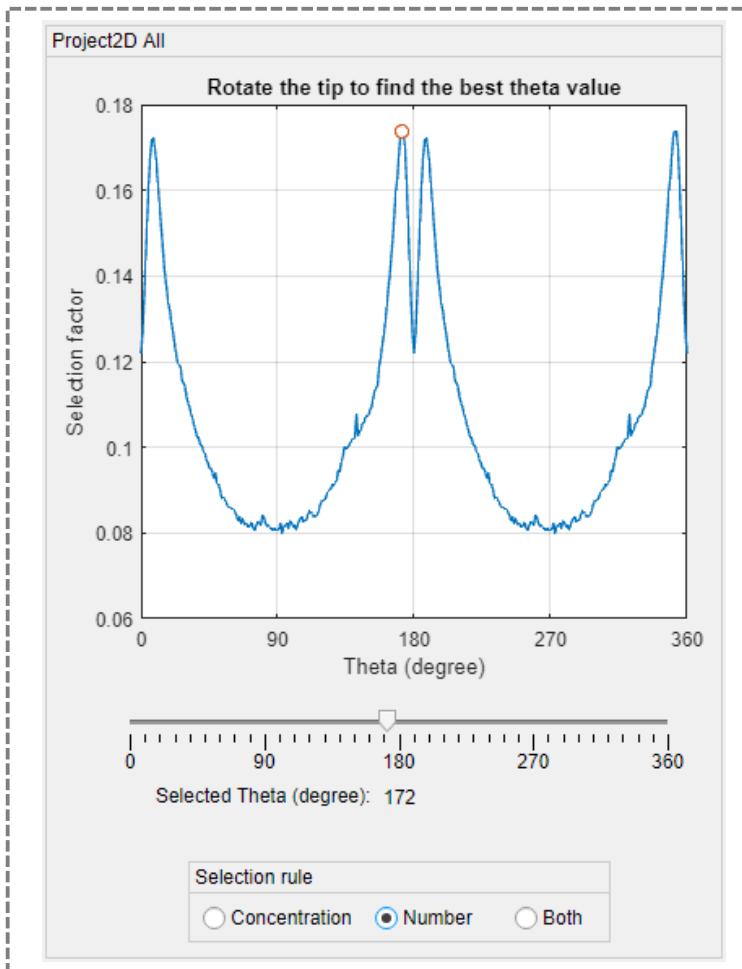
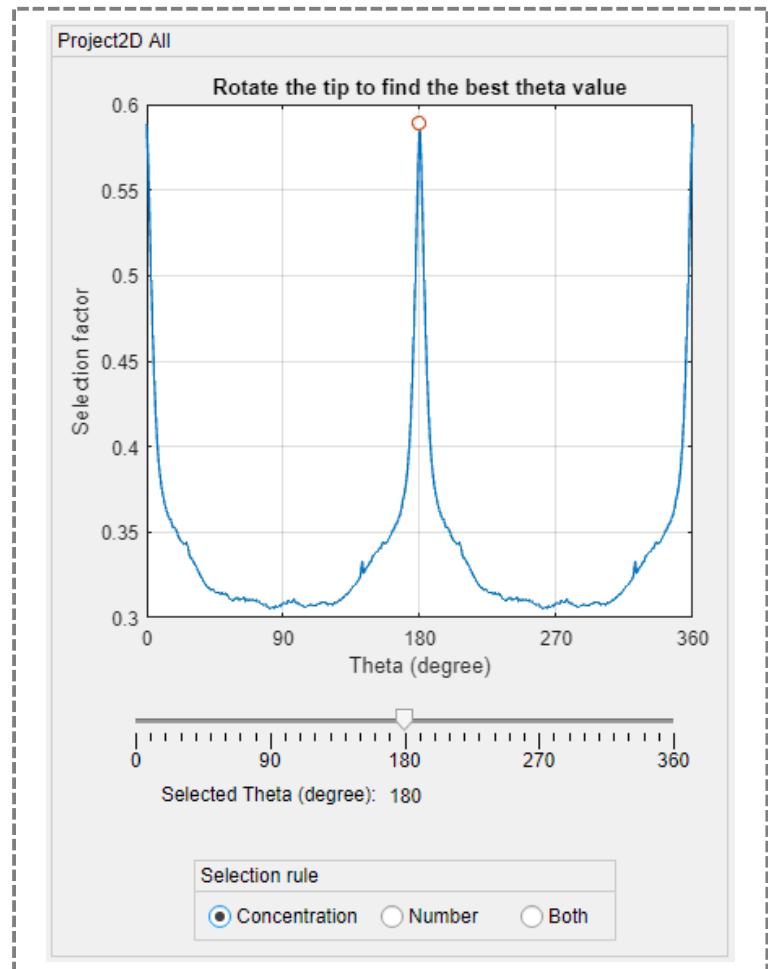
- Axis “Project2D All” (9): The graph for this axis shows the selection factors depending on the value of the rotation theta.
- Slider “Selected Theta (degree)” (10): Click this slider to manually select the best rotation theta value for the GB Edge-on configuration. The image in the “Project2D” axis is automatically updated.
- Ratio Button group “Selection rule” (11): The ideal theta value for the GB edge-on configuration is determined based on different selection rules. Option 1 – “Concentration” gives the average composition of the filtered pixels. Option 2 – “Number” counts the ratio of remaining pixels to all pixels. Option 3 – “Both” used the product of the values from Option 1 and Option 2.



2. 4. Step 2 – Generate 2D projection series (continue 3)



- Axis “Project2D All” shows the ideal theta value for GB edge-on configuration that has been determined based on different selection rules. We have provided multiple selection rules as the real APT can be complicated.

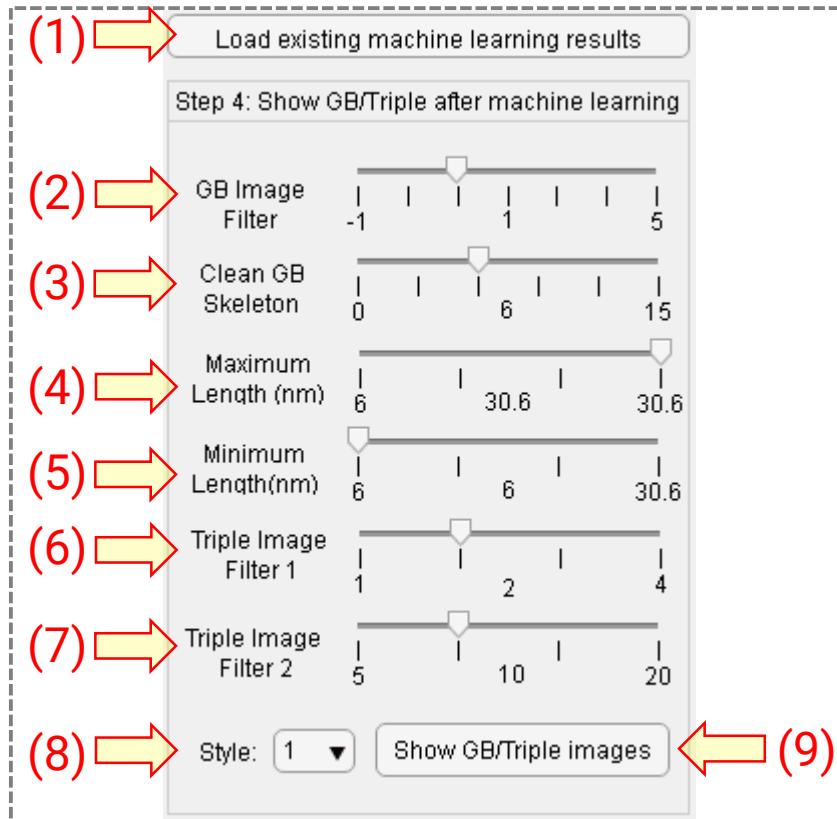


2. 5. Step 3 – Generate 2D projection series



- Drop Down “Version” (1): Click the down-arrow to select a number that indicates the version for the following calculation. The options range from 1 to 9.
- Drop Down “Subimage size (pixel)” (2): Click to select the number of pixels used for image segmentation. The default value is 20 pixels.
- Drop Down “Gap (pixel)” (3): Click here to select the number of pixels between each sliding window. A large gap reduces the resolution of the GB detection, but increases the speed of the calculation.
- Button “Export” (4): Click it to generate an image collection (*.hdf5 file) that contains all image segments for local feature identification (grain interior, GB, or triple junction). This step takes a few minutes, but also depends on the running parameters. All parameters for generating such a file are stored as the name of this *.hdf5 file.
Example: (“..\\example\\Cropped_70_50_50\\CNN\\V1_atom_Cr_0.20_100_0.5_180_20_1.hdf5”)
- Lamp (5): The lamp lights up green when the calculation is in progress. As soon as it is finished, it returns grey.

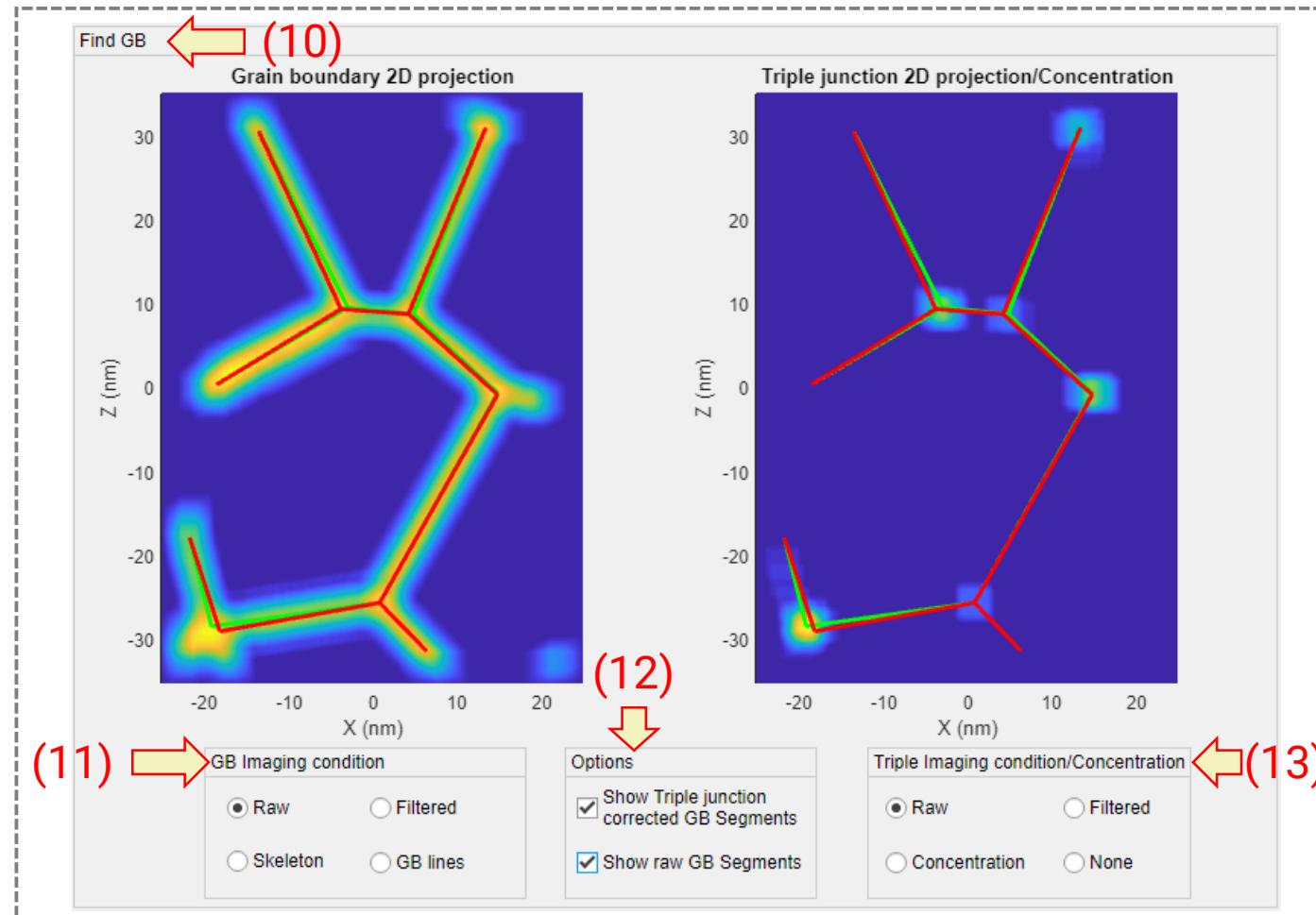
2. 6. Step 4 – Show GB/Triple after machine learning



- Button “Load existing machine learning results” (1): If users need to reload an existing machine learning result (CNN), they can click this button to select one. Example: (“..\example\Crop ped_70_50_50\CNN\V1_atom_Cr_0.20_100_0.5_180_20_1.txt”)
- Slider “GB Image Filter” (2): Click to select the image filter factor. The principle is similar to 2.4. step 2 (3).
- Slider “Clean GB Skeleton” (3): Click to select the strength to remove the dangling pixels for the GB skeleton. If a large value is selected, more pixels will be removed.
- Slider “Maximum Length (nm)” (4): Click to choose the maximum length that individual GB line segment can reached. Automatically updated when one changes (1-2).
- Slider “Minimum Length (nm)” (5): Click to select the minimum length that individual GB line segment can reach.
- Slider “Triple Image Filter 1/2” (6-7): Click to select the Gaussian peak finding filters for locating triple junctions.
- Drop Down “Style” (8): Click the down-arrow to select a number that indicates the style for running parameters.
- Button “Show GB/Triple images” (9): Click to execute the display of GB/Triple images. See next slides for images.



2. 6. Step 4 – Show GB/Triple after machine learning (continue 1)

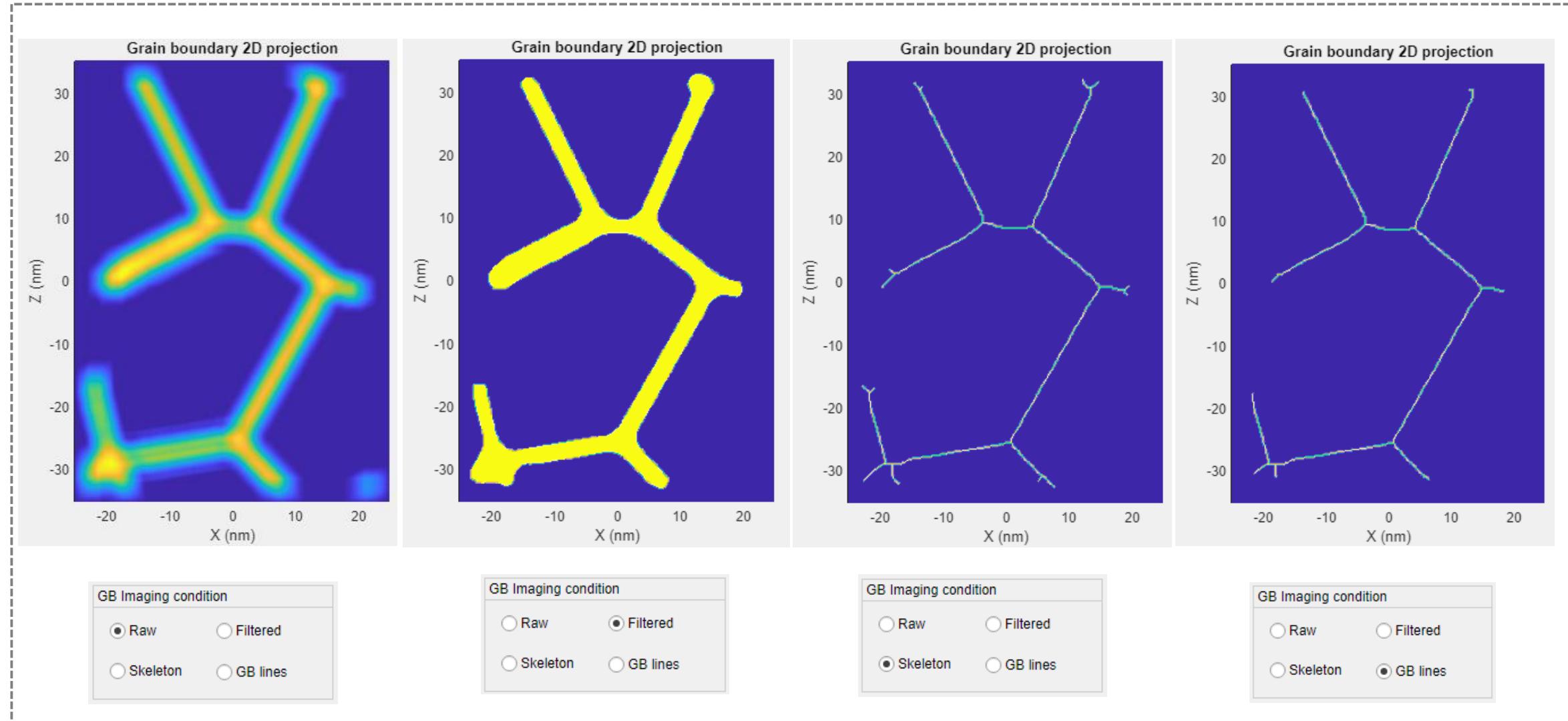


- Axis “Find GB” (10): It shows the Grain boundary 2D projection (left) and Triple junction 2D projection (right) identified by CNN. The red lines overlaying the image show the GB segments identified by the GB criteria, while the green lines (behind the red lines) show those further corrected by the triple junction criteria.
- Ratio Button group “GB Imaging condition” (11): Option 1 – Raw: Raw from CNN recognition. Option 2 – Filtered: Filtered by above mentioned image filter factor. Option 3 – Skeleton: GBs

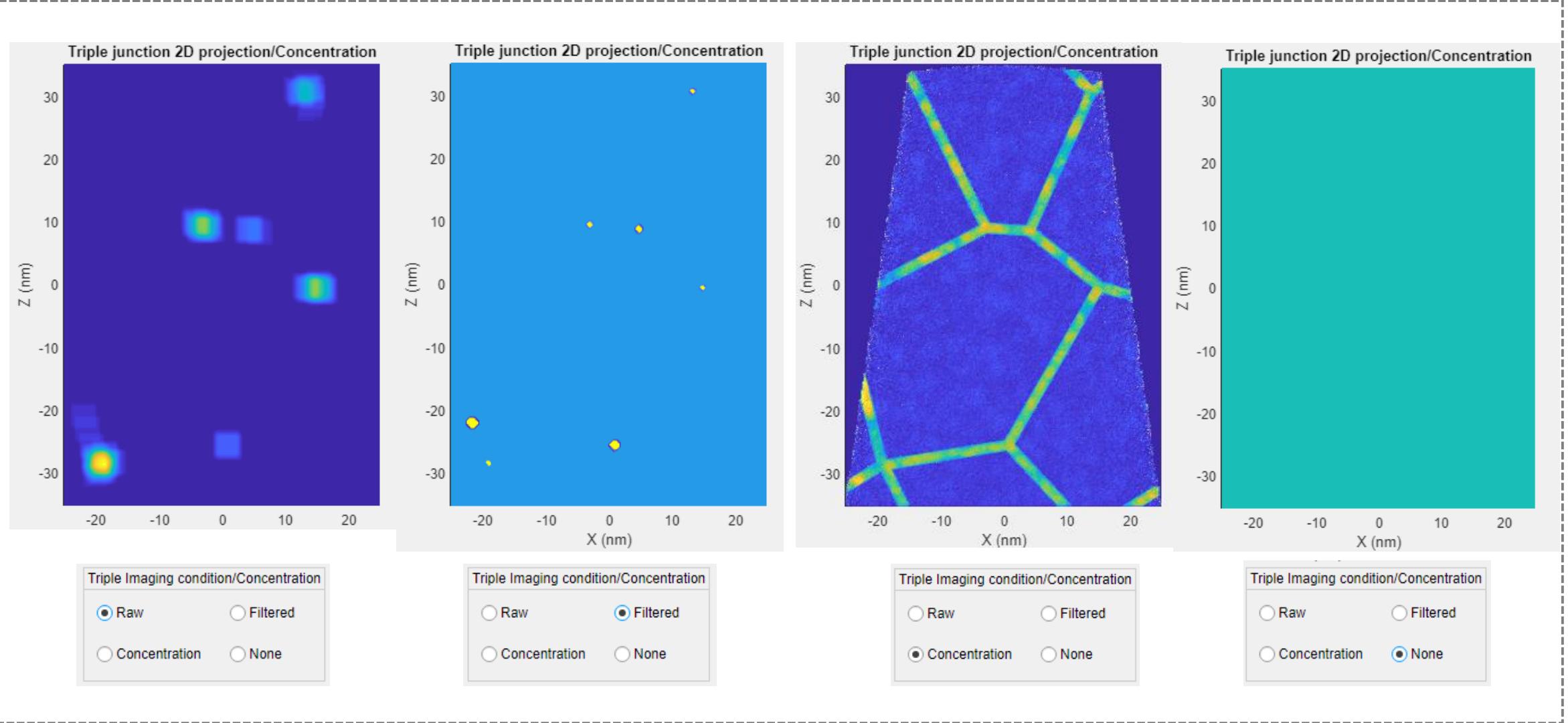
are represented as 1 pixel thick line segments. Option 4 - GB lines: GB lines with the dangling pixels removed.

- Check Box “Options” (12): Select to show GB line segments identified by GB (red lines)/Triple (green) criteria.
- Ration Button group “Triple Imaging condition/Concentration” (13): Similar to 2.6. Step 4 (2).

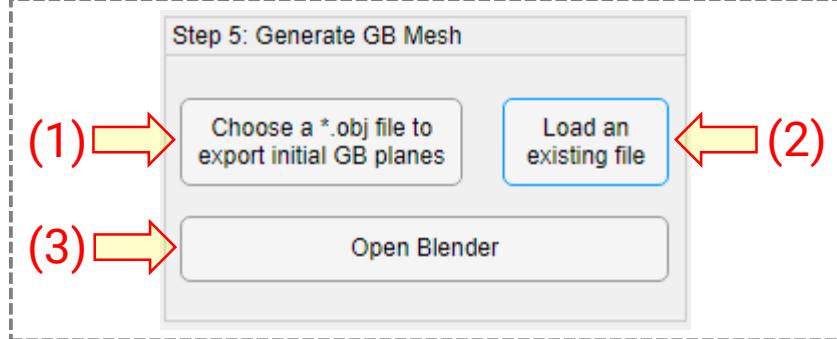
2. 6. Step 4 – Show GB/Triple after machine learning (continue 2)



2. 6. Step 4 – Show GB/Triple after machine learning (continue 3)



2. 7. Step 5 – Generate GB Mesh



- Button “Choose a *.obj file to export initial GB planes” (1): Click to export the initial GB planes as a 3D OBJ file. All parameters to create such a file will be saved as the name of this *.OBJ file. An example of the exported file:

(“..\\example\\Cropped_70_50_50\\CNN\\V1_atom_Cr_0.20_100_0.5_180_20_1_S1_1.5_6_30.6_6_4_20_Tri.obj”)

- Button “Load an existing file” (2): If the users need to reload an existing *.obj file, they can click this button to select one. After loading, all corresponding parameters will be reloaded in the APT-GB program. An example file: (..\\example\\Cropped_70_50_50\\CNN\\V1_atom_Cr_0.20_100_0.5_180_20_1_S1_1.5_6_30.6_6_4_20_Tri.obj”)
- Button “Open Blender” (3): Clicking this button opens the Blender 3D software for the following GB meshing process. Functions in Blender "GBMesh" add-ons help the users to transform these initial GB planes into well-defined 3D GB meshes.

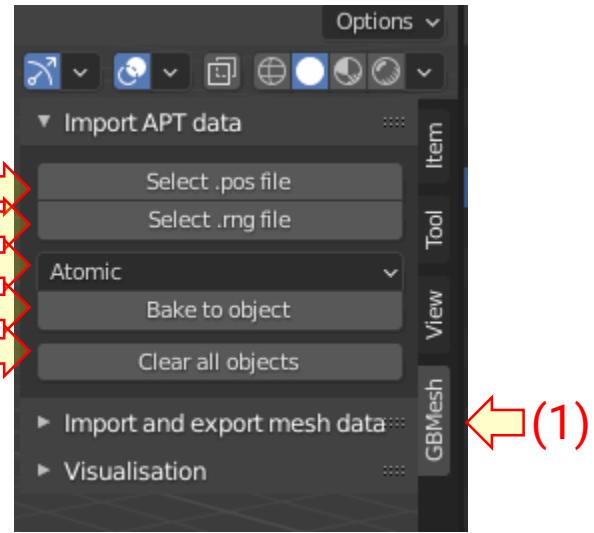
The following GB meshing operation is performed in Blender.

!!Strongly recommend users to learn some basics about Blender before using it!!



2.8. GB Mesh (Blender 2.92.0)

3D Window
Object mode

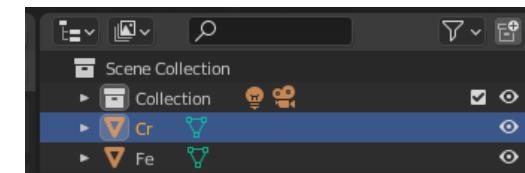


- How to activate the interface of the “GBMesh” Add-on that users have installed for Blender? (1): Move the mouse over the 3D window and type "N" on the keyboard. The toolbars appear in the upper right corner of the 3D Window.
- Button “Select .pos file” (2): Click it to select a POS file to display atoms/ions in Blender. Here, the POS file is the one created from 2.3 Step 1(6). An example of the imported file:

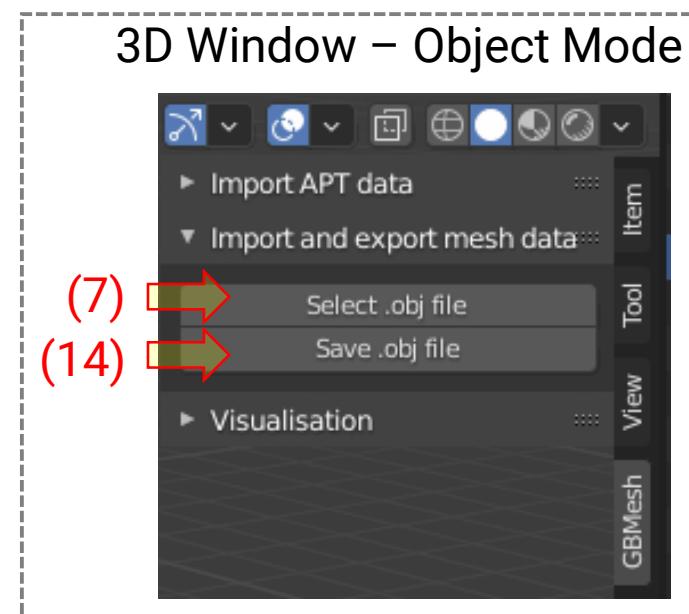
(“..\\example\\Cropped_70_50_50\\blenderImaging\\70_50_50_atom_Cr_10%.pos”)

- Button “Select .rng file” (3): Click it to select the RNG file to import a range file. Here, the RNG file is the one generated from 2.3 Step 1(2). Example (“..\\example\\Cropped_70_50_50\\AB.rng”).
- Drop Down “Atomic/Ionic” (4): Click on one of the options to specify the preferred imaging mode.
- Button “Bake to object” (5): Click to execute the import process. The imported atoms/ions can be found in the “Outliner Window” panel (right image “Cr” and “Fe”).
- Button “Clear all objects” (6): Click to remove all objects.

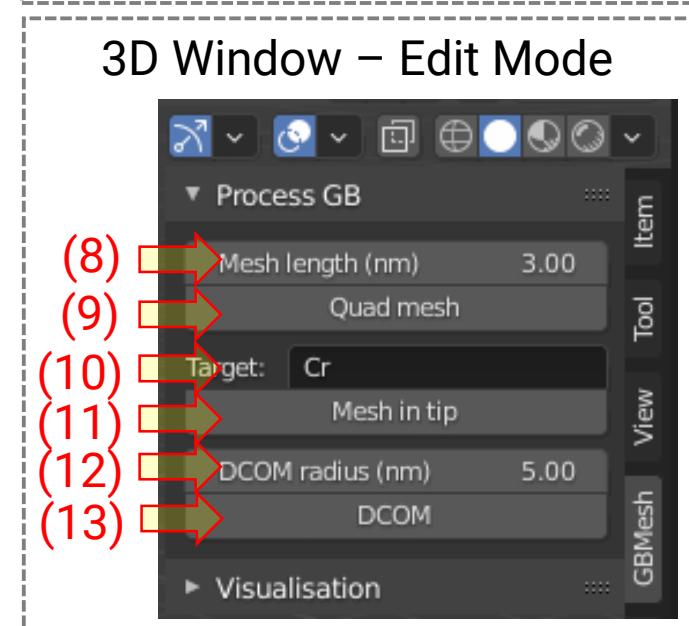
“Outliner Window”.



2.8. GB Mesh (continue 1)

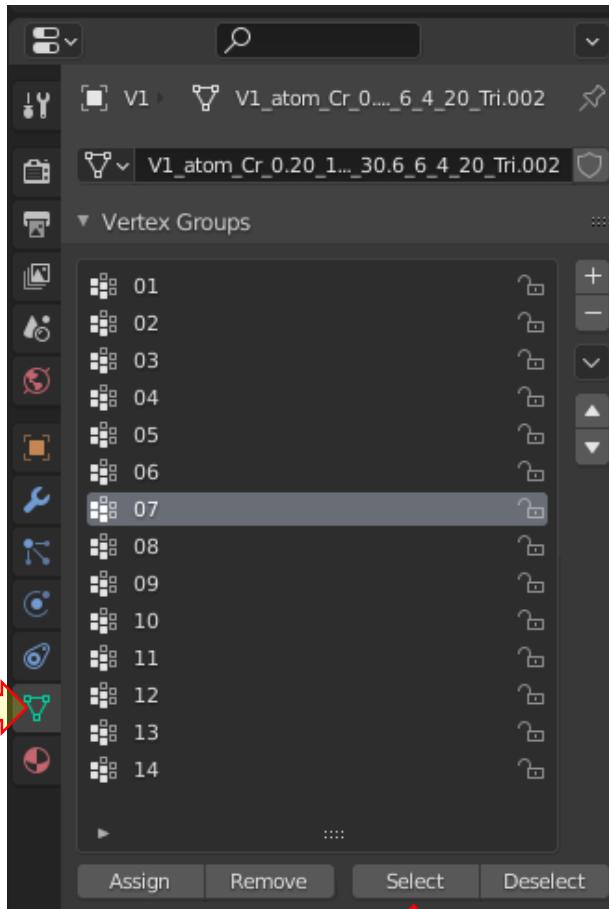


- Button “Select .obj file” (7): Click it to select a OBJ file for the initial GB planes. An example of the imported file: (“..\\example\\Cropped_70_50_50\\V1_atom_Cr_0.20_100_0.5_180_20_1__ S1_1.5_6_30.6_6_4_20_Tri.obj”). The imported OBJ file is automatically renamed to “V1_S1”.
- Select (click) “V1_S1” in the “Outliner Window”
- Switch to edit mode: Move the mouse over the 3D Window, press “Tab” key to switch. See also 1.2 Installation (C).
- Type in “Mesh” (8): Type in the minimal length (nm) of the Quad mesh.
- Button “Quad mesh” (9): Click to execute the automatic Quad mesh.
- Type in “Target” (10): Type in the name of atoms/ions for the following process. The names can be found from the panel “Outliner Window”.
- Button “Mesh in tip (11): Click it to remove meshes outside the tip convex.
- Type in “DCOM radius (nm)” (12): Enter radius for searching the mass center.
- Button “DCOM” (13): Click it to align the GB mesh to solute center of mass (a few mins).
- Button “Save .obj file” (14): Click it to save an OBJ file for the 3D GB meshes.

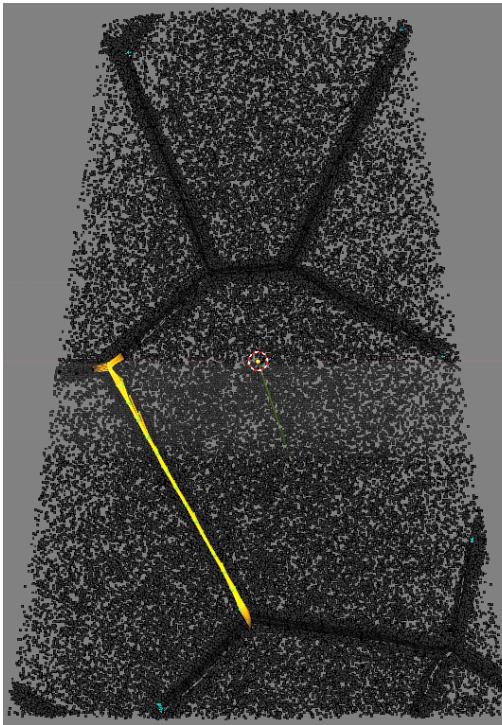


2.8. GB Mesh (continue 2)

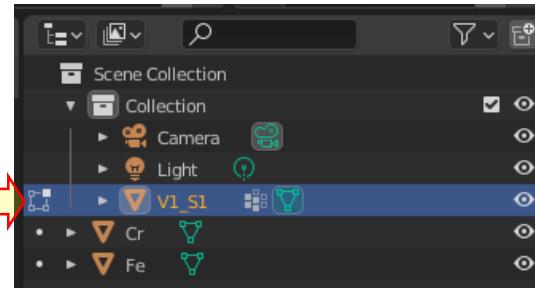
Properties Window



3D Window - Edit Mode



"Outliner Window"

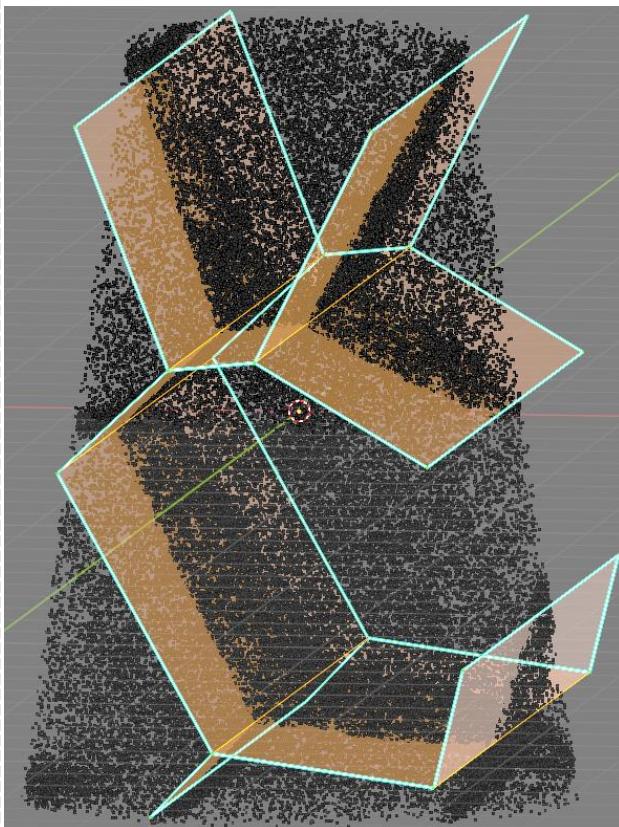


- Each GB has a unique name. Users can find their names by clicking on "Object data property" (15) in the "Properties window". Each GB can be selected individually by clicking on "Select" (16).
- The selected GB will be highlighted in orange in the "3D window".
- Click the 3D GB meshes "V1_S1" (17) (objective mode) and save as described in 2.8. GB mesh (14). ("..\example\Cropped_70_50_50\CNN\V1_S1_QLen2.0_Cr_R5.0.obj")
- Save the Blender file. ("..\example\Cropped_70_50_50\blenderImaging\Crop ped_70_50_50_AfterMesh.blend")
- Close Blender. Otherwise, the "APT-GB" program will not respond to further operation.**

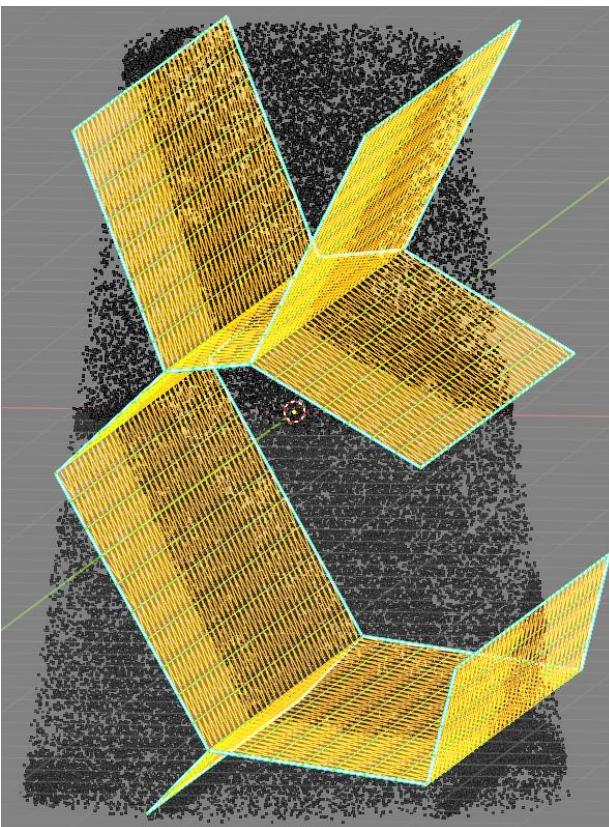
2.8. GB Mesh (continue 3)



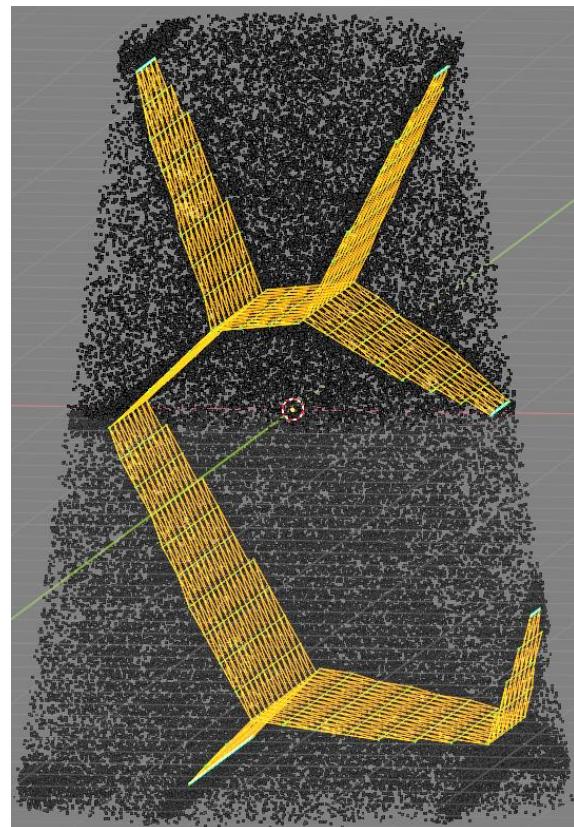
3D Window - Edit Mode



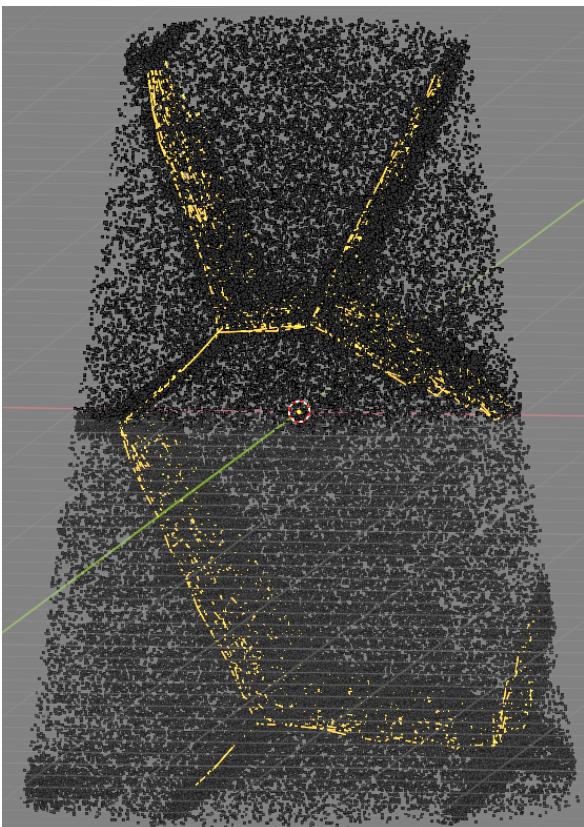
Initial GB planes



Quad mesh



Mesh in tip

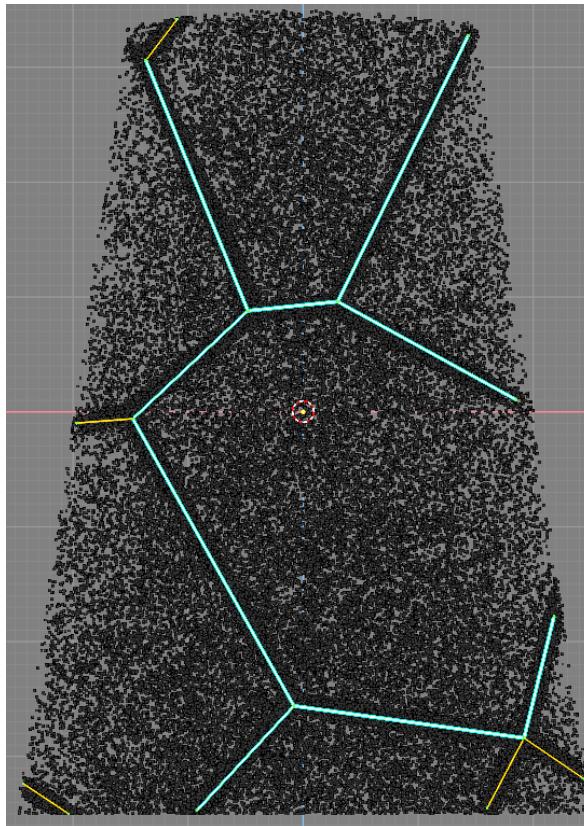


After DCOM

2.8. GB Mesh (continue 4)



3D Window - Edit Mode

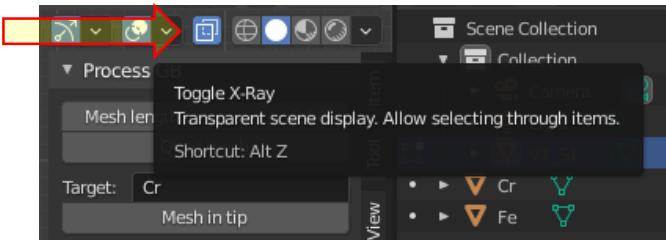


Manually adjustment
Orange lines are newly added

- It is also possible to adjust the location of initial GB planes in Blender.
(The steps in this page are optional. They should be executed before 2.8. GB mesh (8).)
- Make sure that Blender is in edit mode.
- Make sure that Toggle X-Ray is on (18).
- GB is in an edge-on configuration.
- Deselect all the vertices.
- Select the vertices to be adjusted.
- Adjust the position of the selected vertices or add new vertices.
- Make sure that the length of each GB line segment is at least twice the mesh length.
- Select the Blender file for backup as ("..\example\Cropped_70_50_50\blender Imaging\Cropped_70_50_50_Before Mesh.blend")

3D Window - Edit Mode

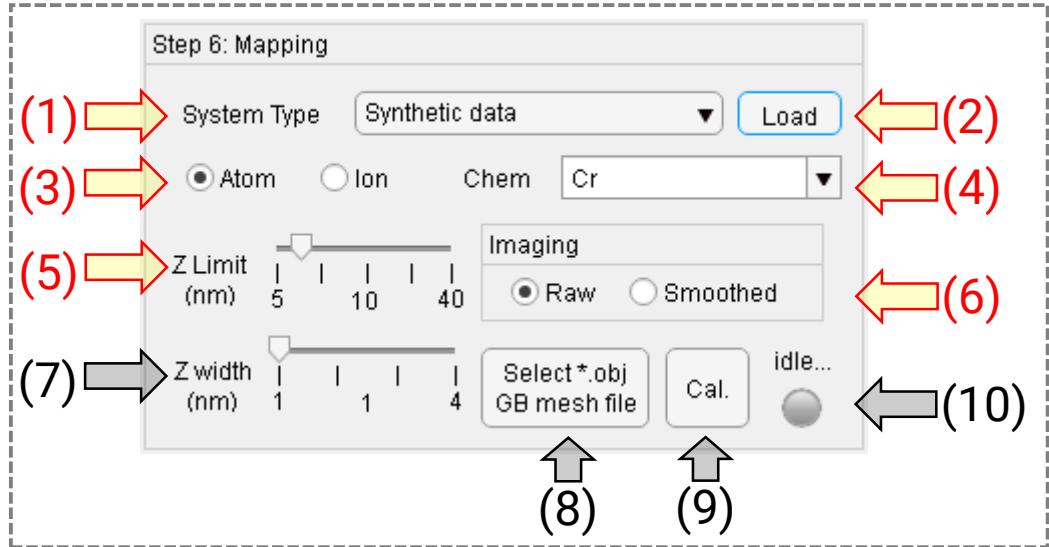
(18)



Tips (in Edit mode):

- > Tap "A", select all vertices.
- > Double Tap "A", unselect all vertices
- > Tap "B", select interesting vertices
- > Tap "E", to add new vertices
- > Tap "G", to change vertices position
- > Tap numbers in Num Pad to change different view directions.

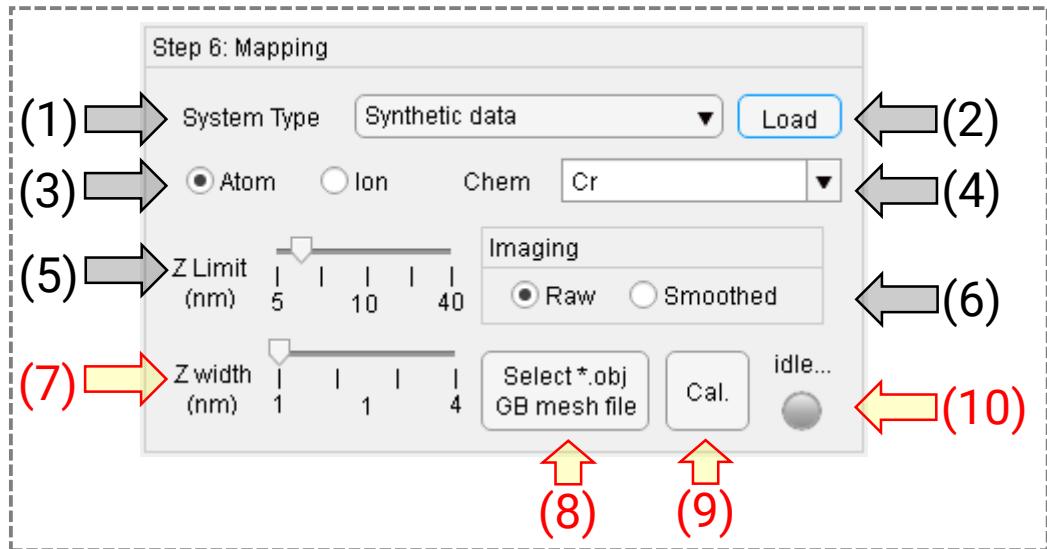
2. 9. Step 6 – Mapping (Matlab 2018a)



- Drop Down “System Type” (1): Click on the down arrow to select the device for data acquisition/generation. This value affects the calculation of the interface excess due to different detection rate. Option 1 -- ‘5000 XS’; Option 2 – ‘5000 XR/3000 XS/4000 XS’; Option 3 – ‘3000 HR/4000 HR’; Option 4 – ‘Synthetic data’.
- Button “Load” (2): Click to load the existing calculation results. Example (“..\example\Cropped_70_50_50\V1_S1_QLen2.0_Cr_R5.0_Cr_10_1_atom\IEC.mat”)
- Ratio Button group “Atom/Ion” (3): Click one of the two options to determine the preferred calculation.
- Drop Down “Chem” (4): Click the down-arrow to select the atom/ion specie for the following calculation. Users can calculate the concentration (C) and interfacial excess (IE) maps based on different elements.
- Slider “Z Limit (nm)” (5): Click to select the limit of thickness of the slabs used for IE calculation.
- Ratio Button group “Imaging” (6): Click to select the display format. Option – 1 Raw: C and IE maps are based on the value for each individual vertex. Option 2 – Smoothed: The values are generated based on the average values of surrounding vertices. Such maps can reduce the errors created by bad vertices and make smooth images.

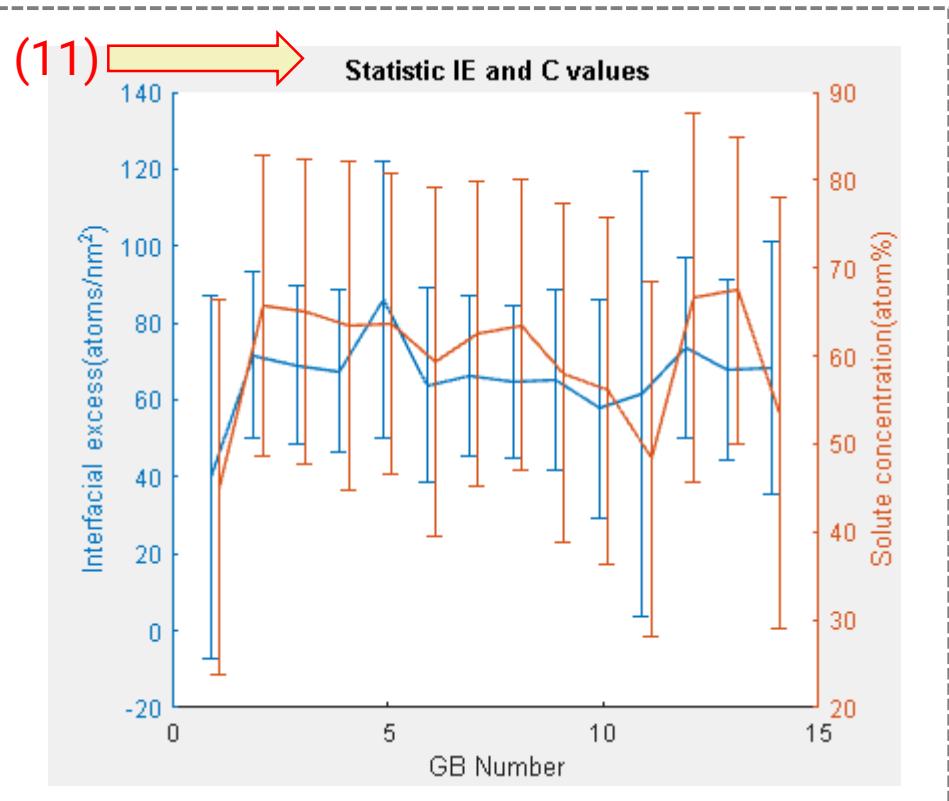


2. 9. Step 6 – Mapping (continue 1)



- Slider “Z Width (nm)” (7): Click to select the limit of thickness of the volume used for calculating local concentration.
- Button “Select *.obj GB mesh file” (8): Click to load the well-defined 3D GB meshes, which has been generated from 2.8. GB Mesh (8). Example (“..\\example\\Cropped_70_50_50\\CNN \\V1_S1_QLen2.0_Cr_R5.0.obj”)
- Button “Cal.” (9): Click to execute the calculation. A folder is automatically created where all calculation results are saved. i.e., (“..\\example\\Cropped_70_50_50\\V1_S1_QLen2.0_Cr_R5.0_Cr_10_1_atom\\”) In this folder, there are seven subfolders -- “values”, “statistics”, “overview”, “histogram”, “ladder”, “maps”, “s_maps” and one file “IEC.mat”. If there is a prefix ‘s_’, it is the 1st neighboring smoothed values. The information of each vertex is storage in the subfolder ‘values’. Each file contains five columns: e.g., “..\\values\\00_data.txt”: area (nm²), raw IE (atoms/nm²), smoothed IE, raw concentration(%), smoothed concentration. The files in other subfolders are explained in the following slides.
- Lamp (10): The lamp lights up green when the calculation is in progress. As soon as it is finished, it returns grey.

2. 9. Step 6 – Mapping (continue 2)

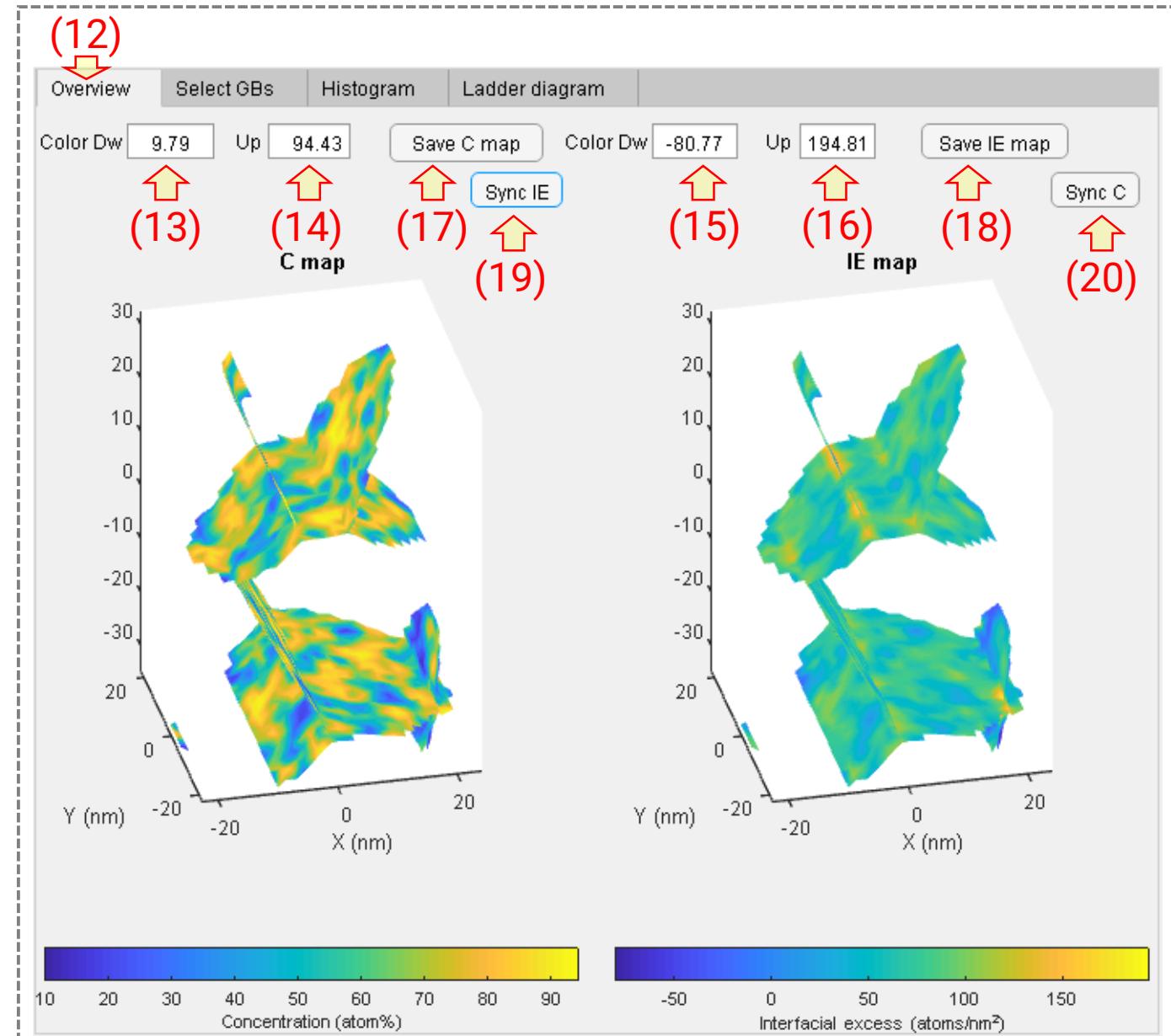


- Axis “Statistic IE and C values” (11): This plot shows the average values of the interfacial excess (left axis) and the solute concentration (right axis) for each individual GB. The error bars represent the standard deviation values within a GB. The GB number corresponds to vertex group number which could be accessed in Blender, 2.8. GB Mesh (16).
- This plot and the correspond data are stored in the folder: (“..\\example\\Cropped_70_50_50\\V1_S1_QLen2.0 _Cr_R5.0_Cr_10_1_atom\\statistics\\”). The data contains

contains five columns, i.e.,

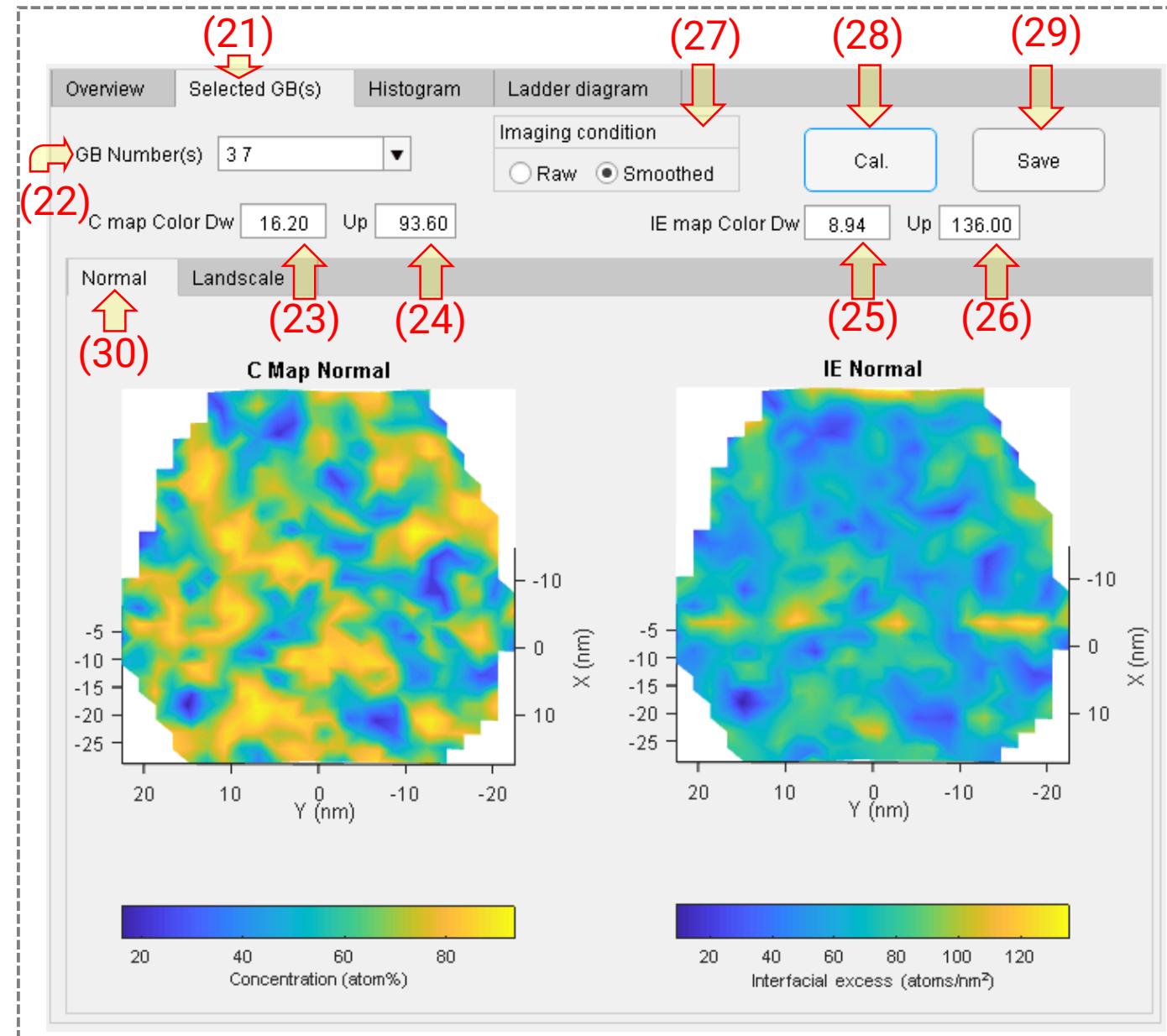
“..\\statistics\\statistic.txt”: GB No., IE(atoms/nm²), IE error bar, Concentration(atoms%), Concentration error bar, area.

2. 9. Step 6 – Mapping (continue 3)



- Sub-panel “Overview” (12): This panel shows the calculated C and IE maps.
- Type in “Color Dw/Up” (13-16): Type in values for setting the low and high limits for the colormap of C and IE maps. The default values are minimal and maximal.
- Button “Save C/IE map” (17-18): Click to save the C/IE map (*.ply file) for imaging in Blender. E.g., : (“..\\example\\Cropped_70_50_50\\V1_S1QLen2.0_Cr_R5.0_Cr_10_1_atom\\overview\\s_CMap.ply”)
- Button “Sync IE/C” (19-20): Click this button to synchronize the fields of the views between the C map and the IE map.

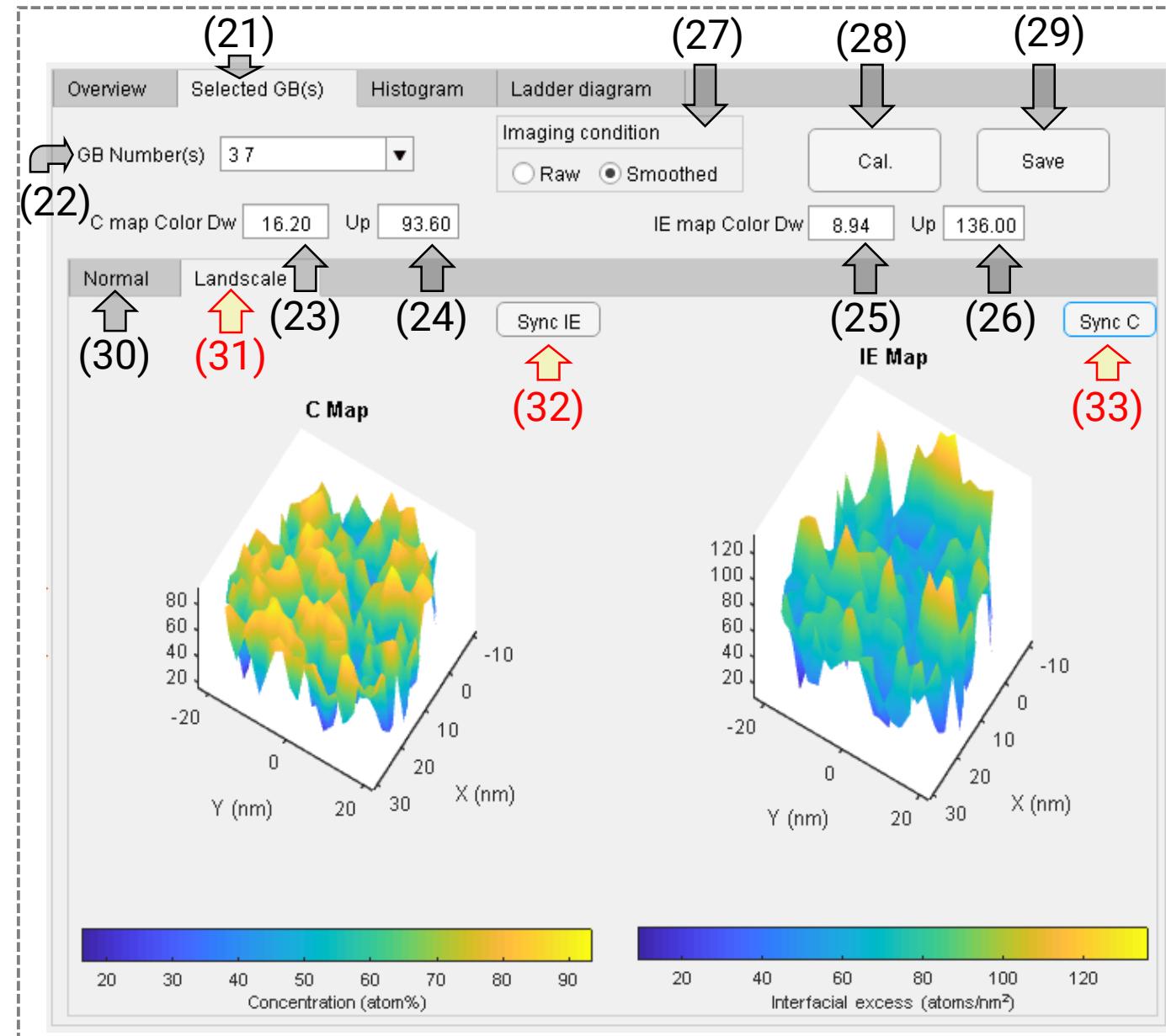
2. 9. Step 6 – Mapping (continue 4)



- Sub-panel “Select GBs” (21): This panel shows the calculated C & IE maps for selected GB(s).
- Type in “GB Number (s)” (22): Enter a number or numbers with blank to select GB(s).
- Type in “Color Dw/Up” (23-26): Enter values for setting the lower and upper limits for the colormap of C & IE maps.
- Ratio Button group “Imaging” (27): Click to select the display format. See 2.9. Step 6(6).
- Button “Cal.” (28): Click to execute the calculation of the maps of selected GB(s).
- Button “Save” (29): Click to save the C and IE maps as .ply file. E.g., (“..\\example\\Cropped_70_50_50\\V1_S1QLen2.0_Cr_R5.0_Cr_10_1_a tom\\s_map\\3_7_CMap.ply”)
- Sub-sub-panel “Normal” (30): Normal view.

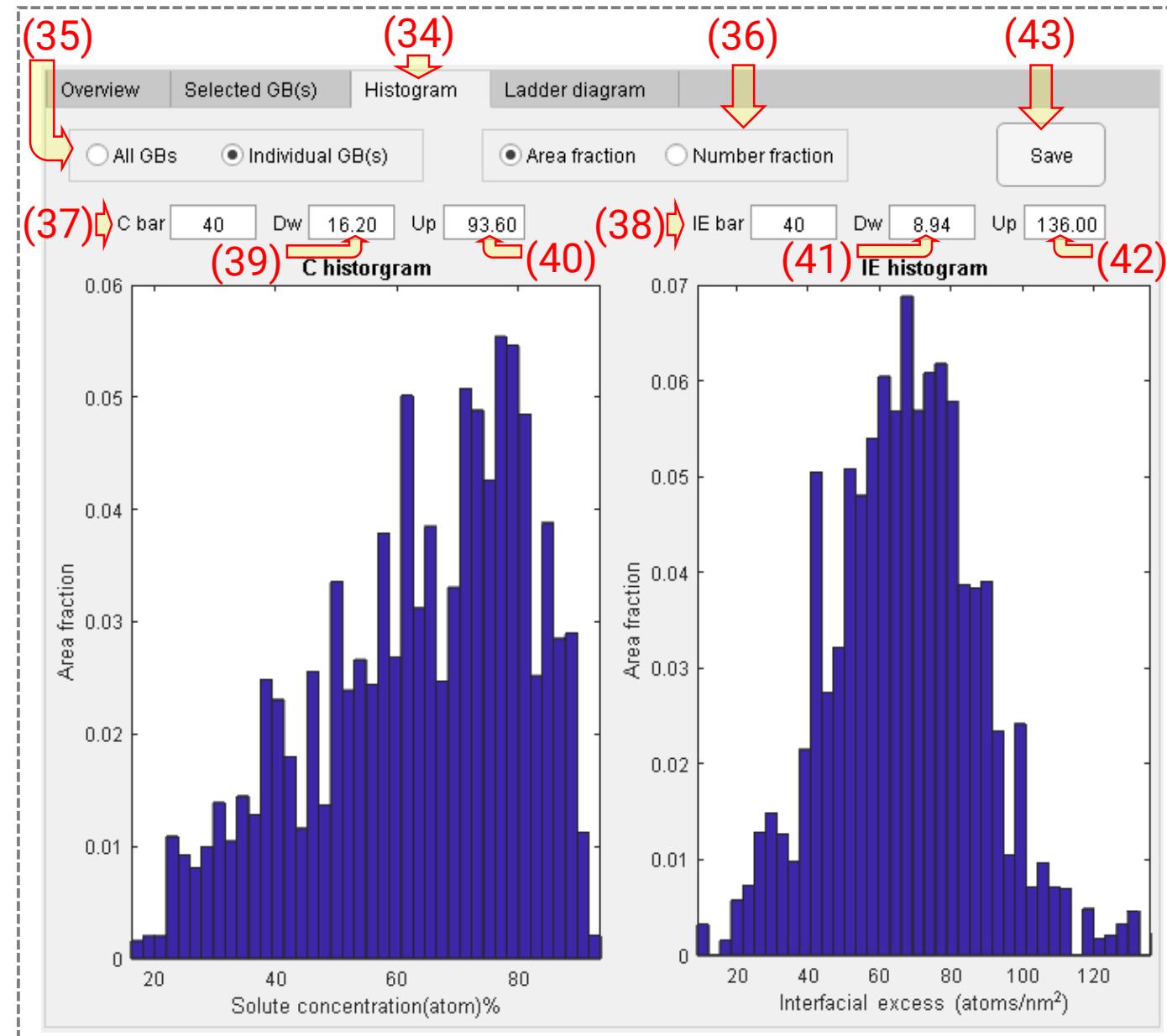


2. 9. Step 6 – Mapping (continue 5)



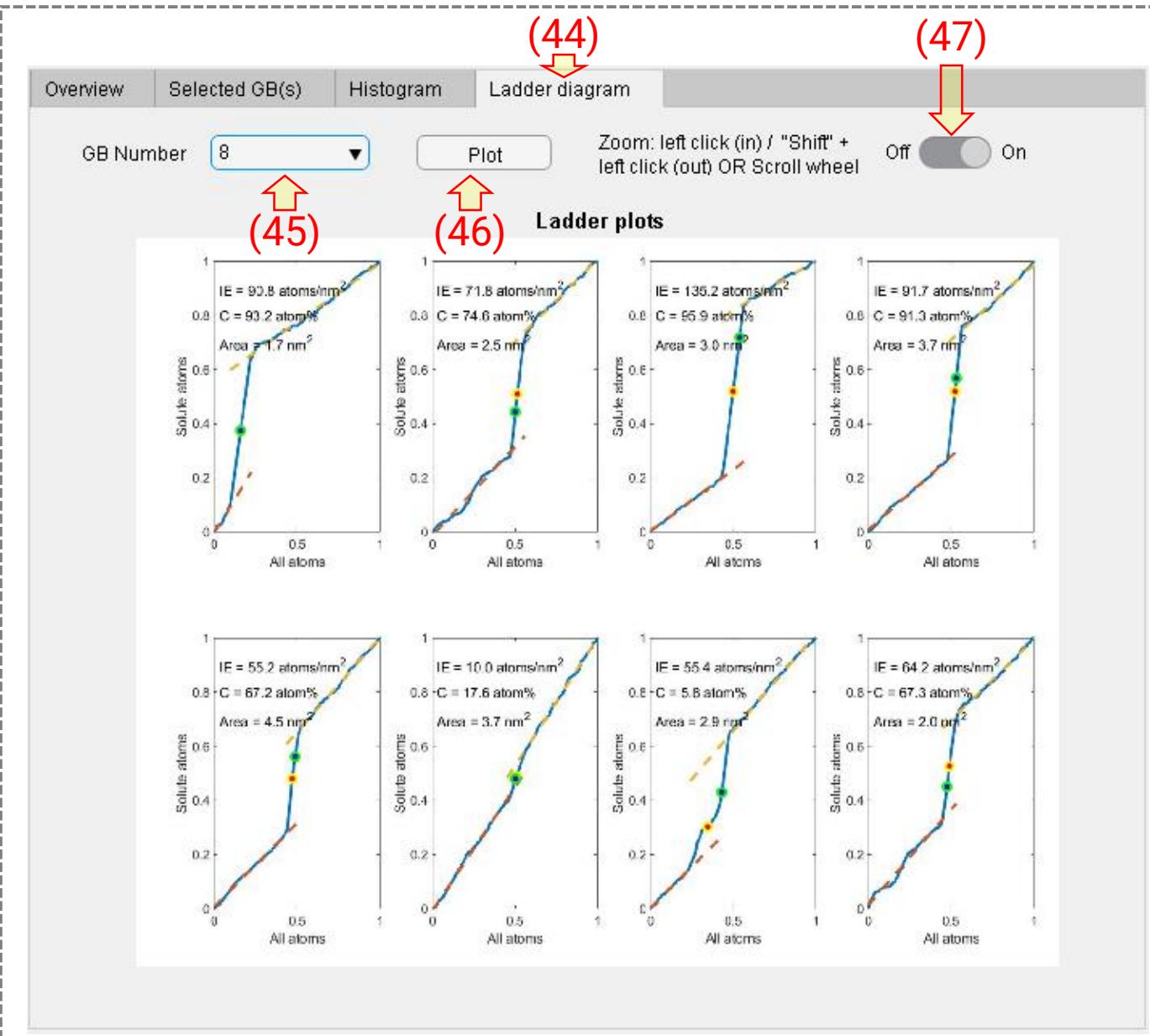
- Sub-sub-panel “Landscape” (31): C map & IE map are displayed in landscape-style figures.
- Button “Sync IE/C” (32-33): Click it to synchronize the view fields between the C map and the IE map.

2. 9. Step 6 – Mapping (continue 6)



- Sub-panel “Histogram” (34): Provides the histograms of C & IE of each vertex in GB(s).
- Ratio Button group “All GBs/Individual GB(s)” (35): Click to select the working data set. Individual GB(s) are from 2.9. Step 6(22).
- Ratio Button group “Area/Number fraction” (36): Click to select how to obtain histogram.
- Type in “C/IE bar” (37-38): Set the numbers of bars for the histogram.
- Type in “Color Dw/Up” (39-42): Enter values for setting the lower and upper limits for the histograms of the C & IE maps.
- Button “Save” (43): Click to save histograms.
e.g. (“..\\example\\Cropped_70_50_50\\V1_S1_Q
Len2.0_Cr_R5.0_Cr_10_1_atom\\histogram\\s_3
7_Chist_16.2_93.6_40A.txt”)

2. 9. Step 6 – Mapping (continue 7)

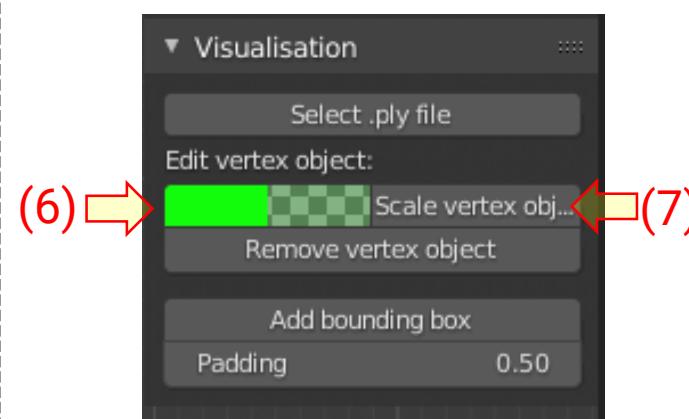
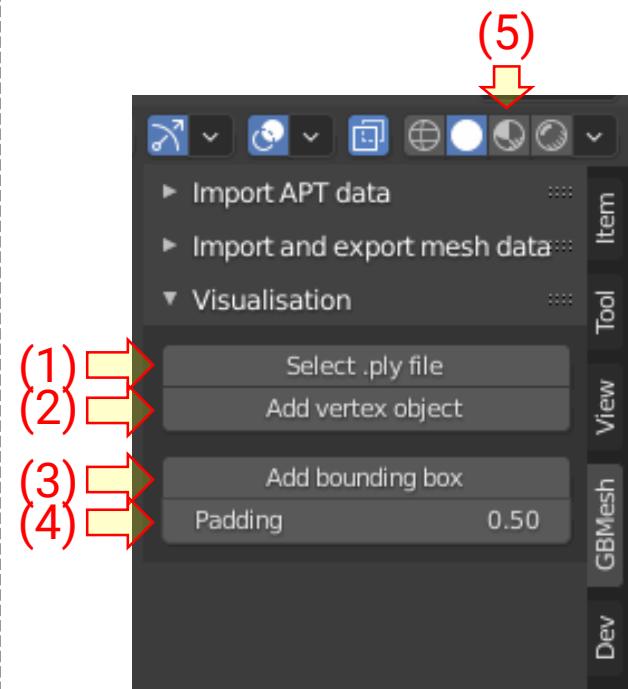


- Sub-panel “Ladder diagram” (44): Presents the ladder diagrams of eight randomly selected vertices in each GB. The goal is to give users an idea of how the IE is calculated.
- Drop Down “GB Number” (45): Click the down arrow to select the number of the GB for which the ladder diagram should be displayed.
- Button “Plot” (46): Click to plot the images. The images of the ladder diagrams for different GBs are stored in the folder: (“ ..\example\Crop ped_70_50_50\V1_S1QLen2.0_Cr_R5.0_Cr_10 _1_atom\ladder\”).
- Switch “Off/on” (47): Toggle the key to disable and enable zoom function. When the switch is off, the plots are reset to the default view.

2. 10. Final imaging in Blender (Blender 2.92.0)



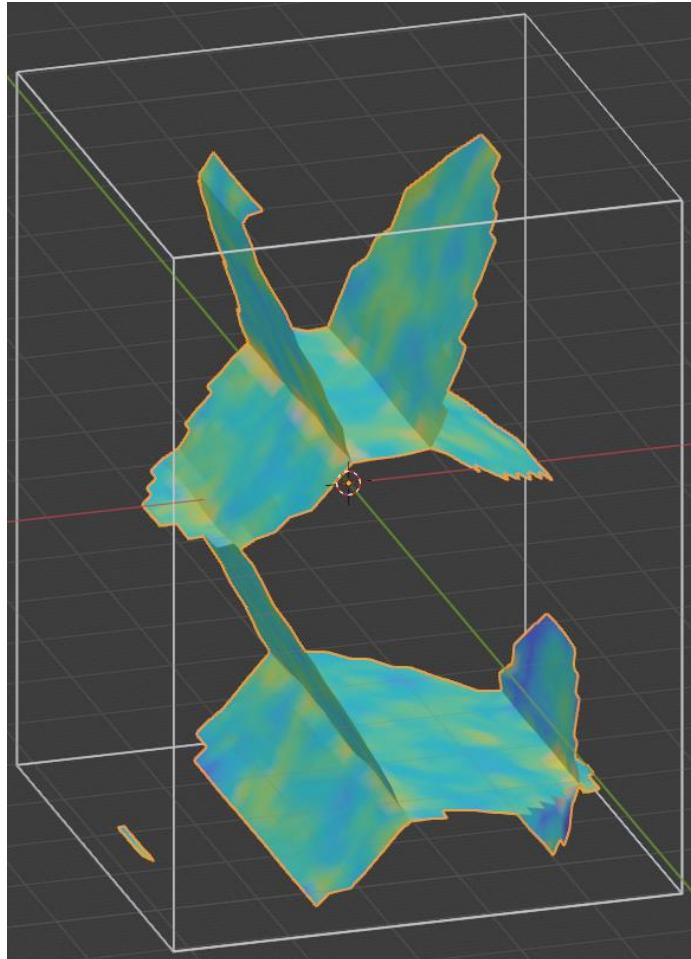
3D Window – Object Mode



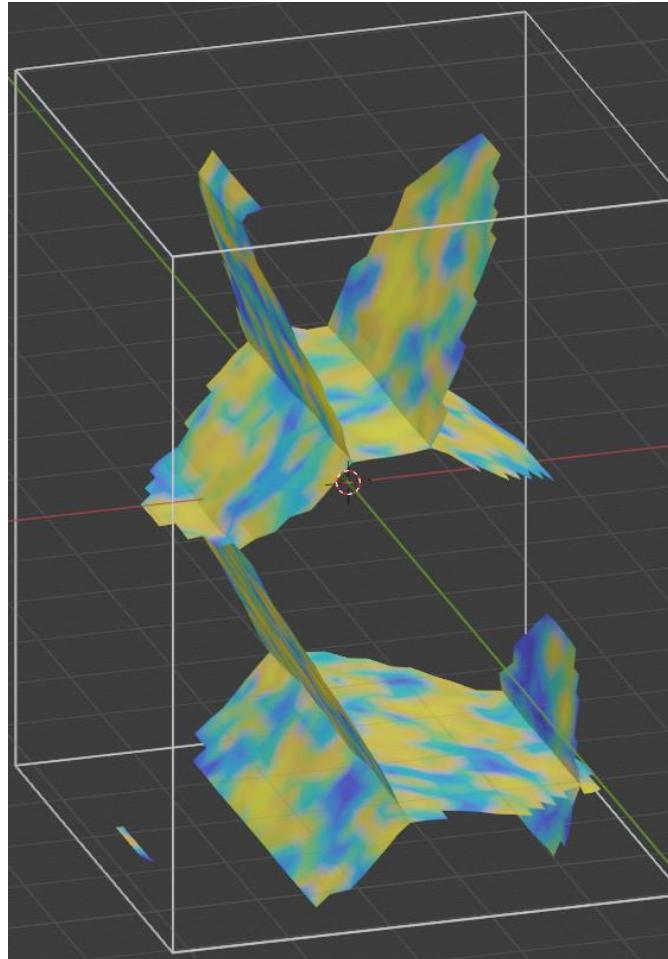
- Button “Select .ply file” (1): Click it to select a PLY file for the C or IE map. An example of the imported file. (“..\example\Cropped_70_50_50\V1_S1QLen2.0_Cr_R5.0_Cr_10_1_atom\overview\s_CMap.ply”)
- Button “Add vertex object” (2): Click to set the color and size of individual atoms. The changes are possible through the pop-up new items (6-7).
- Button “Add bounding box” (3): Click to add a bounding box for the atom cloud.
- Type in Padding (4): Enter the padding for the bounding box.
- Button “Material preview” (5): Click to check the color image of the C map and IE map.
- Button “Diffuse color” (6): Click to set the color for atoms/ions.
- Button “Scale vertex object” (7): Click and shift the mouse to change the size of each atom/ion.

2. 10. Final imaging in Blender (continue 1)

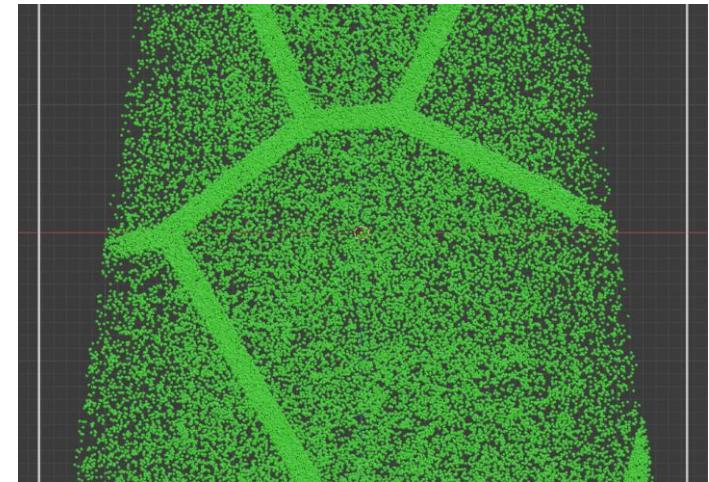
3D Window – Material previewMode



Interfacial excess map



Concentration map



Atom map





Thank you for your attention!

- We thank Prof. Dr. Peter Felfer, Dr. Anna Ceguerra, and Ms. Varvara Efremova for opening their codes.
- Example: X. Zhou, R. Darvishi Kamachali, B. Boyce, B. Clark, D. Raabe, G.B. Thompson, Spinodal Decomposition in Nanocrystalline Alloys, *Acta Mater* **Accepted**, 117054 (2021)..



Appendix

--For developer



A1. 1. Installation – Spyder

Version: Spyder **3**, Python **3.7.3**, Tensorflow **2.0.0-beta1**

A. Download Anaconda <https://www.anaconda.com/distribution/> and install it.

B. Create a new environment for python 3.7

- Run Anaconda Prompt as administrator
- Enter: conda create -n py37 python=3.7.3 anaconda
- Enter: conda activate py37
- Enter: spyder

C. Install Tensorflow package

- In Ipython console
- Enter: pip install opencv-python
- Restart the kernel
- Enter: pip install tensorflow==2.0.0-beta1
- Restart the kernel

A1. 2. Installation – (Spyder Continue 1) Create Executable from Python Script using Pyinstaller



D. Download python 3.7.3

<https://www.python.org/downloads/windows/>

and install it.

(check the box “Add Python 3.7 to PATH”).

E. Install pip

- Open Command Prompt (cmd)
- Open folder “..\\codes\\python_spyder\\source code\\”
- Enter: py get-pip.py

F. Install pyinstaller

- Enter: pip install pyinstaller==3.6

G. Install required packages

- Enter: pip install opencv-python
- Enter: pip install tensorflow==2.0.0-beta1
- Enter: pip install astor==0.8.0
- Enter: pip install h5py==2.10.0

H. Create Executable

- Enter: pyinstaller --onefile cnn.py

I. Users can the find executable file “cnn.exe” in “..\\codes\\python_spyder\\source code\\dist\\”.

- **Copy “cnn.exe” to “..\\codes\\matlab\\source code\\cnn\\”**

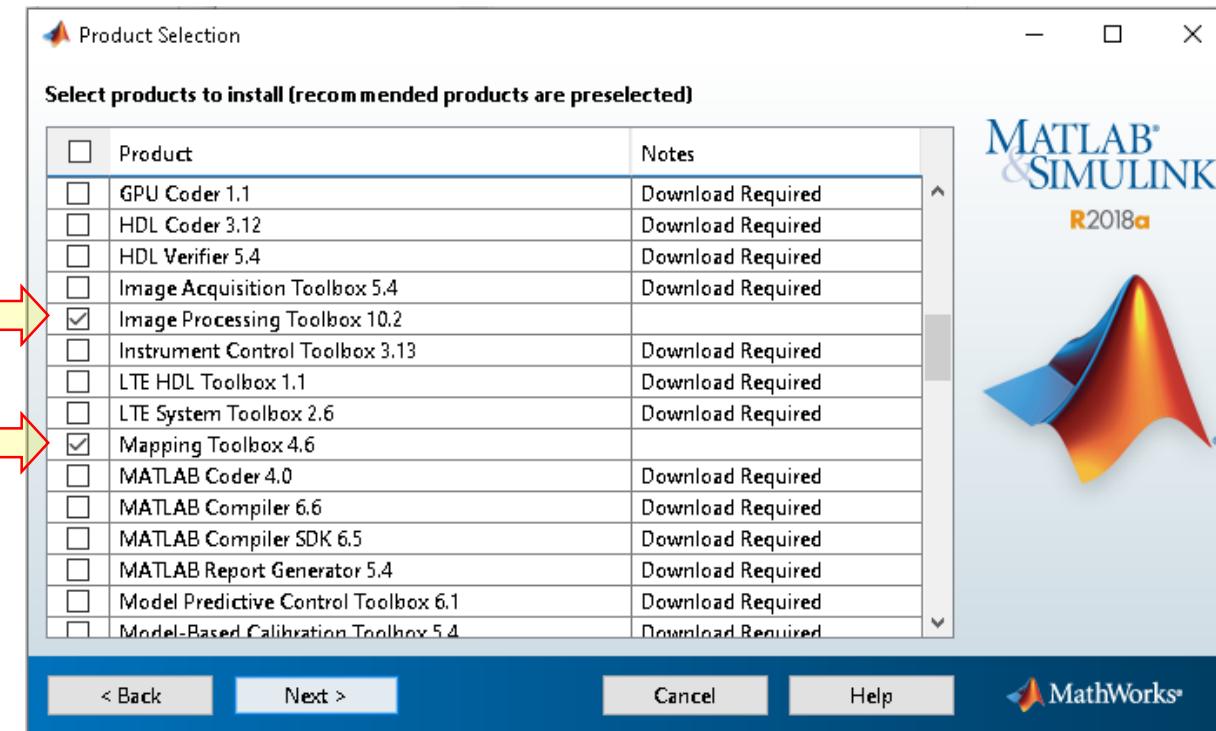
Reference: <https://datatofish.com/executable-pyinstaller/p>

A2. Installation - Matlab

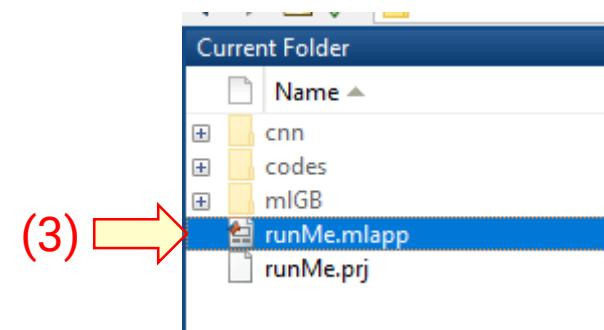


Version: Matlab 2018a

- The program was developed in Matlab **2018a**. It has been tested successfully in a later version Matlab 2020b.
- Please also select “Image Processing Toolbox” **(1)** and “Mapping Toolbox” **(2)** during installation.



- Open Installed Matlab **2018a**.
- Set the current folder as “..\\codes\\matlab\\source code”.
- Right click “runMe.mlapp” **(3)** and choose Run
- Now you can use the APT-GB program.



A3. Installing jupyter_contrib_nbextensions for reviewing the training and testing results (Optional)



A. Installation: Command Prompt:

- pip install jupyter_contrib_nbextensions
- pip install https://github.com/ipython-contrib/jupyter_contrib_nbextensions/tarball/master
- jupyter contrib nbextension install –user
- jupyter nbextension enable codefolding/main
- pip install jupyter-tensorboard

Reference: <https://jupyter-contrib-nbextensions.readthedocs.io/en/latest/install.html>

B. After installation: Open the logs/ folder in Jupyter and then open Tensorboard here by red arrow (1).



A4. Generating training data set for CNN (Optional)



(1) Restart point of GB structure units 1

(2) Number of GB structure units 15

(3) Number of "Training + Testing" groups 1 ▾

(4) Only needs to be done once, it works for all data sets

- Type in “Restart point of GB structure units” (1): The first GB structural units for training data generation. The default value is 1, but if the calculation was interrupted, the user can restart at the break point. .
- Type in “Number of GB structure units” (2): Each structural unit can generate 100 images of the training dataset. The user can set the number of GB structural units as needed. The model with this software package was generated with 200 structural units.
- Drop Down “Number of “Training + Testing” groups” (3): Click here to select the subgroup that the user wants to specify for their training dataset. The goal is to investigate the impact of the number of training data on the accuracy of the CNN.
- Button “Only needs to be done once, it works for all data sets” (4): Click it to perform the calculation.