Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

Exercise 2

Prof. Junhe Lian
Wenqi Liu (Teaching assistant)

Outline

- Software introduction
  - Microstructure modeling
  - DREAM.3D
  - ParaView
- Feedback on Assignment
- Questions

Microstructure modeling

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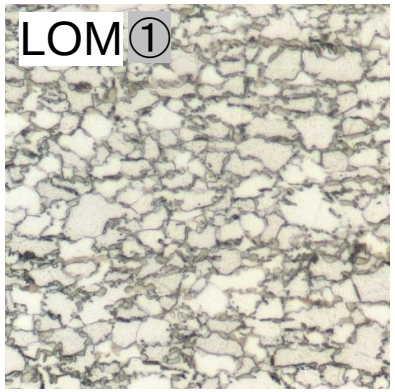
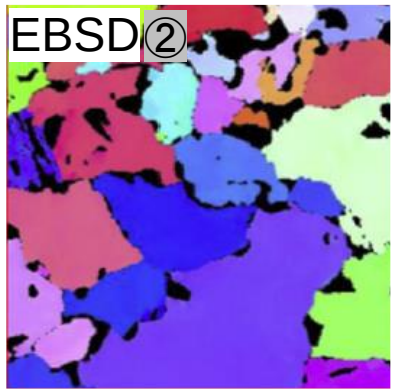
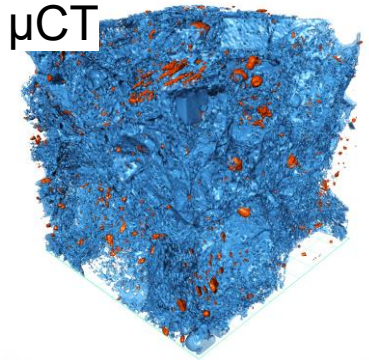
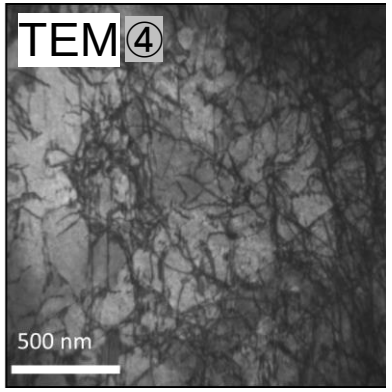
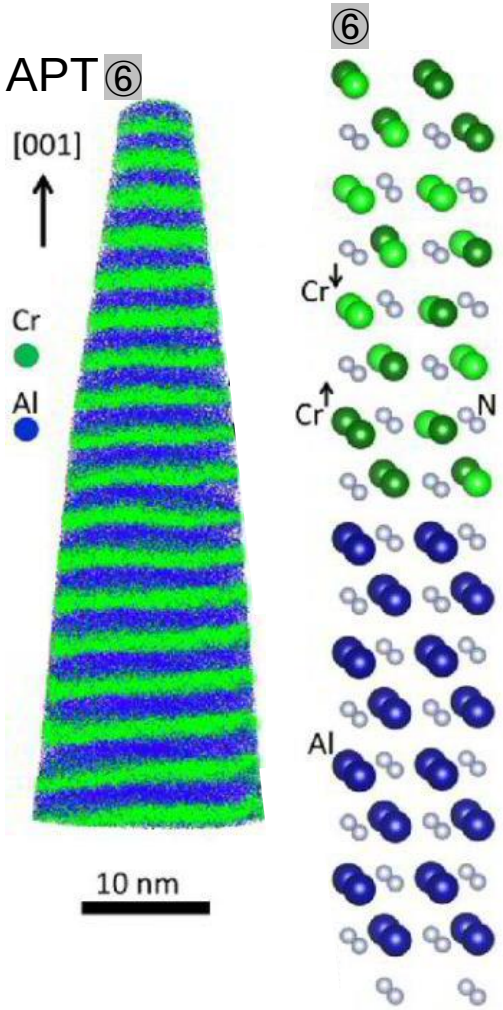
Microstructure modeling

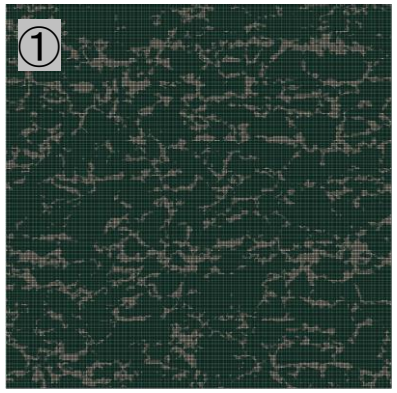


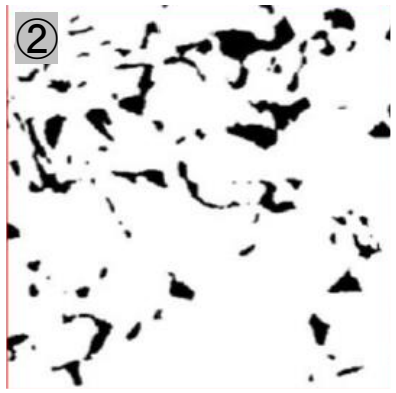


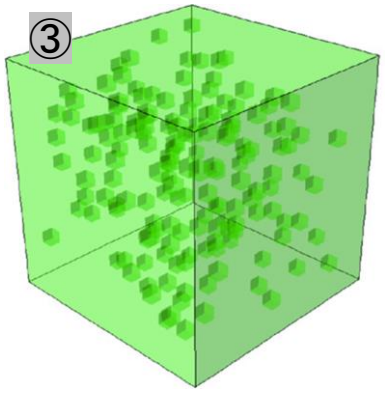


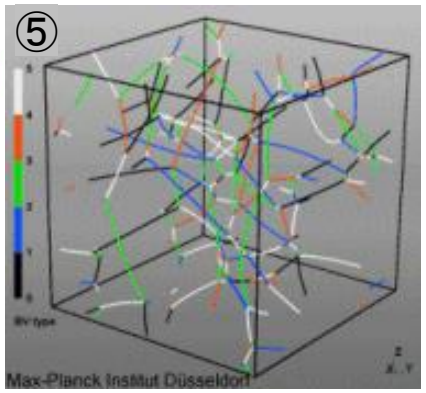










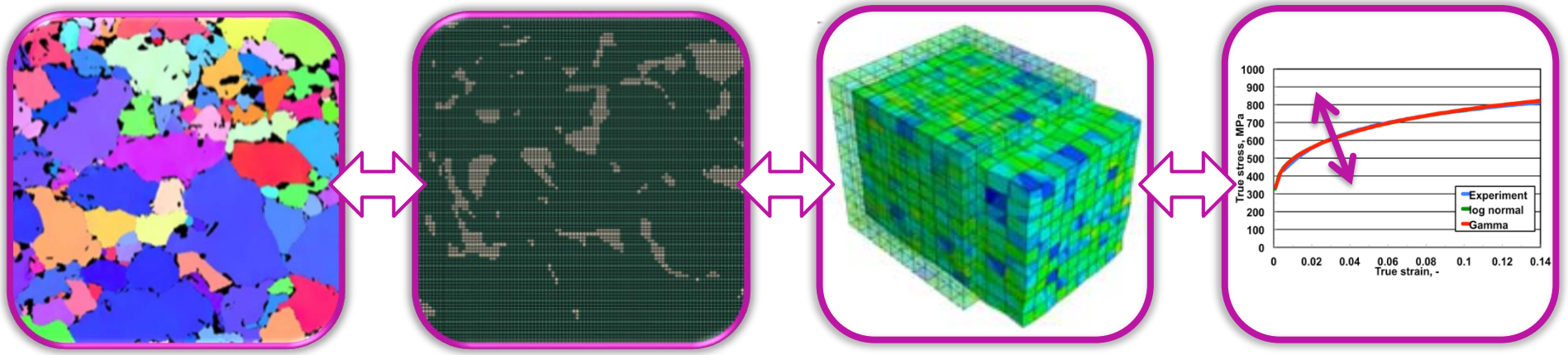


LOM - Light Optical Microscopy; **TEM** - Transmission Electron Microscopy;
EBSD - Electron Backscatter Diffraction; **μCT** - micro Computed Tomography; **APT** - atom probe tomography

① IEHK, ICME lecture.
② https://doi.org/10.1016/j.commatsci.2014.05.051
③ https://onlinelibrary.wiley.com/doi/full/10.1002/adem.202000641
④ S. Zaefferer (MPIE): Microstructures, Microscopy & Modelling.
⑤ http://www.dierk-raabe.com/ddd-discrete-dislocation-dynamics/
⑥ http://www.dierk-raabe.com/atom-probe-and-atomistic-simulations/

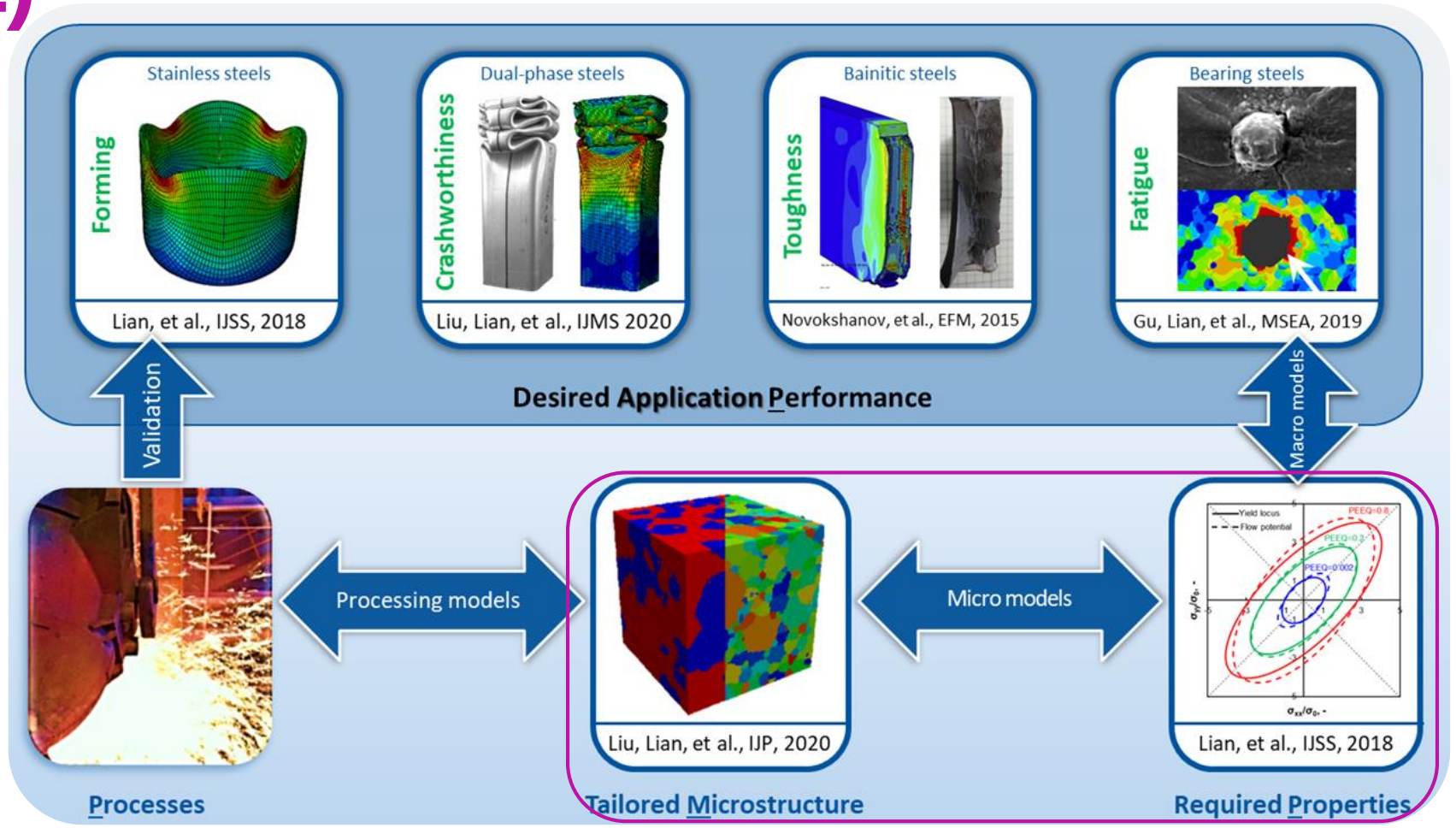
Microstructure modeling

Microstructure - property relation & microstructure -based material design



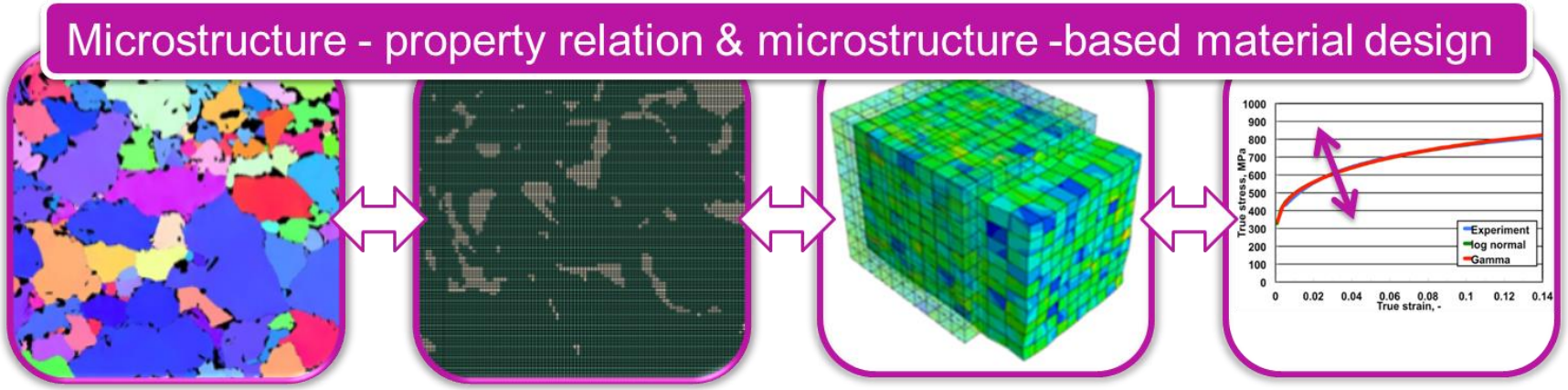
Microstructure measurement | Microstructure modeling | Virtual laboratory | Mechanical properties

Integrated computational materials engineering (ICME)



https://www.researchgate.net/lab/Junhe-Lian-Lab

Microstructure modeling - RVE



***Representative volume element (RVE)**: a sub-volume with sufficient size of the heterogeneous material that provides necessary statistical information about the material, i.e. its effective behavior is representative of the whole material. [1]*

- large enough to be statistically representative;
- contains all relevant heterogeneities;
- small enough to be regarded as point in continuum.

Mesoscale, μm

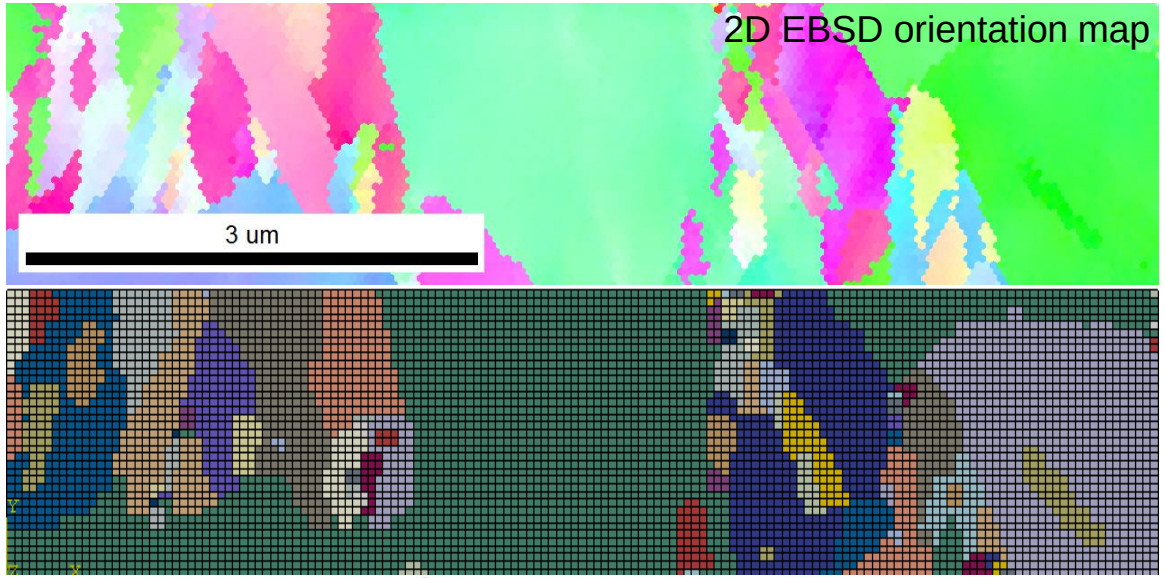
$$\Rightarrow \quad L^M \gg L^{RVE} \gg L^\mu$$

L^M: characteristic length scale of material (scale on which the material or load case exists)
L^{RVE} : size of RVE
L^μ: characteristic length scale of microstructure (e.g. size of inclusion, grain, etc.)

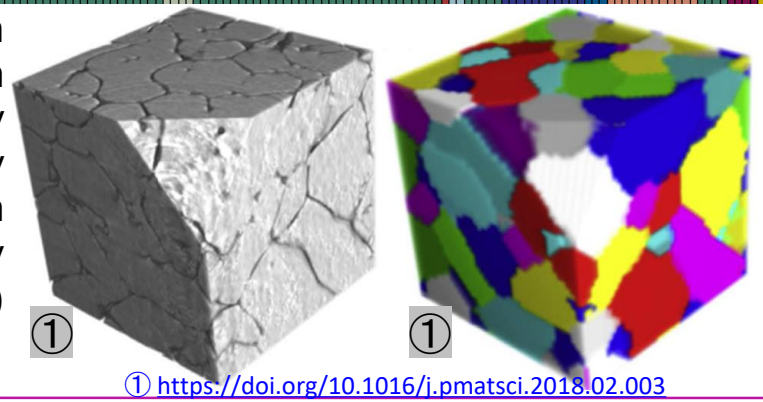
[1] https://doi.org/10.1016/j.pmatsci.2018.02.003

Microstructure modeling - RVE

- *Real microstructure RVE*

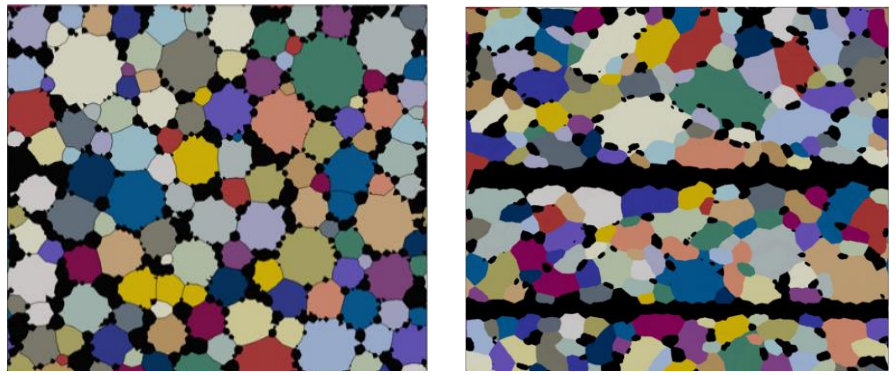


Grain reconstruction by high-energy X-ray diffraction microscopy (3DXRD)

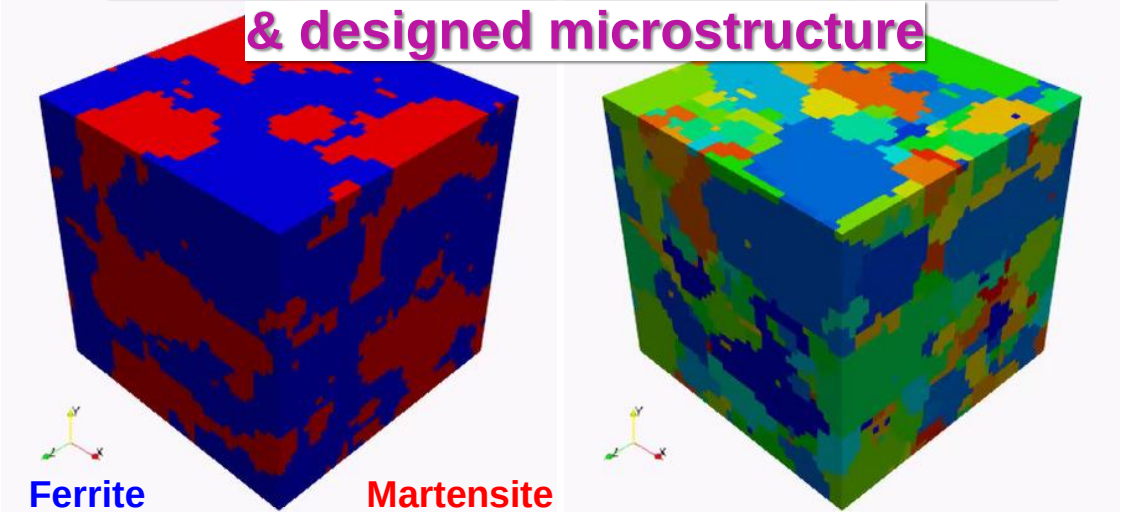


① https://doi.org/10.1016/j.pmatsci.2018.02.003

- *Artificial/synthetic microstructure RVE*



Statistical microstructure information & designed microstructure

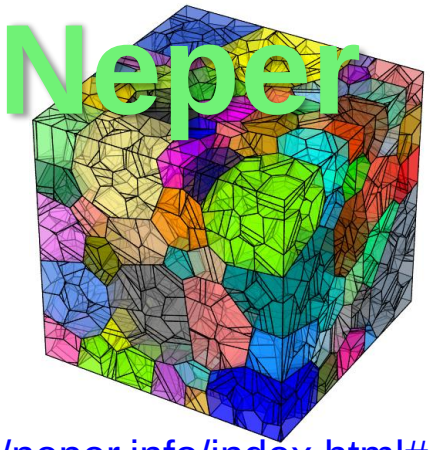


Microstructure modeling - RVE

- Generation

Digimat

https://www.e-xstream.com



https://neper.info/index.html#

GEODICT
The Digital Material Laboratory

https://www.geodict.com/

DREAM.3D
BlueQuartz Edition

http://dream3d.bluequartz.net

simpleware

https://www.synopsys.com/simpleware.html

- Visualization

ParaView

https://www.paraview.org

micress®

https://micress.rwth-aachen.de/index.html

DREAM.3D & ParaView preparation

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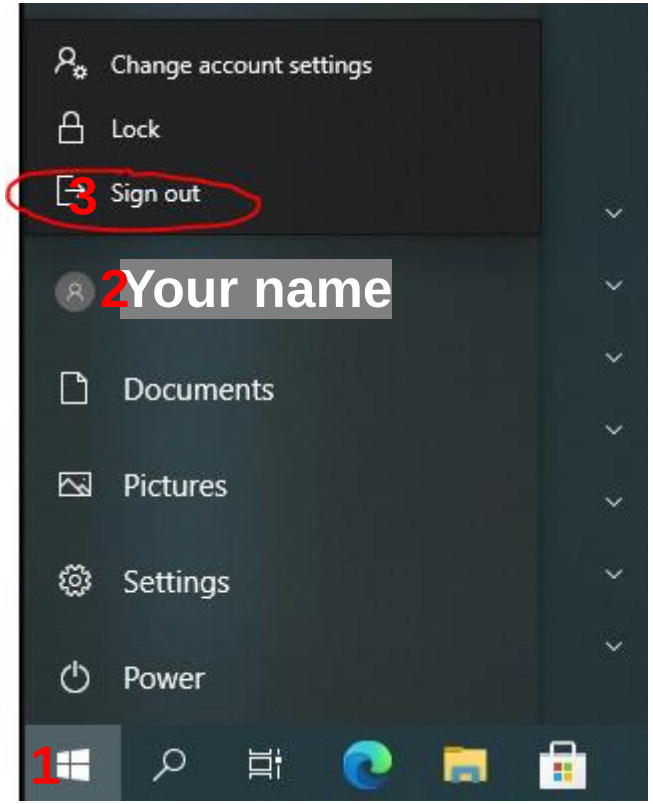
Software preparation

DREAM.3D: open-source/freeware software http://dream3d.bluequartz.net
ParaView: freeware software https://www.paraview.org/download/
Aalto VDI system: **mfavdi.aalto.fi**, or VMware Horizon Client **vdi.aalto.fi**, for more information, please refer to Remote access to Windows classroom computers.
IMPORTANT! Please remember to do '**Sign Out**' after the session (NOT Disconnect). Click your username in Start and click 'Sign Out'.

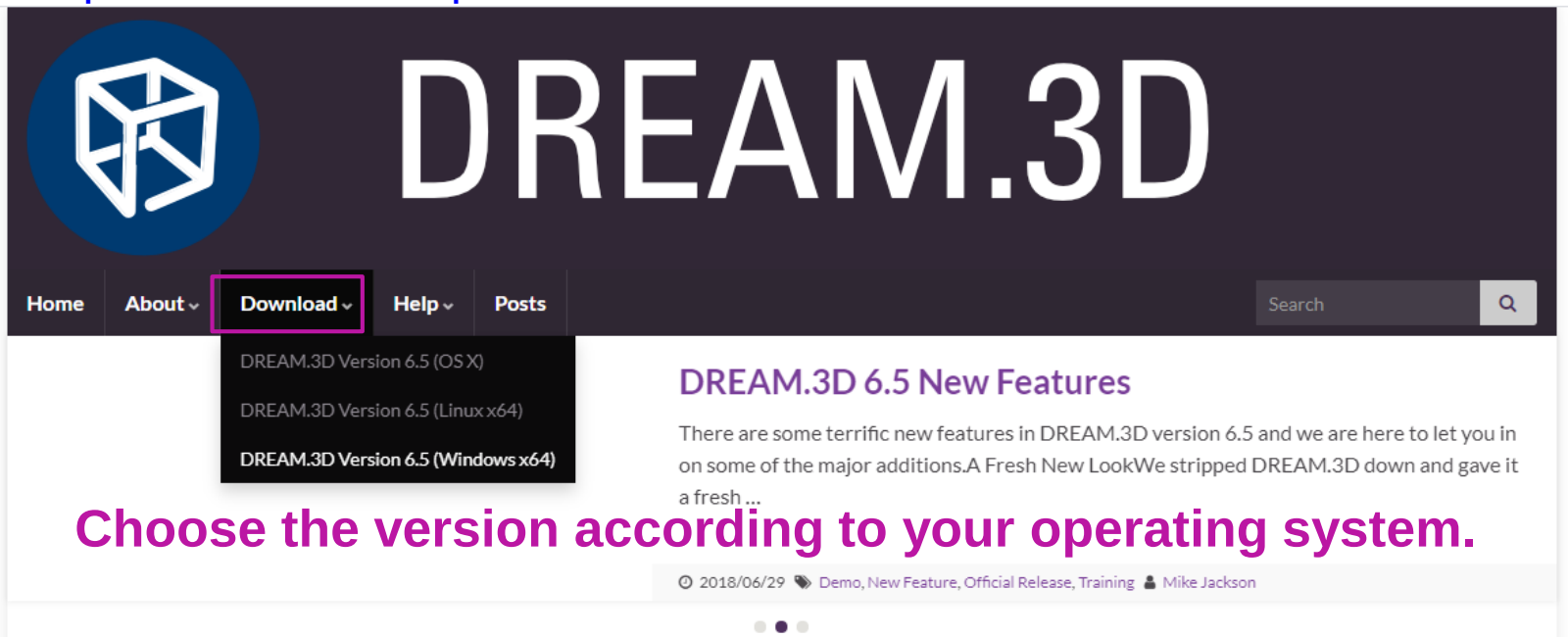
Basic Rule: Please use POINT as the decimal separator, NO COMMA!

Please download and extract the zip file of DREAM.3D and ParaView, and copy it to your work direction. No installation needed, just unzip package and start.



DREAM.3D Download

http://dream3d.bluequartz.net



Choose the version according to your operating system.

Home

DREAM.3D consists of data analysis tools (***Filters***) that allow for the construction of customized workflows (***Pipelines***) to analyze data. DREAM.3D provides a flexible and extensible data structure that eases data transport between collaborators by storing data in a non-proprietary format.

DREAM.3D makes the reconstruction of 3D data simple and straight forward. The development of additional features is ongoing and the DREAM.3D development team welcomes your feedback whether you are a first time user or seasoned user.

All source codes are publicly available through the GitHub repository. The GitHub web site also has the official bug tracker.

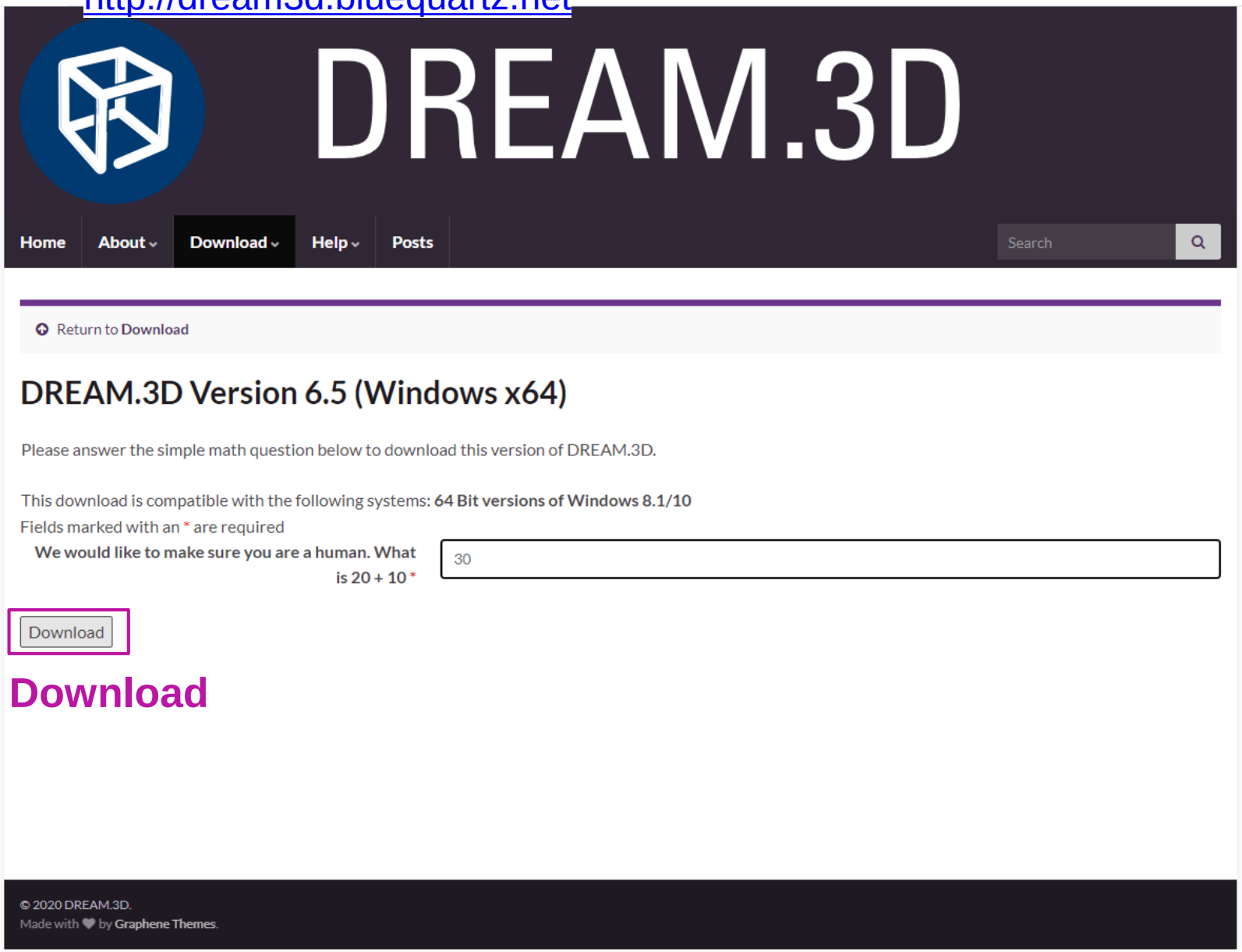
DREAM.3D is completely open source and ***free*** for anyone to use whether that is in a commercial, academic or research setting. We encourage every one to give it a try and provide feedback about your experience.

Features of DREAM.3D

1. 3D Reconstruction of EBSD data from EDAX (.ang), Oxford (.ctf) and Bruker (.ctf) data files. The reconstructions can utilize an array of alignment, cleaning, segmentation algorithms and coloring algorithms.

DREAM.3D Download

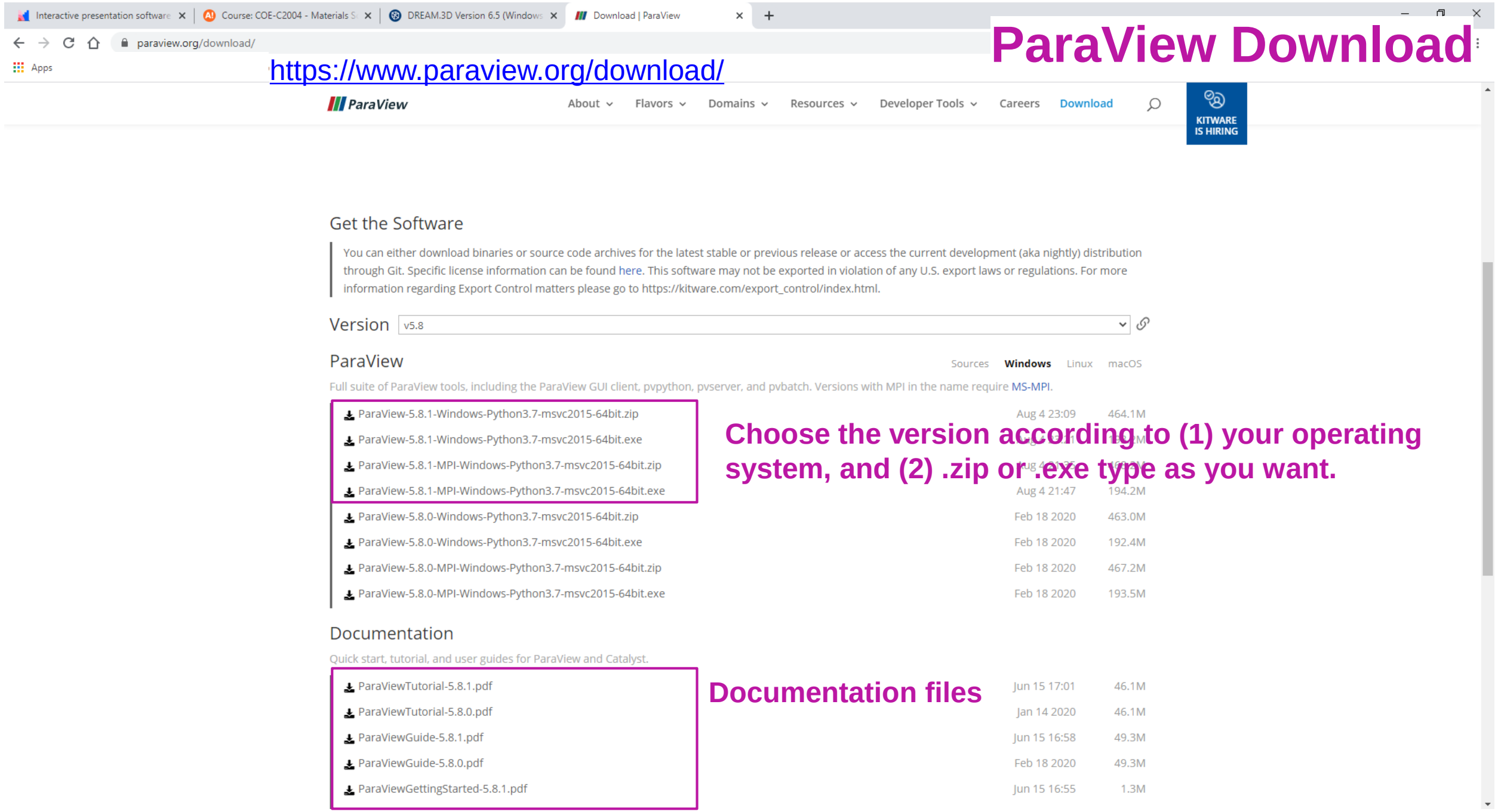
http://dream3d.bluequartz.net



Download

ParaView Download

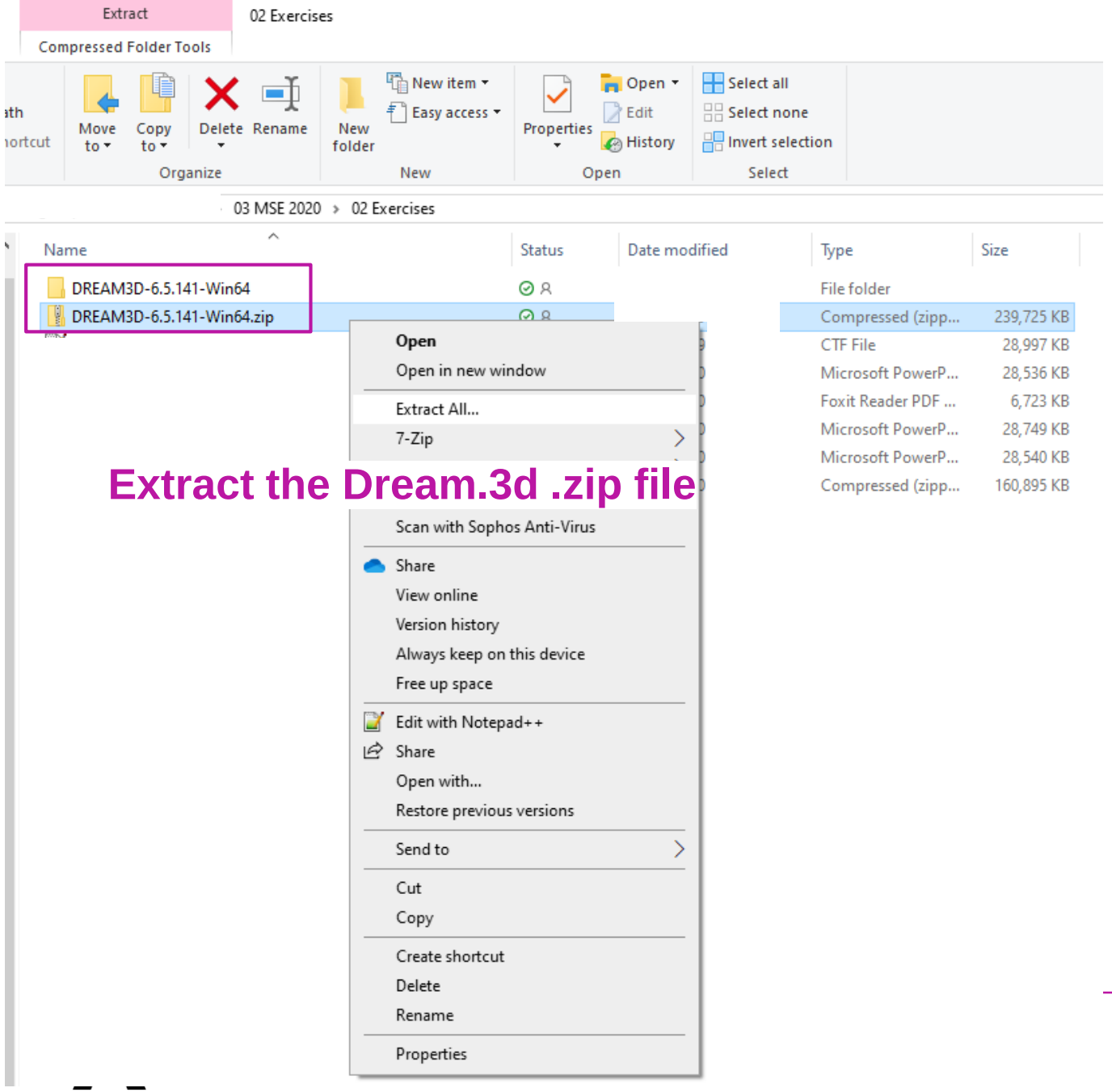
https://www.paraview.org/download/



Choose the version according to (1) your operating system, and (2) .zip or .exe type as you want.

Documentation files

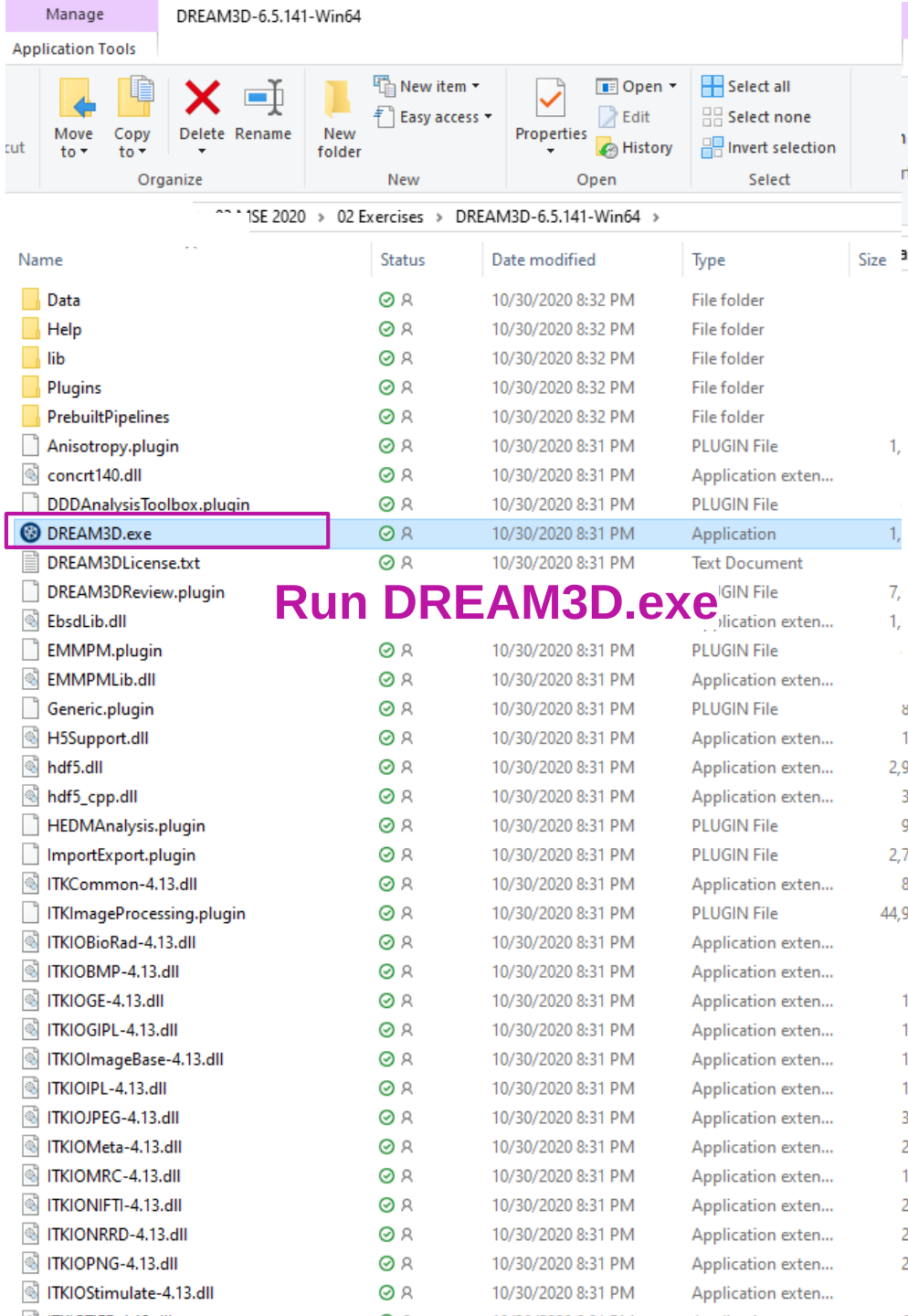
DREAM.3D & ParaView Extraction



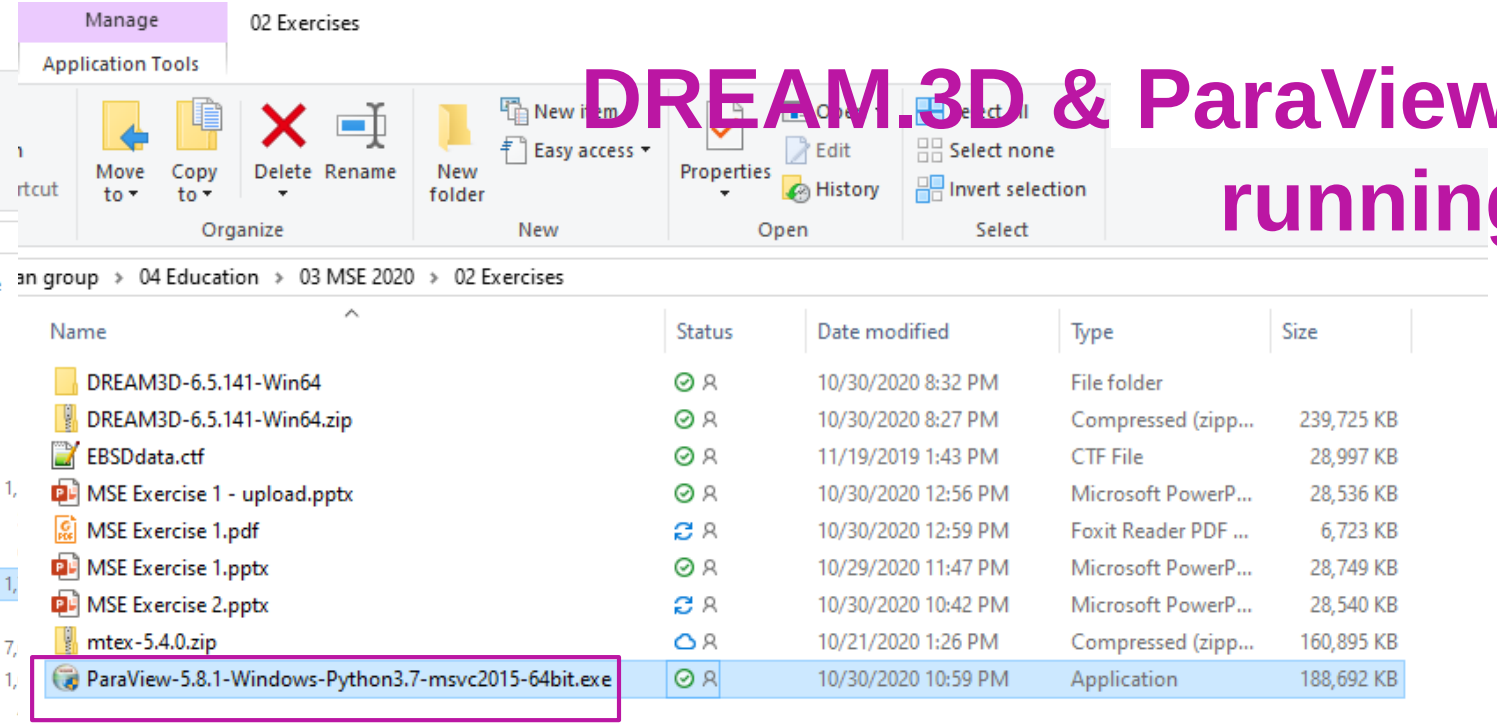
Extract the Dream.3d .zip file

Do the extract again if you also choose the .zip file for ParaView.

DREAM.3D & ParaView running



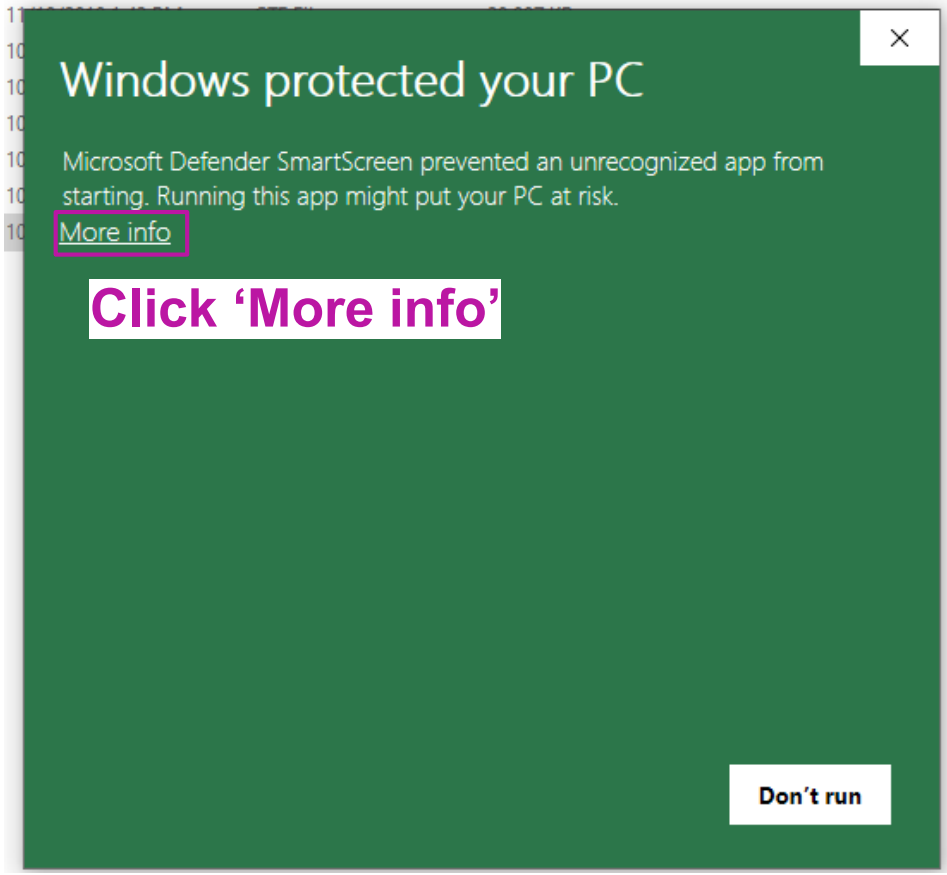
Run DREAM3D.exe

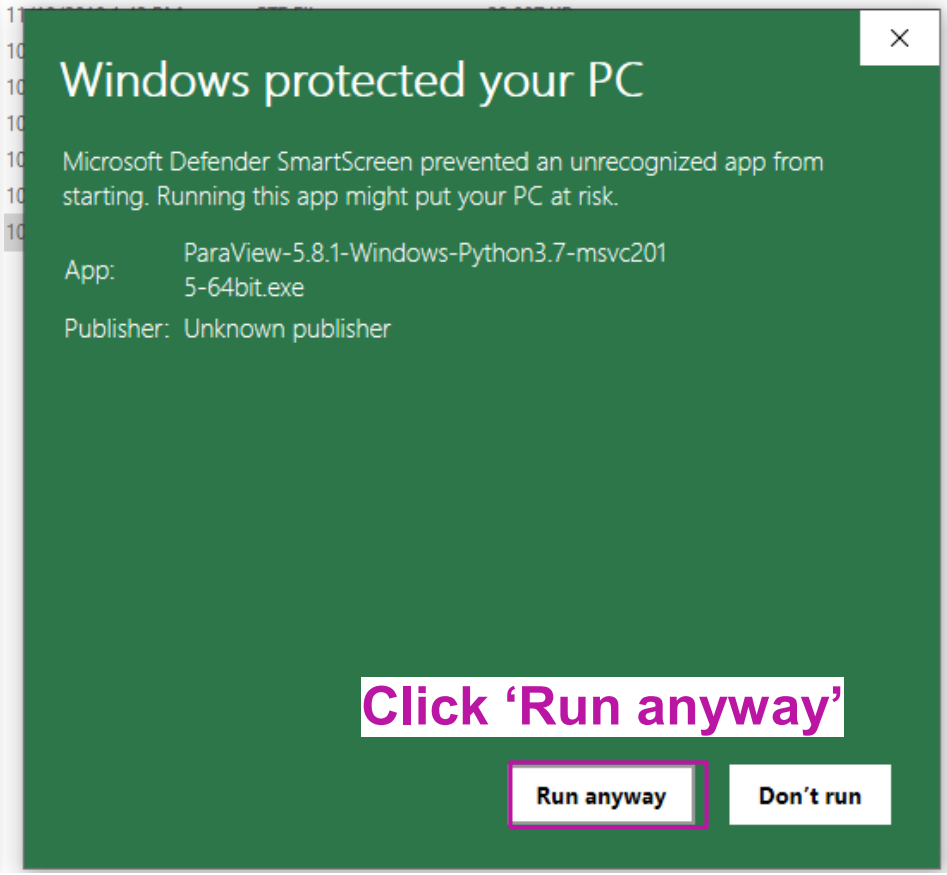


If you download the exe version, you need to install it first.
If you download the zip version, directly run the application.

DREAM.3D & ParaView installation

To run an .exe application in windows system





Basic DREAM.3D operation (Equiaxed single phase)

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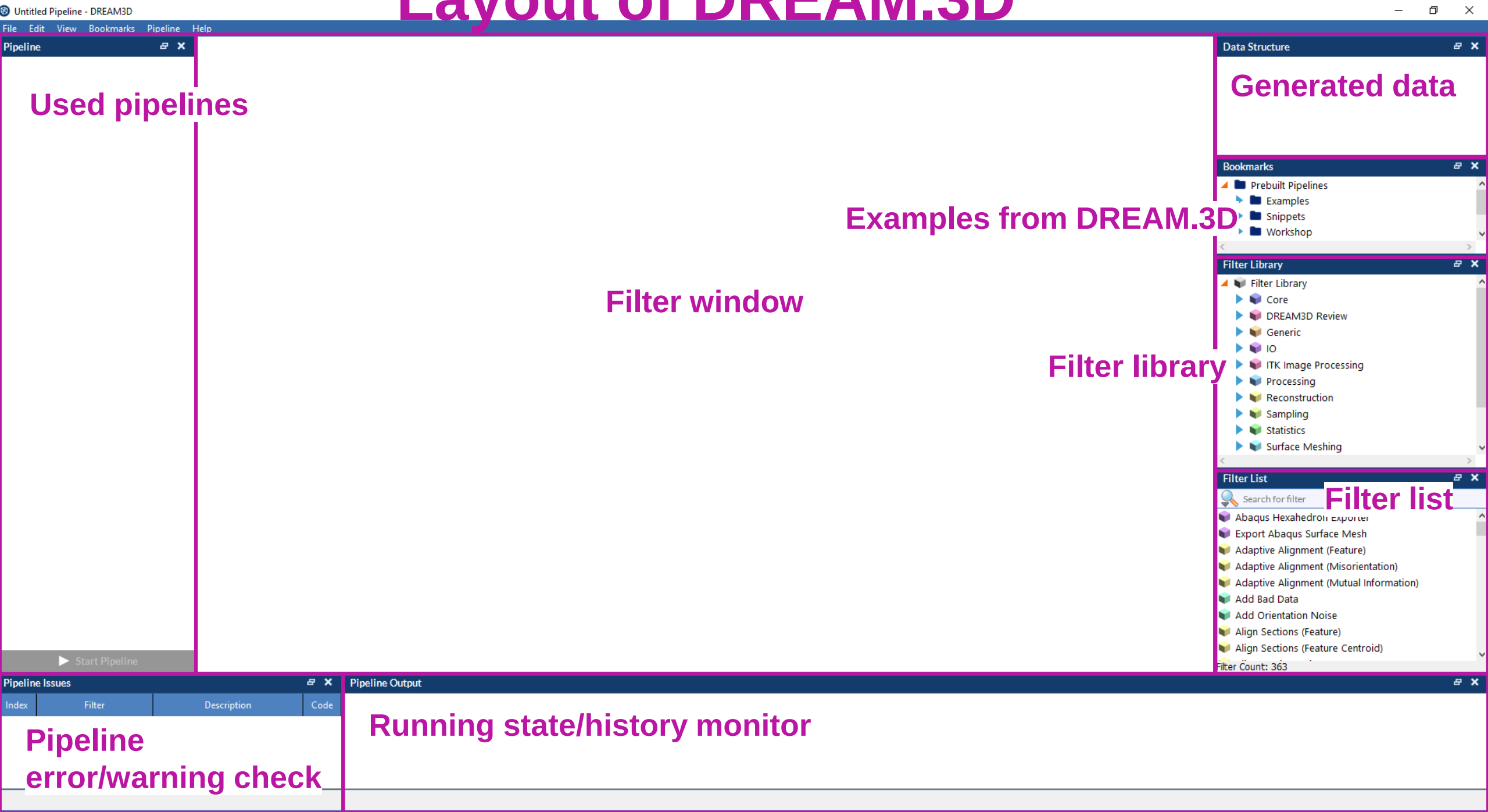
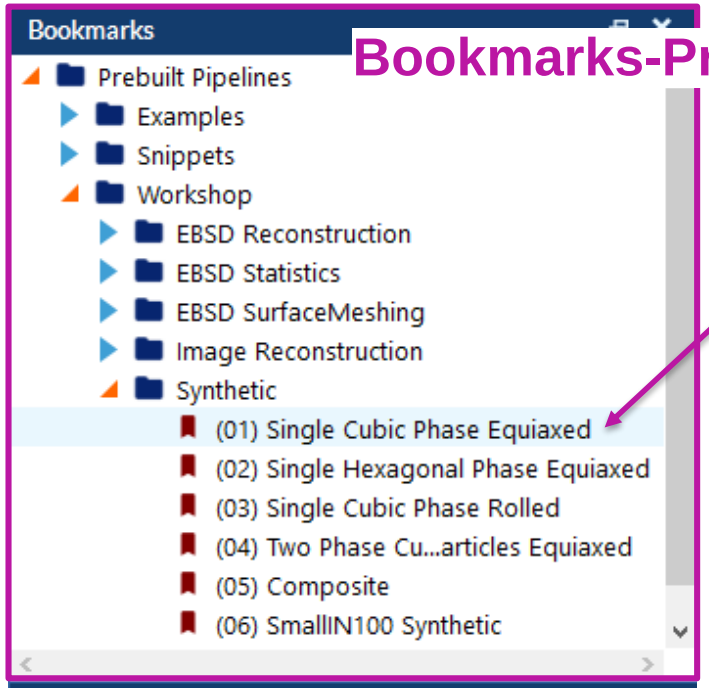
Layout of DREAM.3D

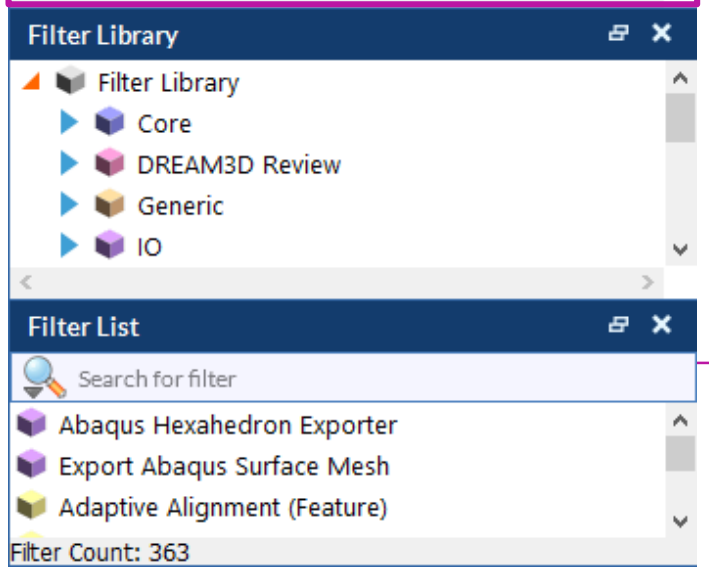


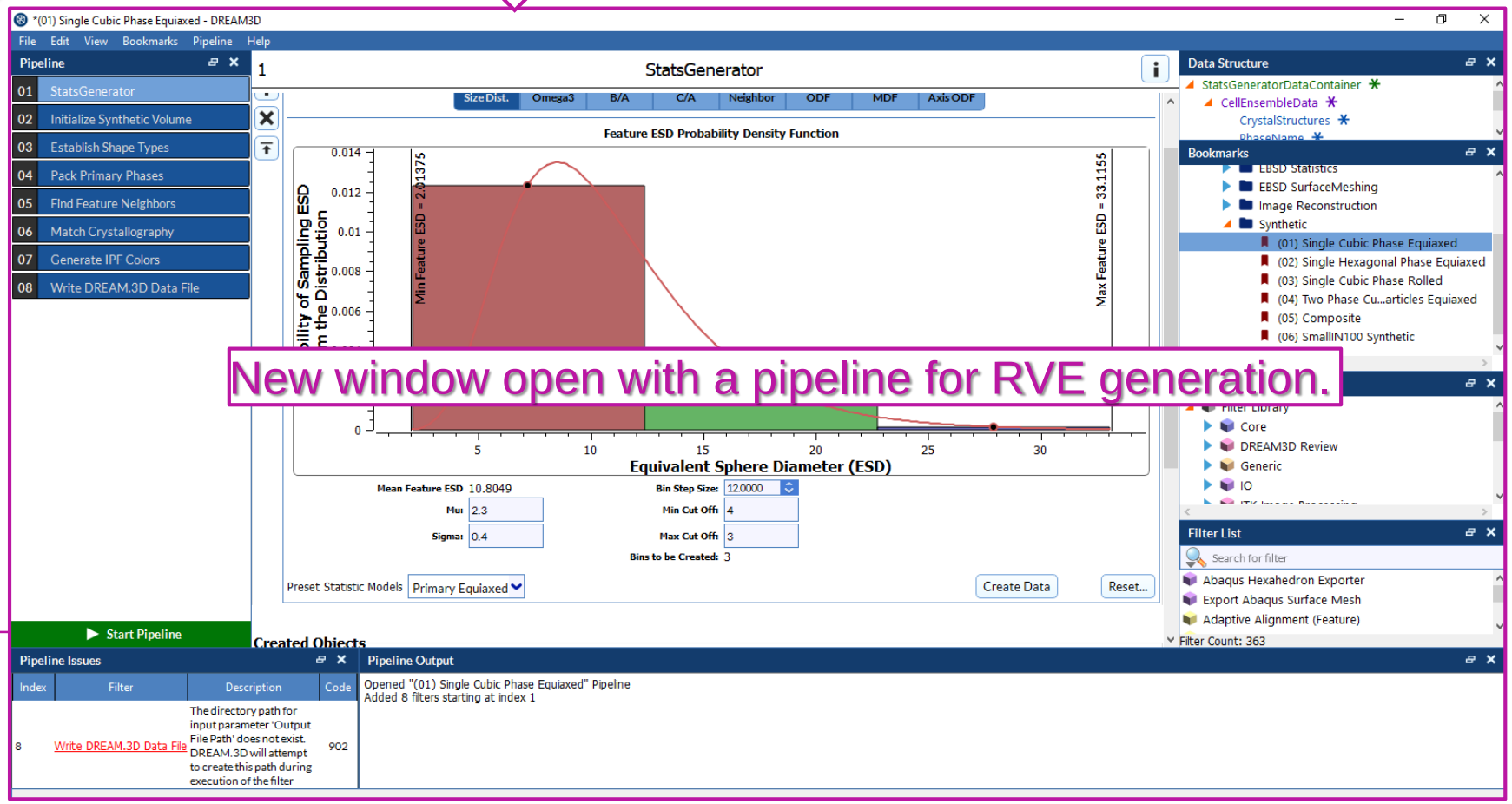
Build up a pipeline

Bookmarks-Prebuilt pipelines: Examples from DREAM.3D

Start from the single-phase cube structure.
Click '(01) Single Cubic Phase Equiaxed'

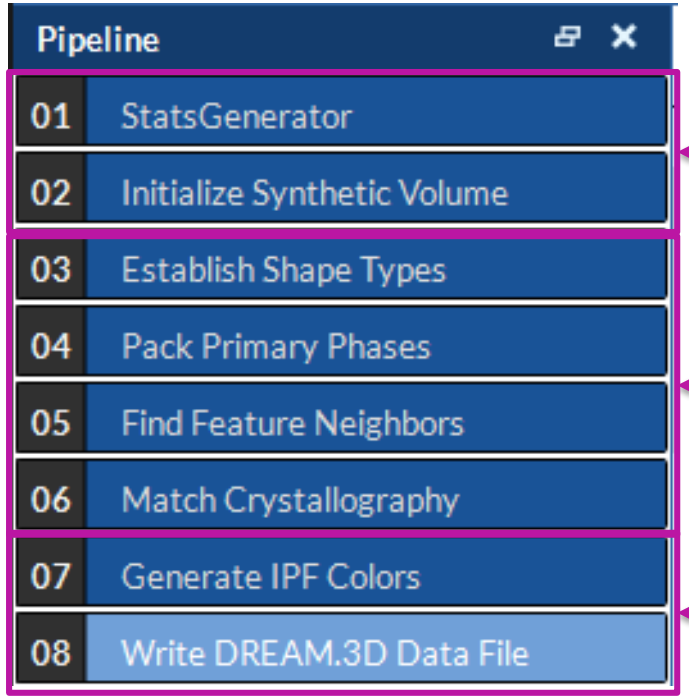






New window open with a pipeline for RVE generation.

DREAM.3D pipelines

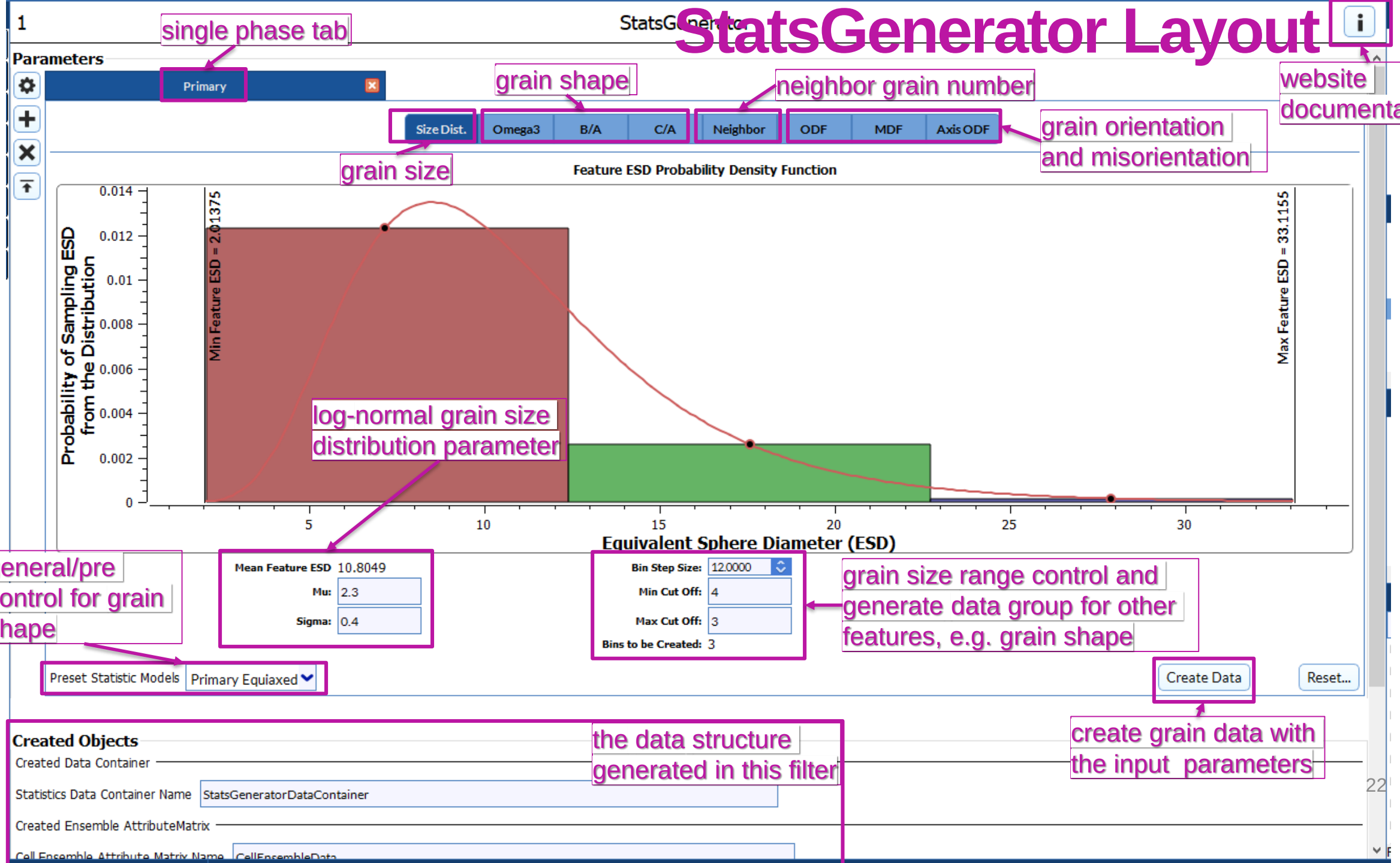


Pre-setting for input features & aimed RVE parameters

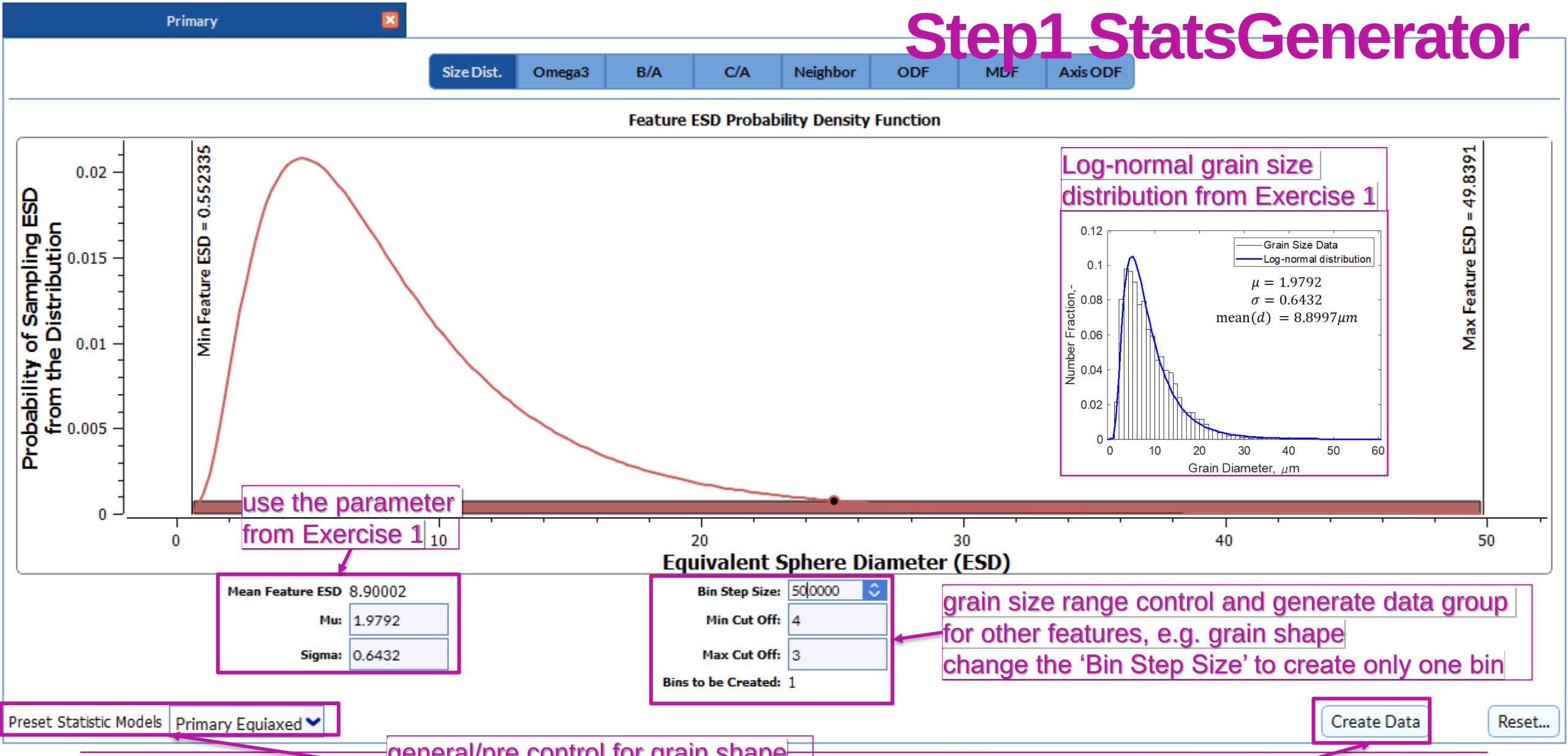
Feature packing and RVE generation process

Output setting for generated RVE

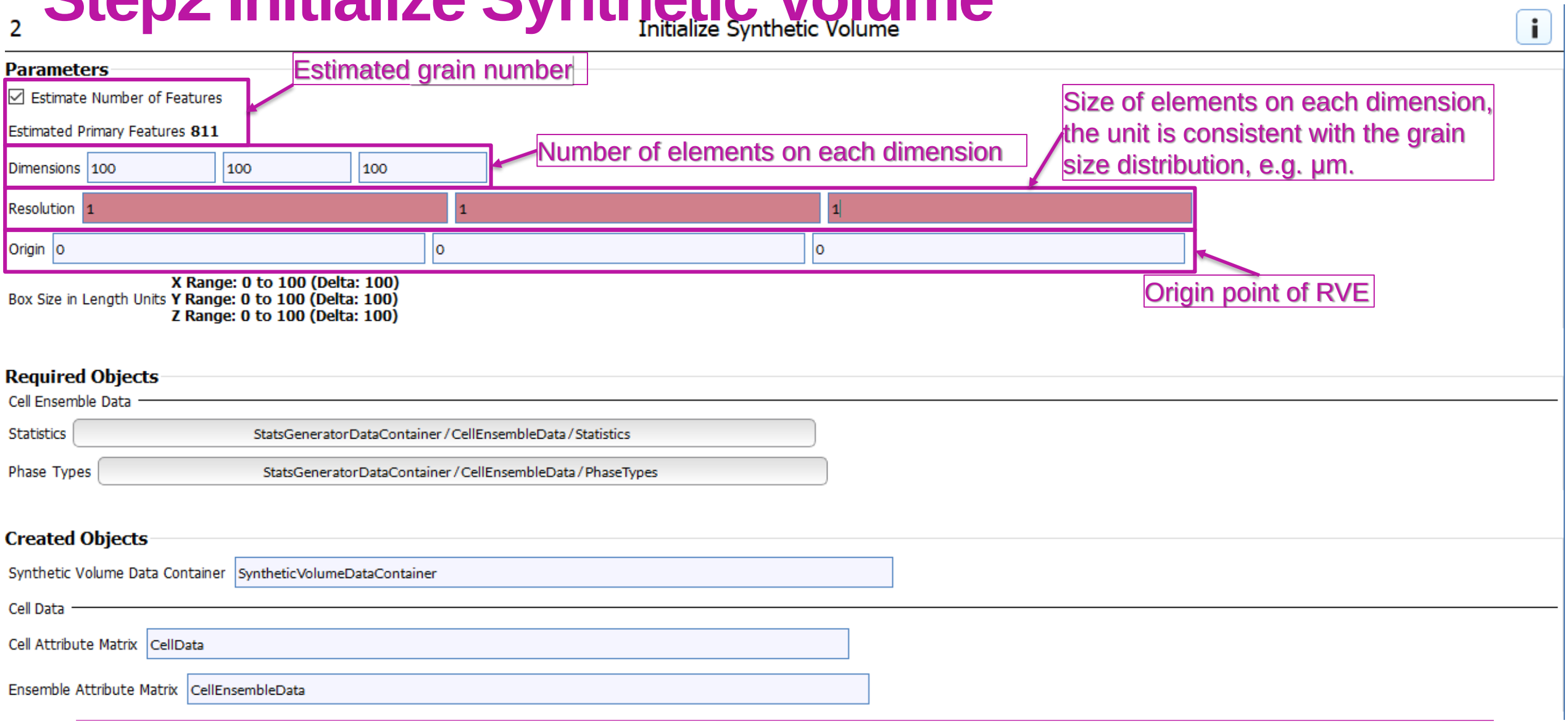
StatsGenerator Layout



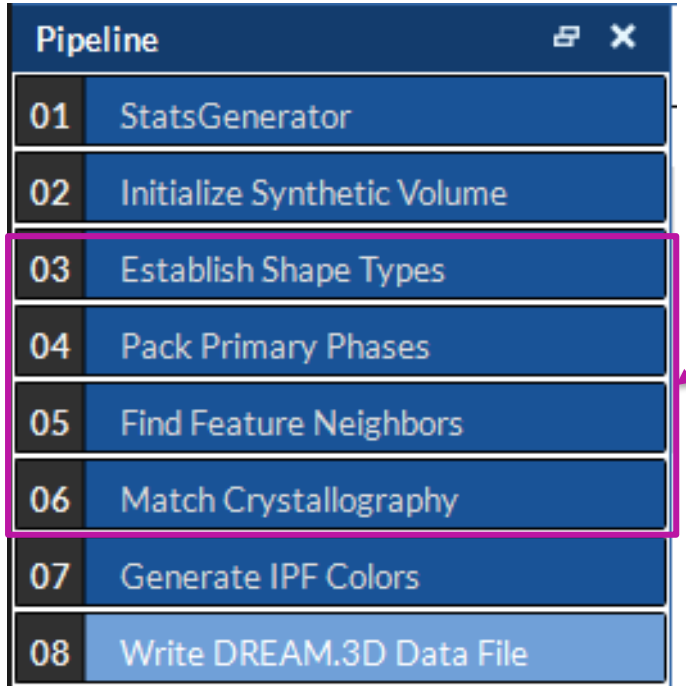
Step1 StatsGenerator



Step2 Initialize Synthetic Volume



DREAM.3D - Generation process



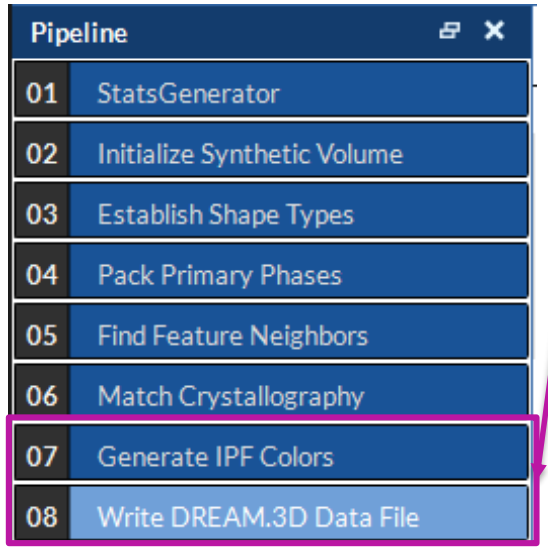
Feature packing and RVE generation process:

- Assign a specific shape type according to user definition in StatsGenerator, e.g. ellipsoid
- Synthetic microstructure building (packing process)
- Determine the number of other grains that are in contact with one grain.
- Match the grain orientation distribution
- Add more Filters here is possible to achieve more functions, like packing the precipitates
- More information is regarding to DREAM.3D tutorial system: http://127.0.0.1:32456/2_Tutorials/SyntheticSinglePhase/

Step3 Generation process:

for these filters, directly use the default setting without any changes, but you need to click and review one by one and solve the probable error/missing data structure, which is shown in the 'Pipeline Issues'.

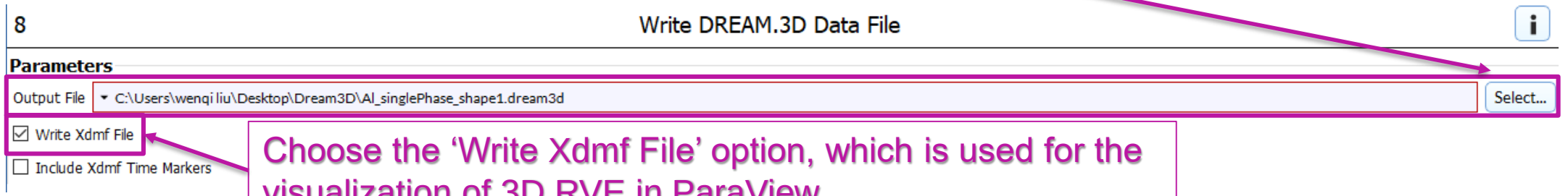
DREAM.3D - RVE output



Step4 Output setting for generated RVE

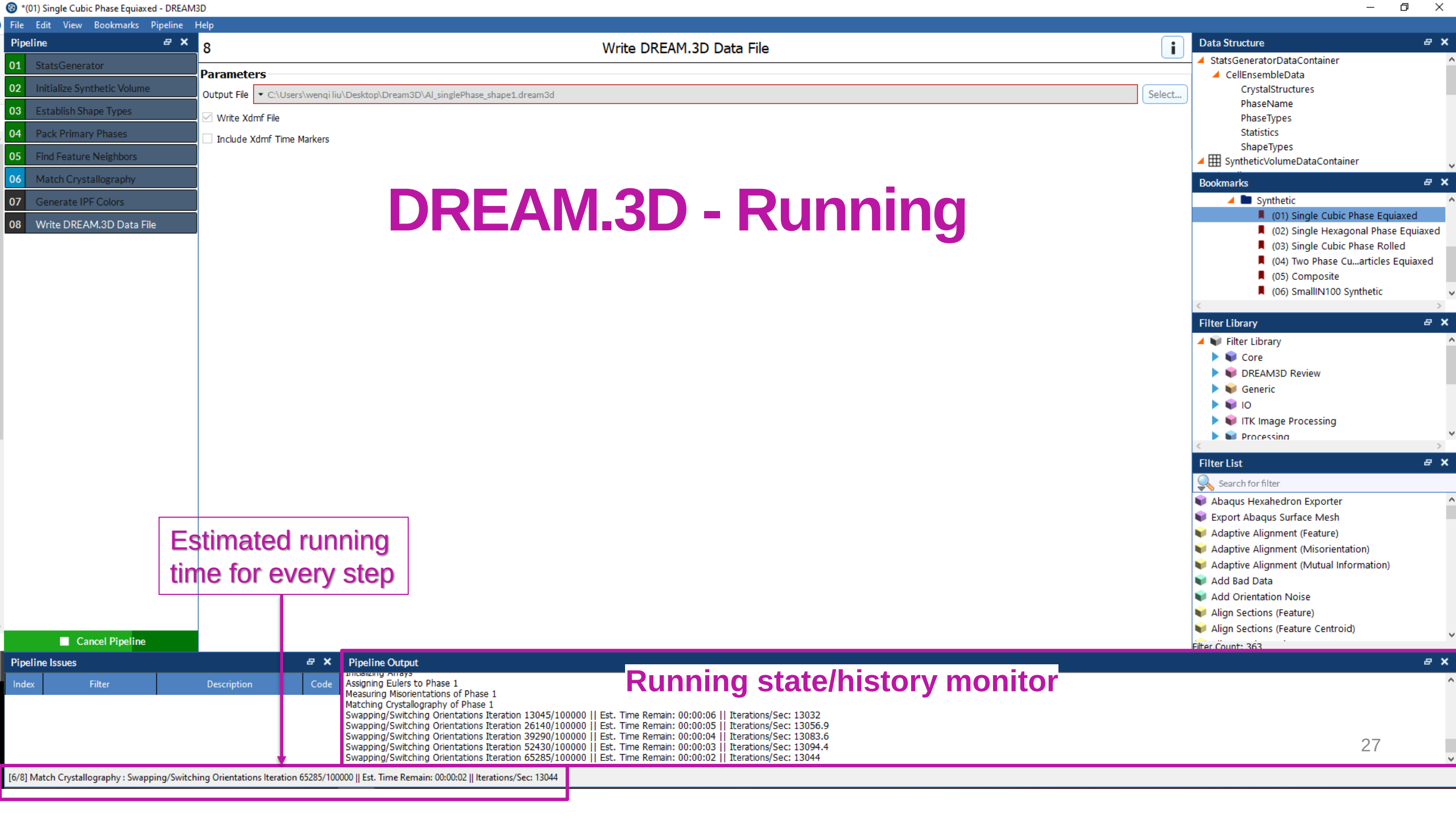
- 'Generate IPF Colors' is set for the grain orientation distribution. Use the default setting.

- 'Write GREAM.3D Data File': click 'Select' to choose the path for your output data here and name the output .dream3d file.

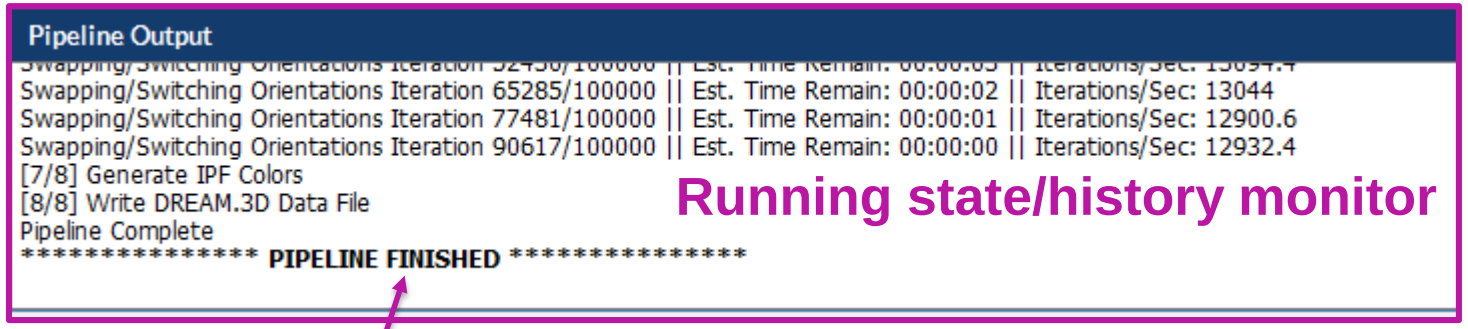


Choose the 'Write Xdmf File' option, which is used for the visualization of 3D RVE in ParaView.

Step5: Click to run the generator


*(01) Single Cubic Phase Equiaxed - DREAM3D
File Edit View Bookmarks Pipeline Help
Pipeline
01 StatsGenerator
02 Initialize Synthetic Volume
03 Establish Shape Types
04 Pack Primary Phases
05 Find Feature Neighbors
06 Match Crystallography
07 Generate IPF Colors
08 Write DREAM.3D Data File
8
Write DREAM.3D Data File
Parameters
Output File
C:\Users\wenqi liu\Desktop\Dream3D\AI_singlePhase_shape1.dream3d
Select...
Write Xdmf File
Include Xdmf Time Markers
DREAM.3D - Running
Data Structure
StatsGeneratorDataContainer
CellEnsembleData
CrystalStructures
PhaseName
PhaseTypes
Statistics
ShapeTypes
SyntheticVolumeDataContainer
Bookmarks
Synthetic
(01) Single Cubic Phase Equiaxed
(02) Single Hexagonal Phase Equiaxed
(03) Single Cubic Phase Rolled
(04) Two Phase Cu...articles Equiaxed
(05) Composite
(06) SmallIN100 Synthetic
Filter Library
Filter Library
Core
DREAM3D Review
Generic
IO
ITK Image Processing
Processing
Filter List
Search for filter
Abaqus Hexahedron Exporter
Export Abaqus Surface Mesh
Adaptive Alignment (Feature)
Adaptive Alignment (Misorientation)
Adaptive Alignment (Mutual Information)
Add Bad Data
Add Orientation Noise
Align Sections (Feature)
Align Sections (Feature Centroid)
Filter Count: 363
Estimated running time for every step
Cancel Pipeline
Pipeline Issues
Index
Filter
Description
Code
Pipeline Output
Assigning Eulers to Phase 1
Measuring Misorientations of Phase 1
Matching Crystallography of Phase 1
Swapping/Switching Orientations Iteration 13045/100000 || Est. Time Remain: 00:00:06 || Iterations/Sec: 13032
Swapping/Switching Orientations Iteration 26140/100000 || Est. Time Remain: 00:00:05 || Iterations/Sec: 13056.9
Swapping/Switching Orientations Iteration 39290/100000 || Est. Time Remain: 00:00:04 || Iterations/Sec: 13083.6
Swapping/Switching Orientations Iteration 52430/100000 || Est. Time Remain: 00:00:03 || Iterations/Sec: 13094.4
Swapping/Switching Orientations Iteration 65285/100000 || Est. Time Remain: 00:00:02 || Iterations/Sec: 13044
Running state/history monitor
[6/8] Match Crystallography : Swapping/Switching Orientations Iteration 65285/100000 || Est. Time Remain: 00:00:02 || Iterations/Sec: 13044

DREAM.3D - Data files

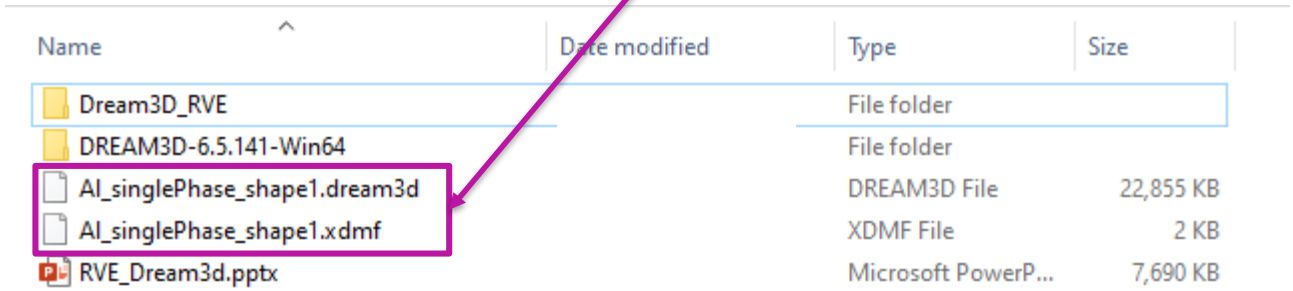


Running state/history monitor

Successfully finished

Check your DREAM.3D output folder:

- '.dream3d' DREAM.3D type data
- '.xdmf' type file for ParaView



ParaView operation

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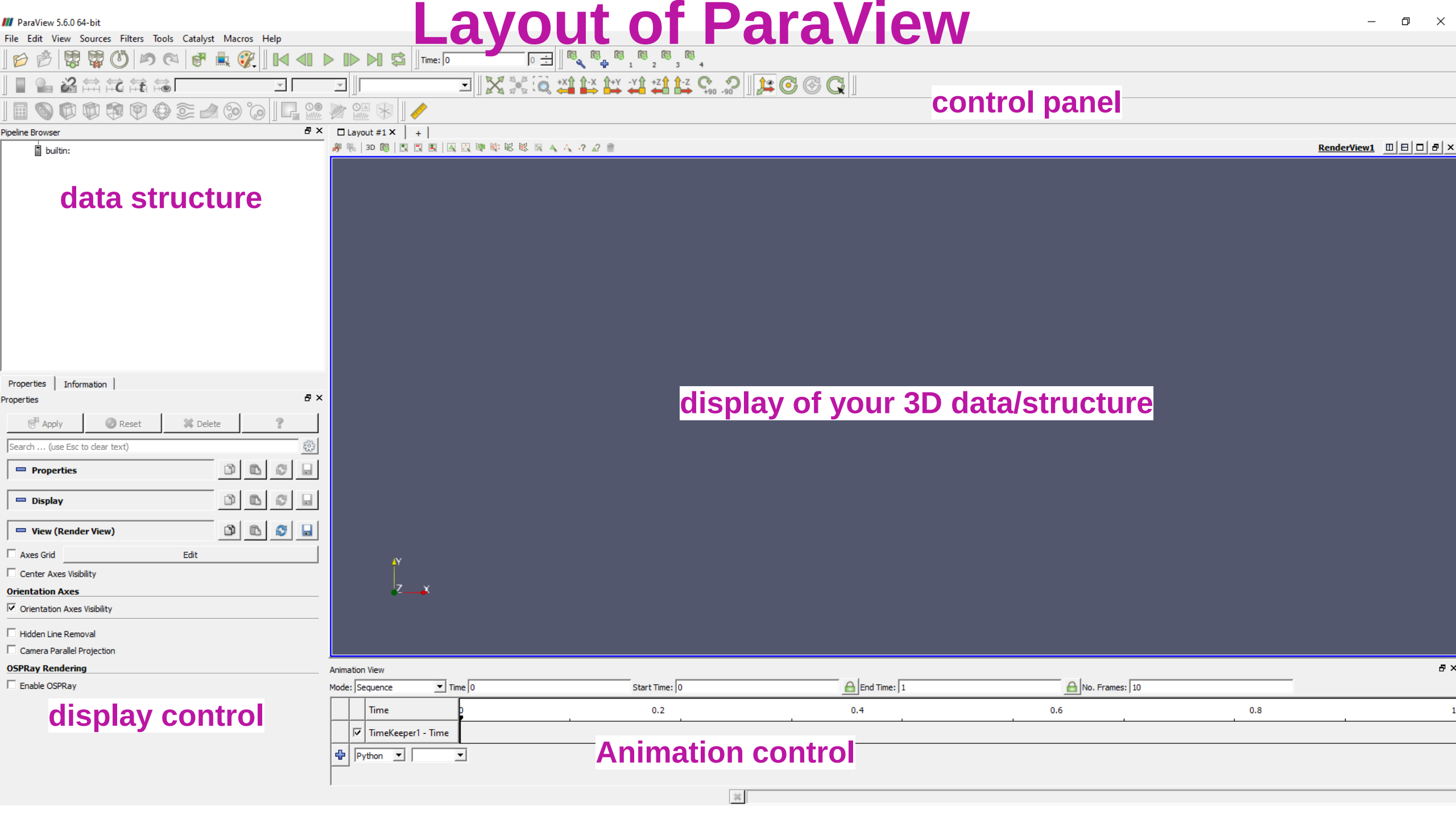
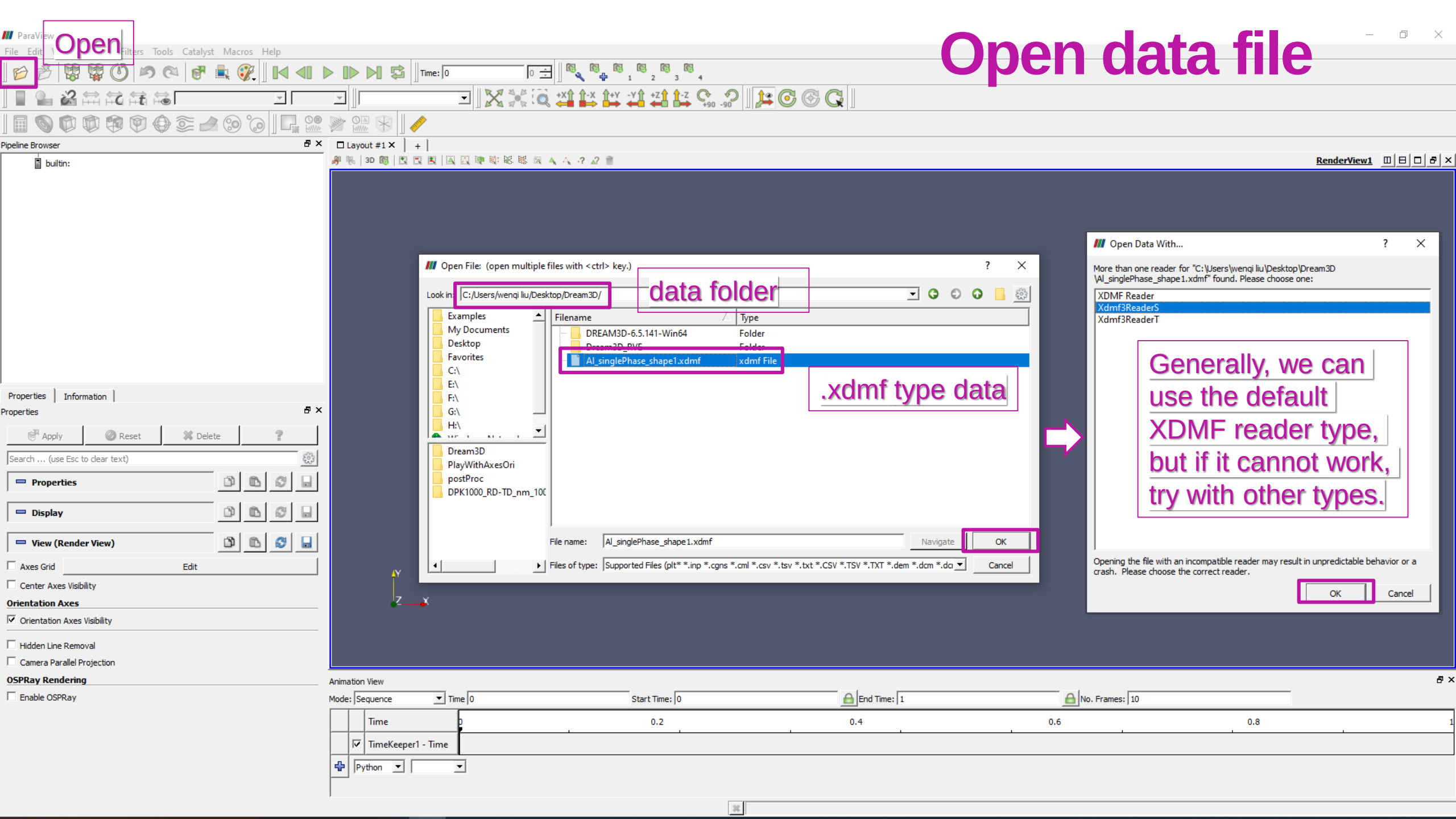
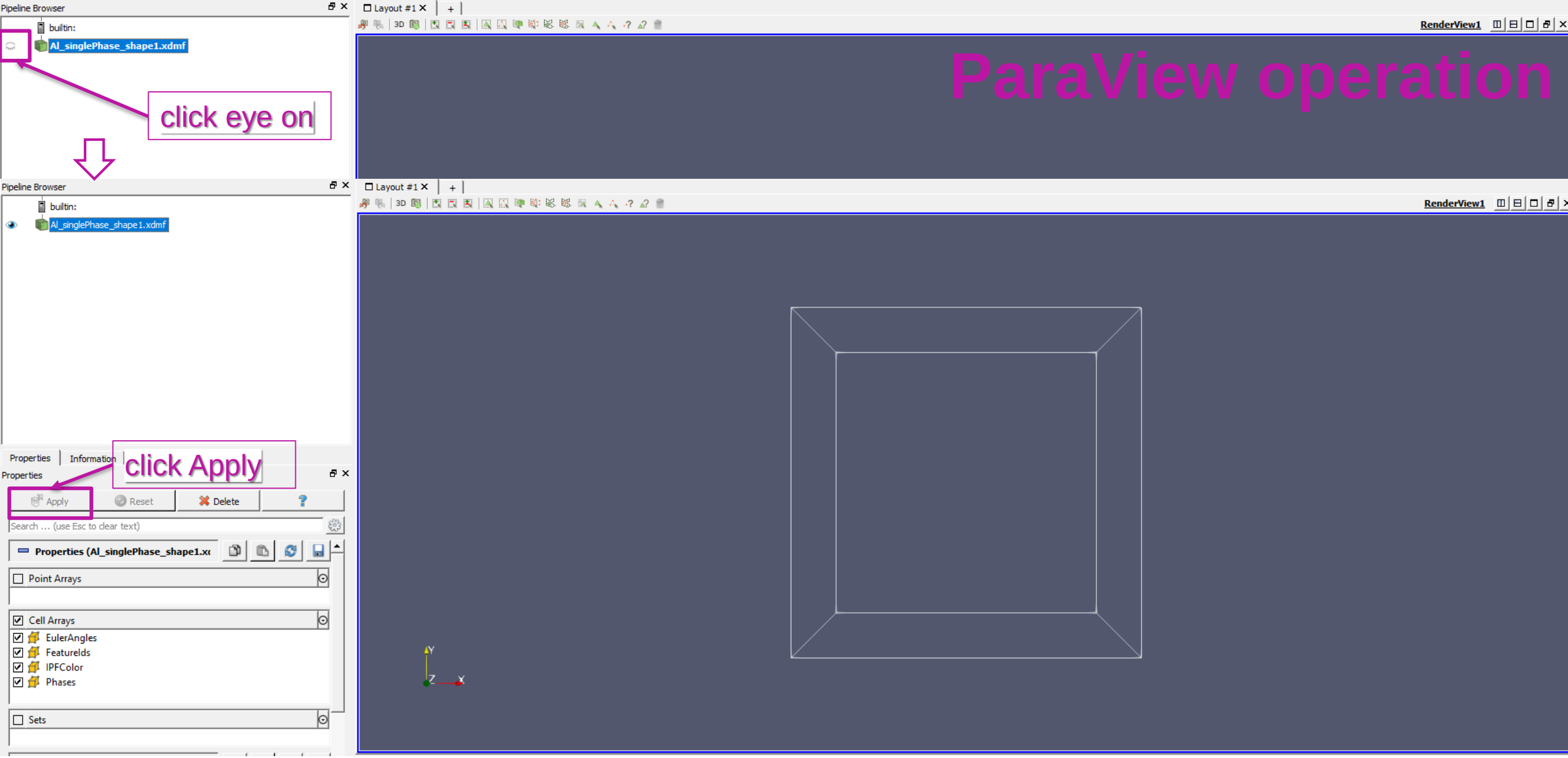
Layout of ParaView

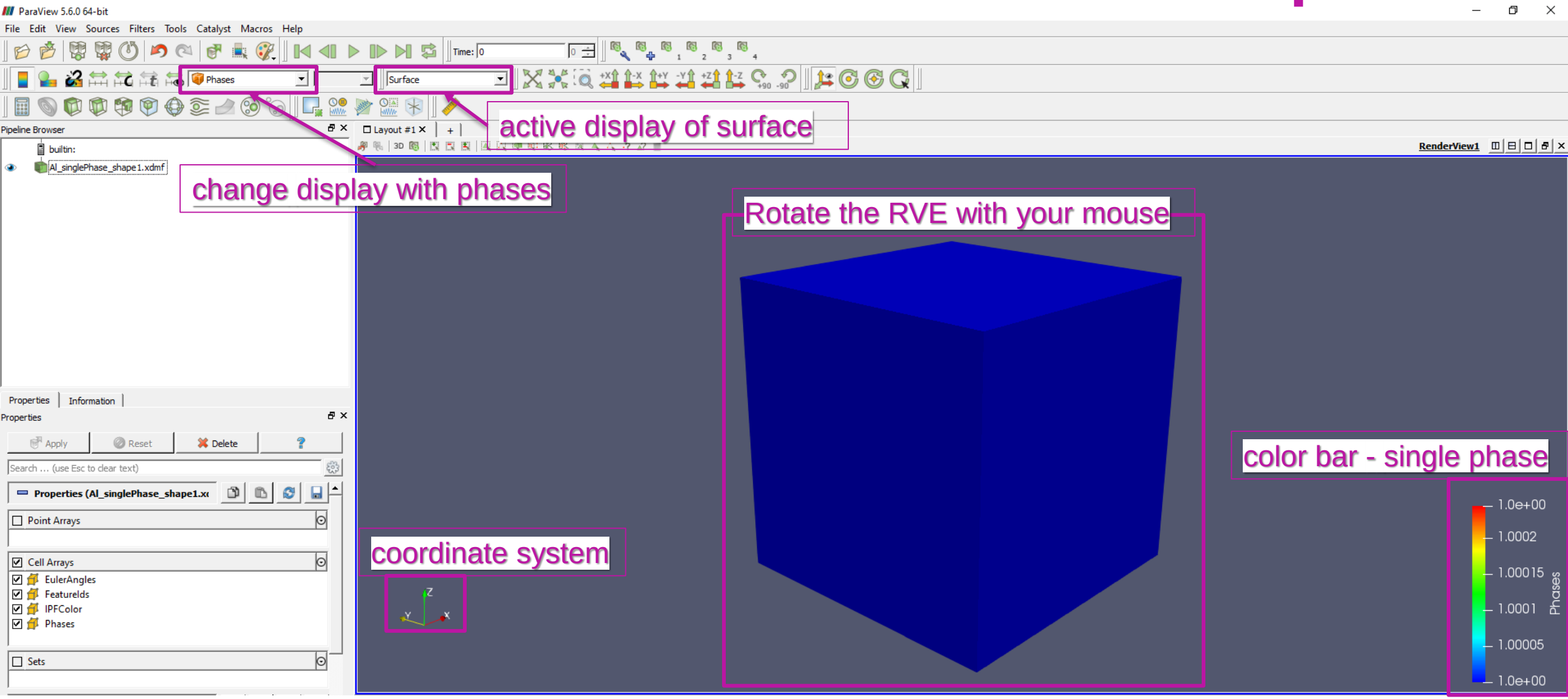


Open data file

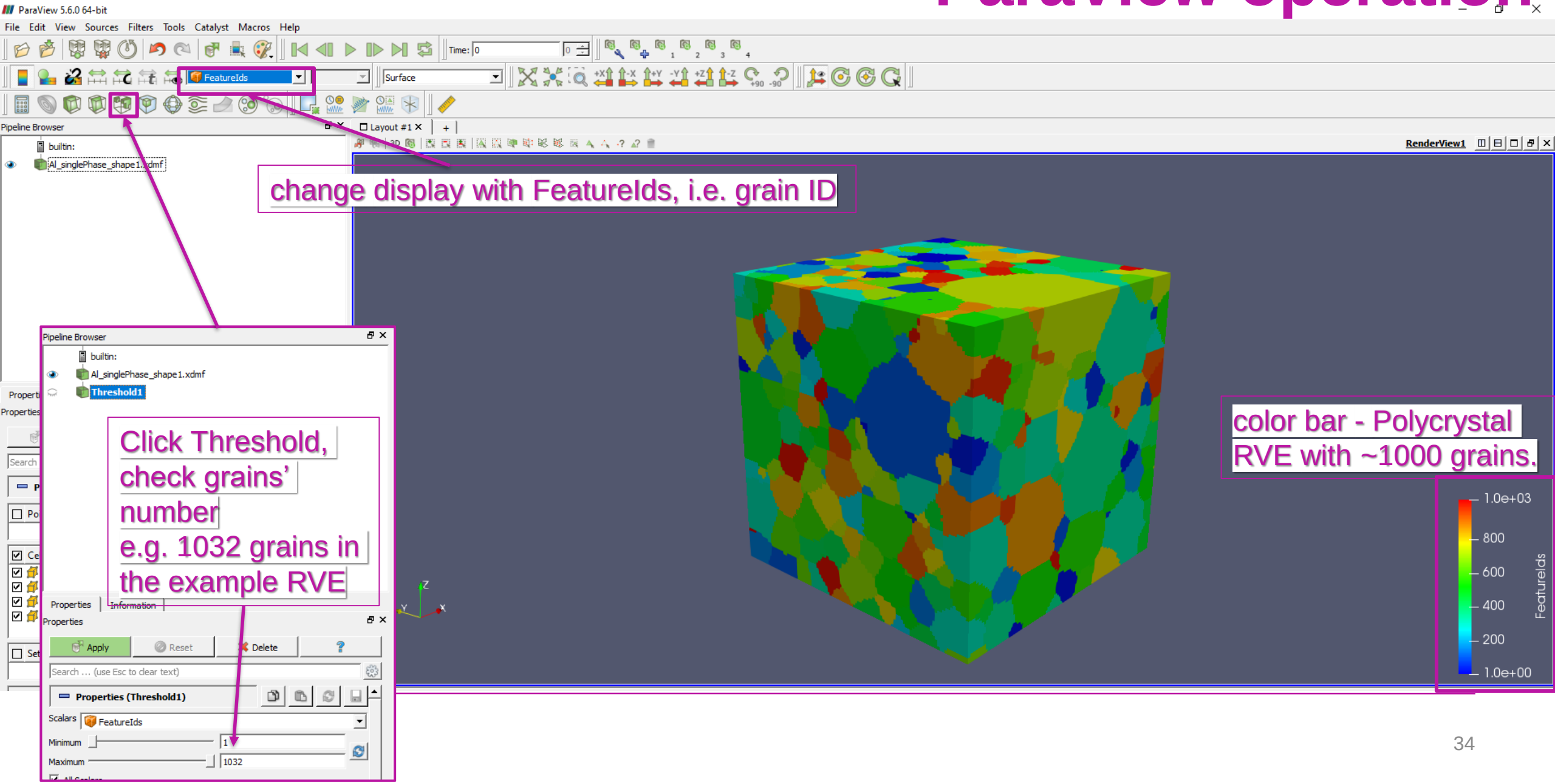



Pipeline Browser
builtin:
Al_singlePhase_shape1.xdmf
click eye on
ParaView operation
Layout #1
RenderView1
Pipeline Browser
builtin:
Al_singlePhase_shape1.xdmf
Layout #1
RenderView1
Properties
Information
click Apply
Properties
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties (Al_singlePhase_shape1.x
Point Arrays
Cell Arrays
EulerAngles
FeatureIds
IPFColor
Phases
Sets

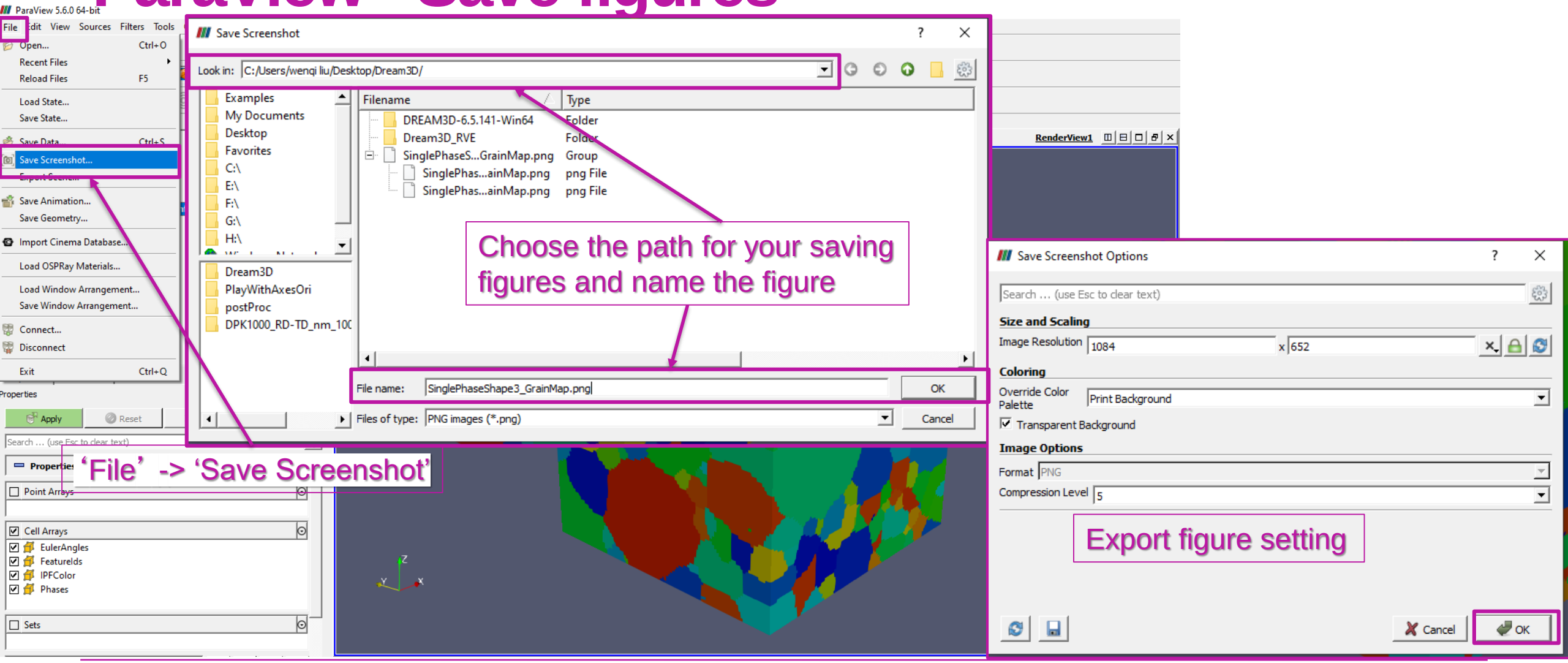
ParaView operation



ParaView operation



ParaView - Save figures



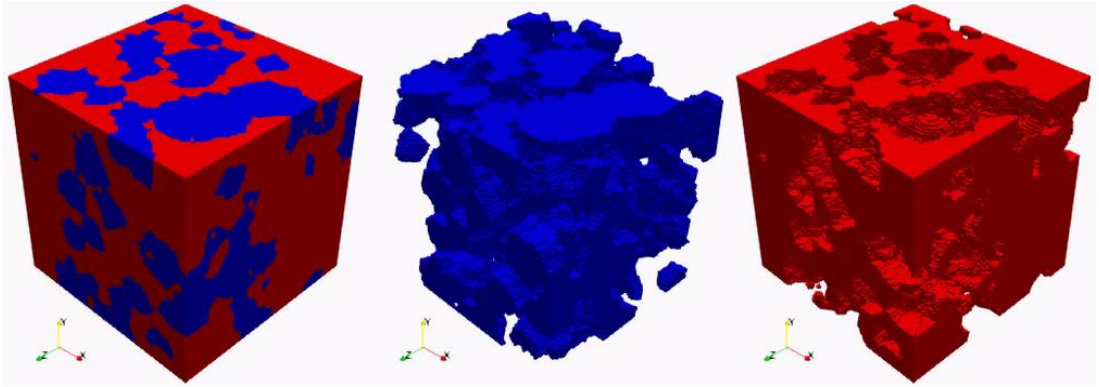
Advanced DREAM.3D operation

Aalto University
School of Engineering

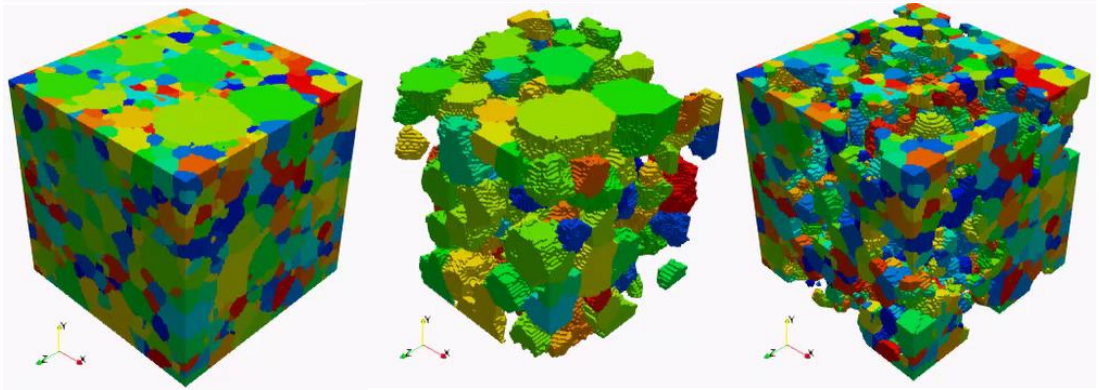
DREAM.3D For more features

- Rolled grain structure
- Grain shape distribution
- Dual-/multi-phase structure

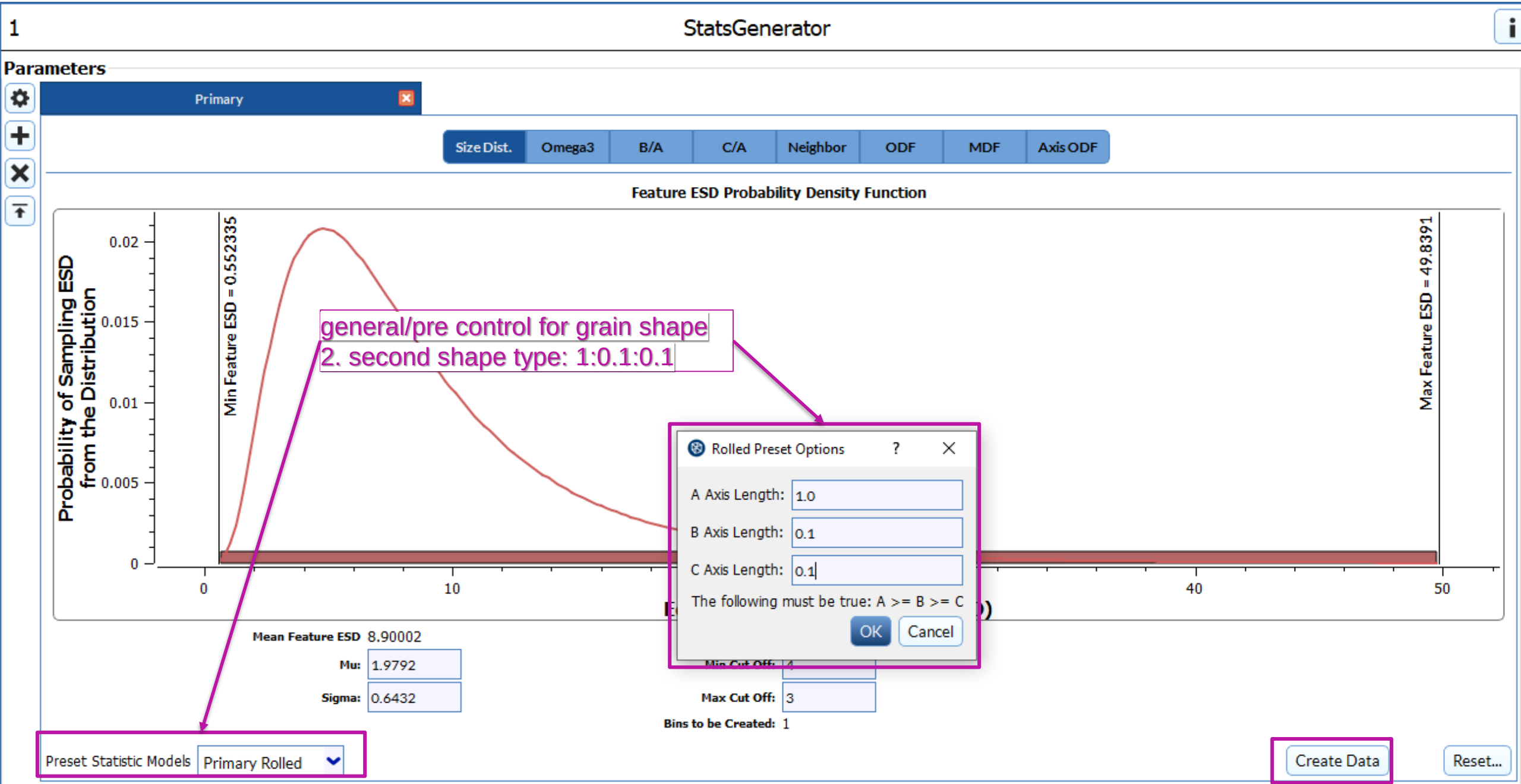
Phase map



Grain map



DREAM.3D - Rolled grain structure



DREAM.3D - Rolled grain structure

*(01) Single Cubic Phase Equiaxed - DREAM3D

File Edit View Bookmarks Pipeline Help

Pipeline

01 StatsGenerator
02 Initialize Synthetic Volume
03 Establish Shape Types
04 Pack Primary Phases
05 Find Feature Neighbors
06 Match Crystallography
07 Generate IPF Colors
08 Write DREAM.3D Data File

Start Pipeline

8 Write DREAM.3D Data File

Parameters

Output File: C:\Users\wenqi liu\Desktop\Dream3D\Al_singlePhase_shape2.dream3d Select...

Write Xdmf File

Include Xdmf Time Markers

Change output filename to avoid overwrite

Start running

Open new RVE in ParaView

Open File: (open multiple files with <ctrl> key.)

Look in: C:/Users/wenqi liu/Desktop/Dream3D/

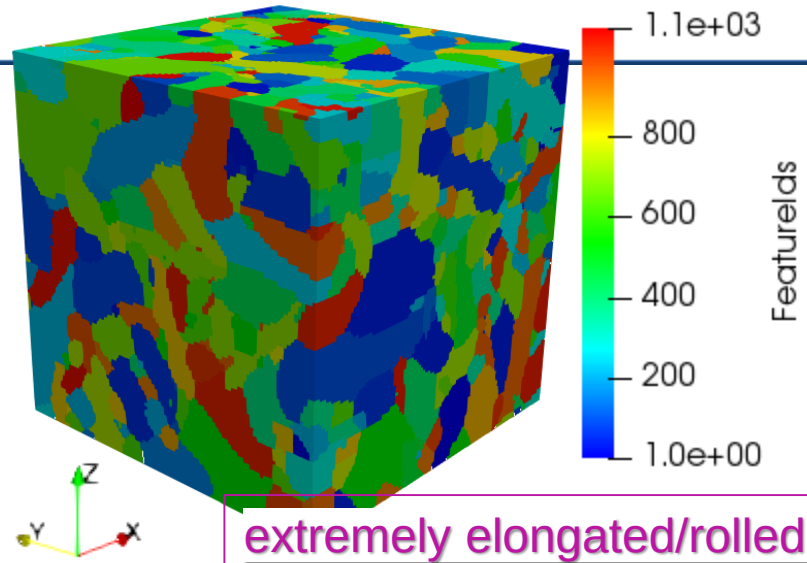
Examples
My Documents
Desktop
Favorites
C:\
E:\
F:\
G:\
H:\

Dream3D
PlayWithAxesOri
postProc
DPK1000_RD-TD_nm_100

Filename	Type
DREAM3D-6.5.1-Win64	Folder
Dream3D_RVE	Folder
Al_singlePhase_shape..xdmf	Group
Al_singlePhase_shape1.xdmf	xdmf File
Al_singlePhase_shape2.xdmf	xdmf File

File name: Al_singlePhase_shape2.xdmf Navigate OK

Files of type: Supported Files (plt* *.inp *.cgns *.cml *.csv *.tsv *.txt *.CSV *.TSV *.TXT *.dem *.dcm *.dc Cancel



extremely elongated/rolled grains

DREAM.3D - Grain shape distribution

1

StatsGenerator

Parameters

Primary

Change grain shape distribution for both planes, first 'B/A' then 'C/A', but with the same parameters.

Size Dist. | Omega3 | B/A | C/A | Neighbor | ODF | MDF | Axis ODF

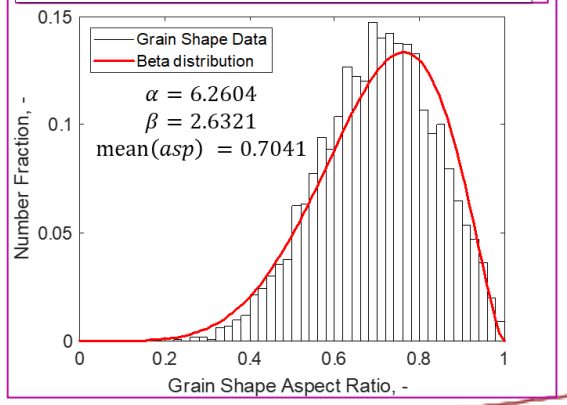
Right click in the figure area, then click 'Edit Data'

Edit Data

Edit B/A Distribution Values Data

Bin	Alpha	Beta
0.552335	6.2604	2.6321

Beta grain shape distribution from Exercise 1

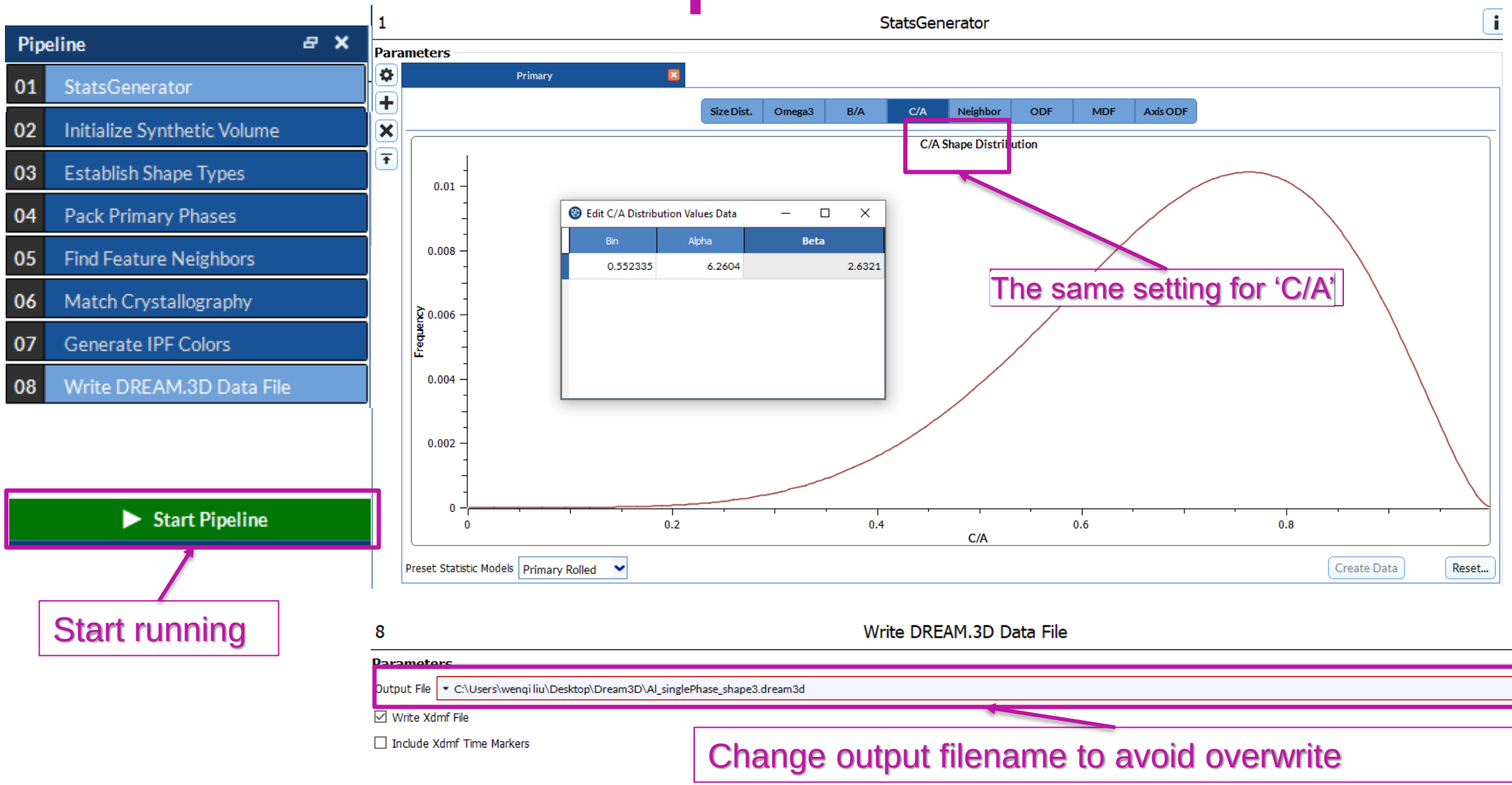


Preset Statistic Models: Primary Rolled

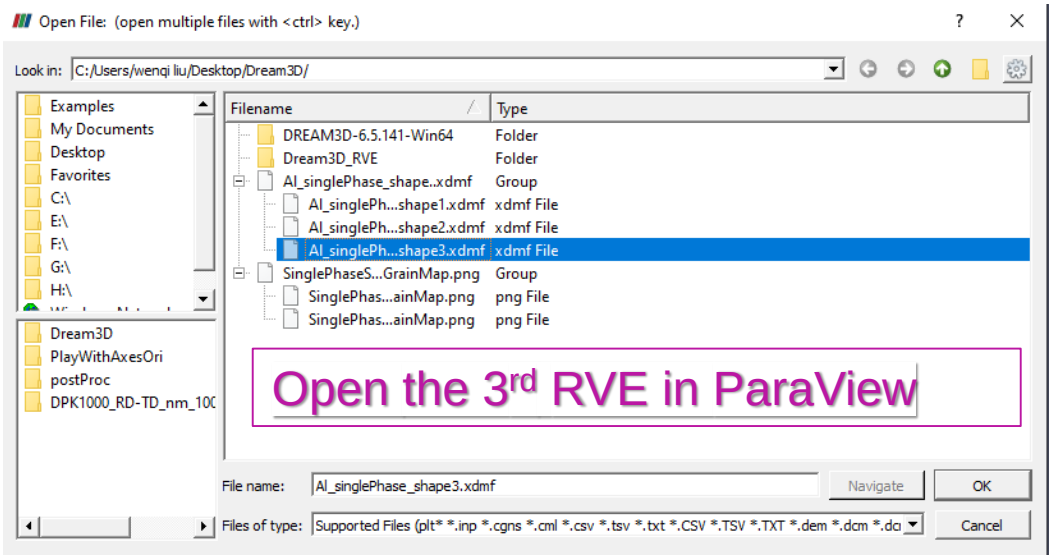
Create Data

Reset...

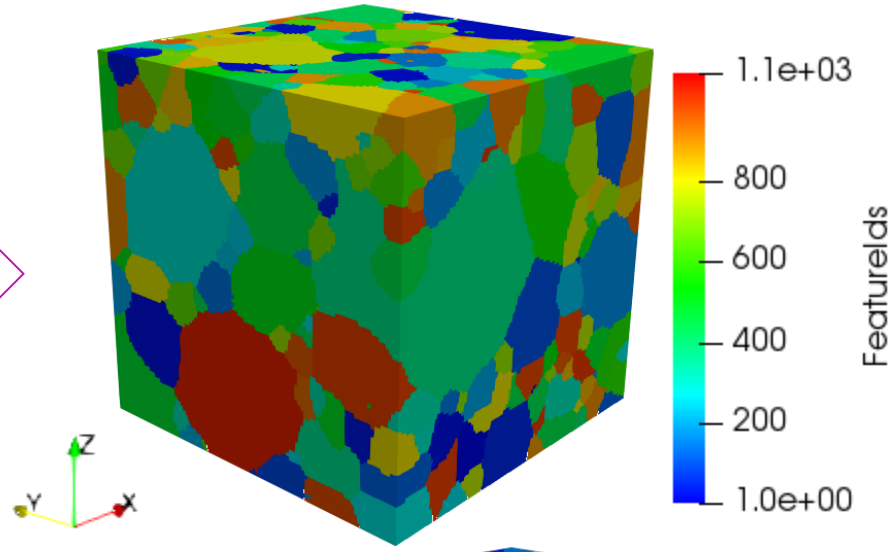
DREAM.3D - Grain shape distribution



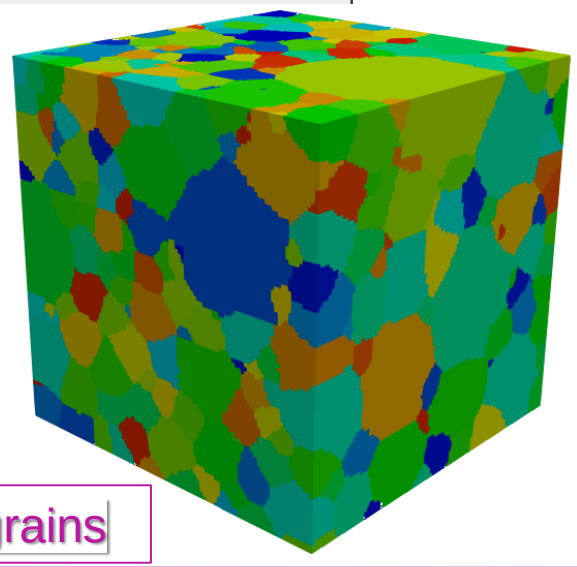
DREAM.3D - Grain shape distribution



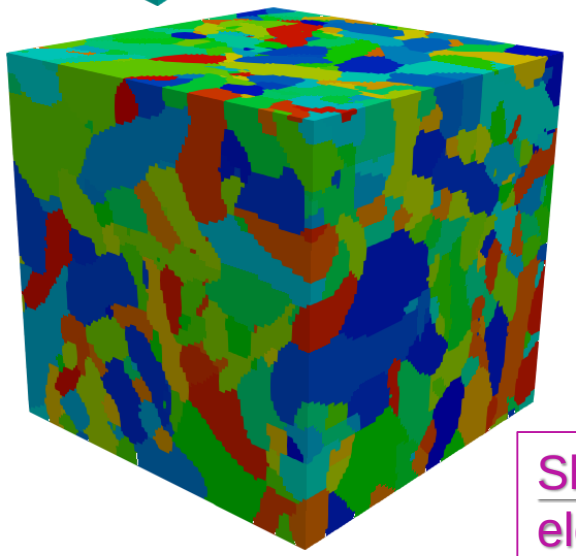
Open the 3rd RVE in ParaView



Shape 3: Elongated/rolled grains based on EBSD measured data



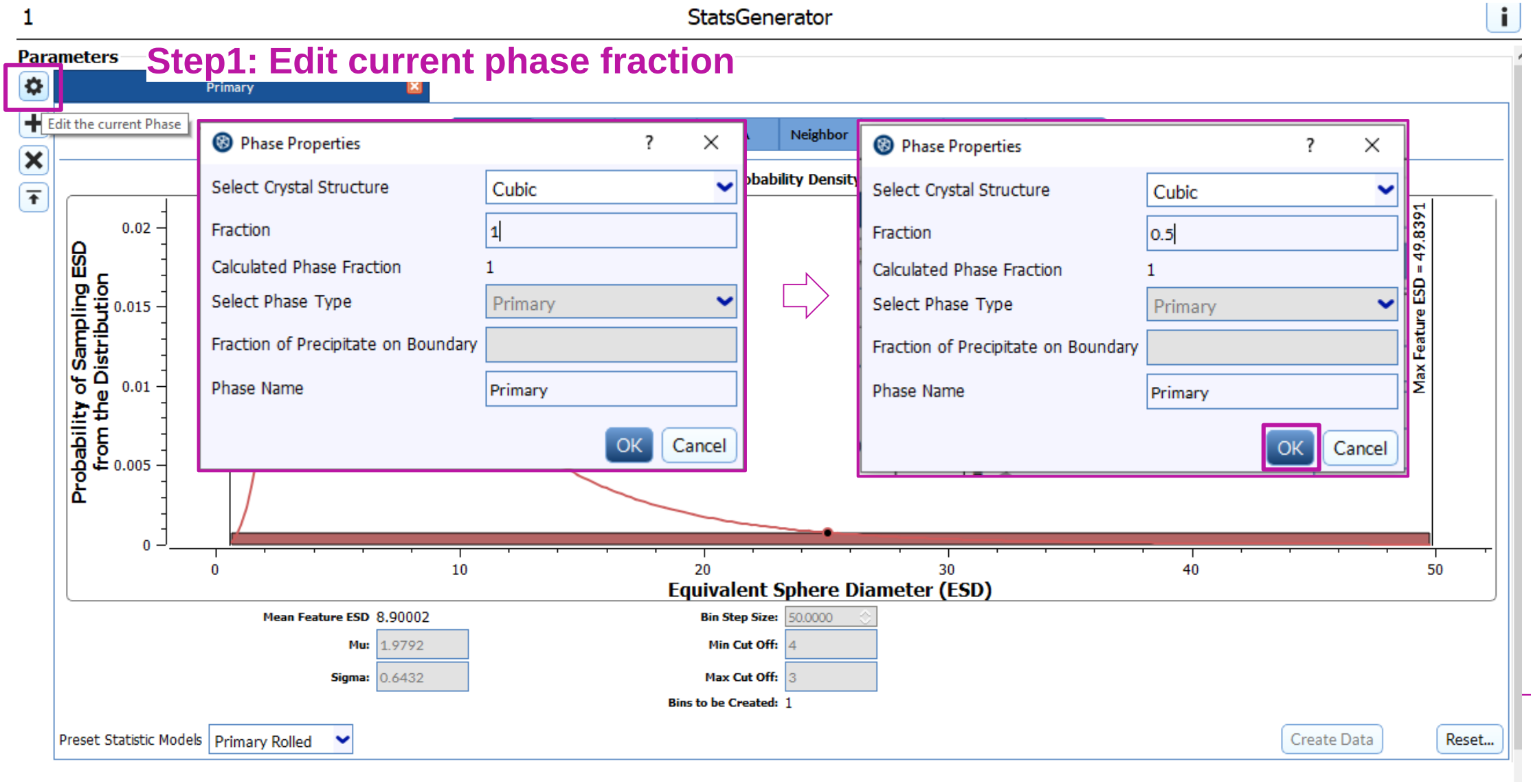
Shape 1: Equiaxed grains



Shape 2: Extremely elongated/rolled grains

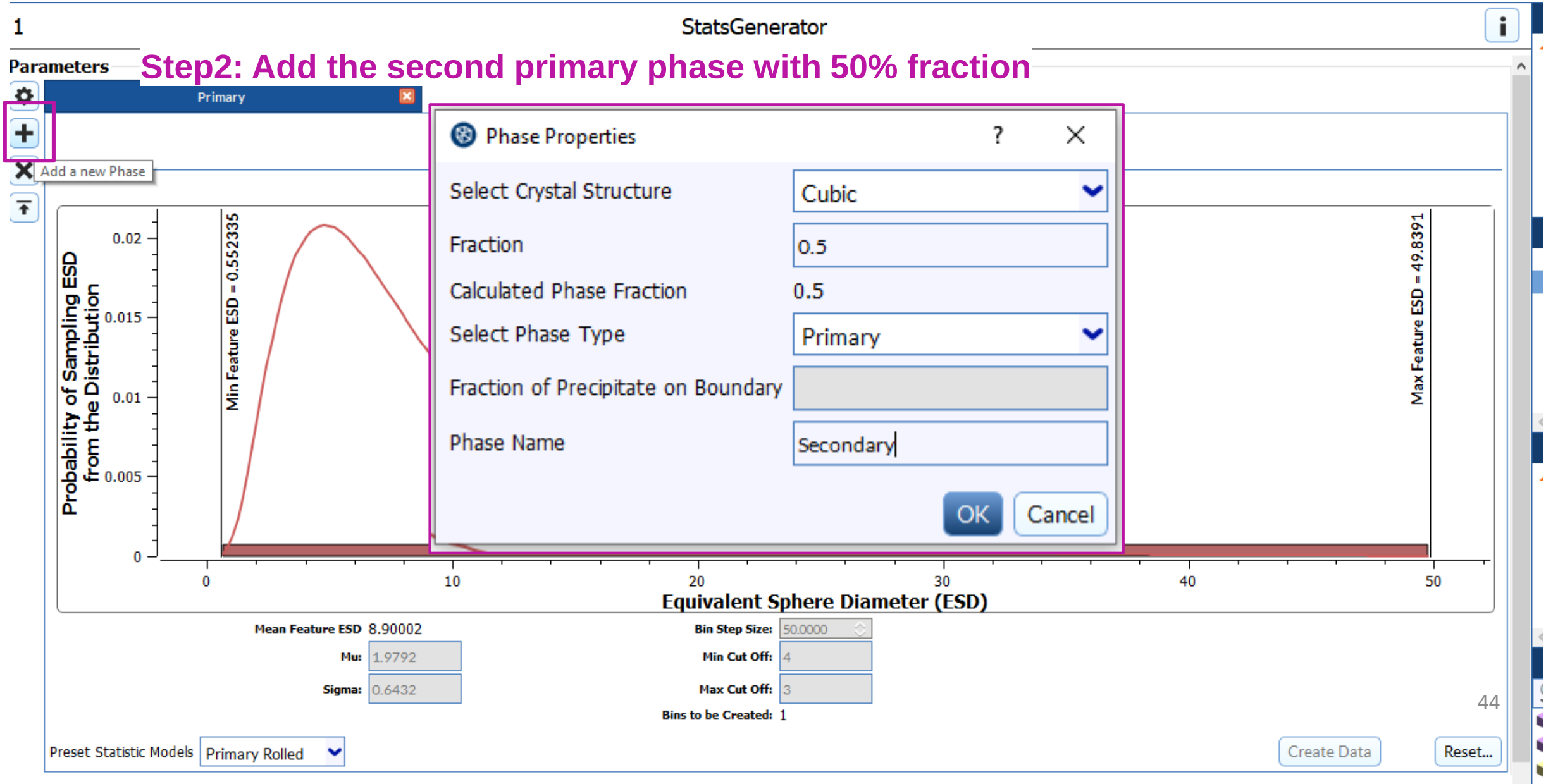
DREAM.3D - Dual-phase structure

- *E.g. duplex phase structure with two equal-fraction primary phases, phase fraction: 50% + 50%*

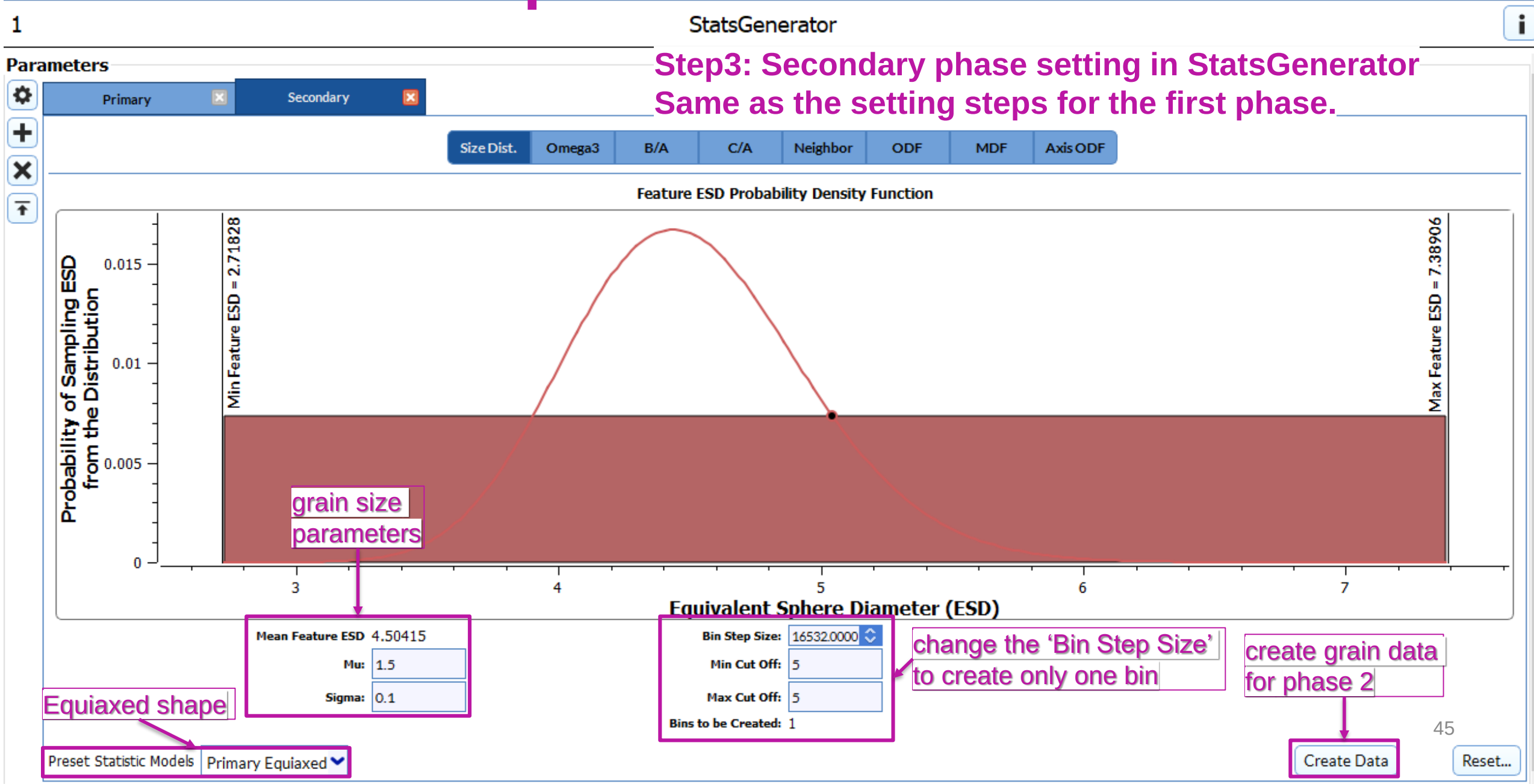


DREAM.3D - Dual-phase structure

- *E.g. duplex phase structure with two equal-fraction primary phases, phase fraction: 50% + 50%*



DREAM.3D - Dual-phase structure



DREAM.3D - Dual-phase structure

File Edit View Bookmarks Pipeline Help

Pipeline

01 StatsGenerator
02 Initialize Synthetic Volume
03 Establish Shape Types
04 Pack Primary Phases
05 Find Feature Neighbors
06 Match Crystallography
07 Generate IPF Colors
08 Write DREAM.3D Data File

Cancel Pipeline

8 Write DREAM.3D Data File

Parameters

Output File: C:\Users\wenqi liu\Desktop\Dream3D\AI_DualPhase_shape1.dream3d Select...

Write Xdmf File

Include Xdmf Time Markers

Step5: Change output filename to avoid overwrite

Step4: Check every filter to solve errors/warnings.

Step6: Start running

Waiting a while for running

Data Structure

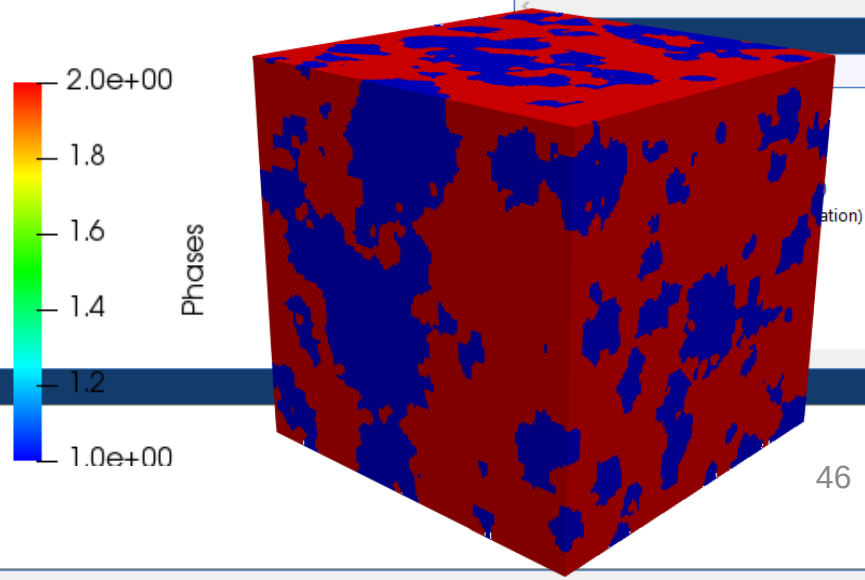
- StatsGeneratorDataContainer
  - CellEnsembleData
    - CrystalStructures
    - PhaseName
    - PhaseTypes
    - Statistics
    - ShapeTypes
- SyntheticVolumeDataContainer

Bookmarks

- Synthetic
  - (01) Single Cubic Phase Equiaxed
  - (02) Single Hexagonal Phase Equiaxed
  - (03) Single Cubic Phase Rolled
  - (04) Two Phase Cu...articles Equiaxed
  - (05) Composite
  - (06) SmallIN100 Synthetic

Filter Library

- Filter Library
  - Core
  - DREAM3D Review
  - Generic
  - IO
  - ITK Image Processing
  - Processing



Pipeline Issues

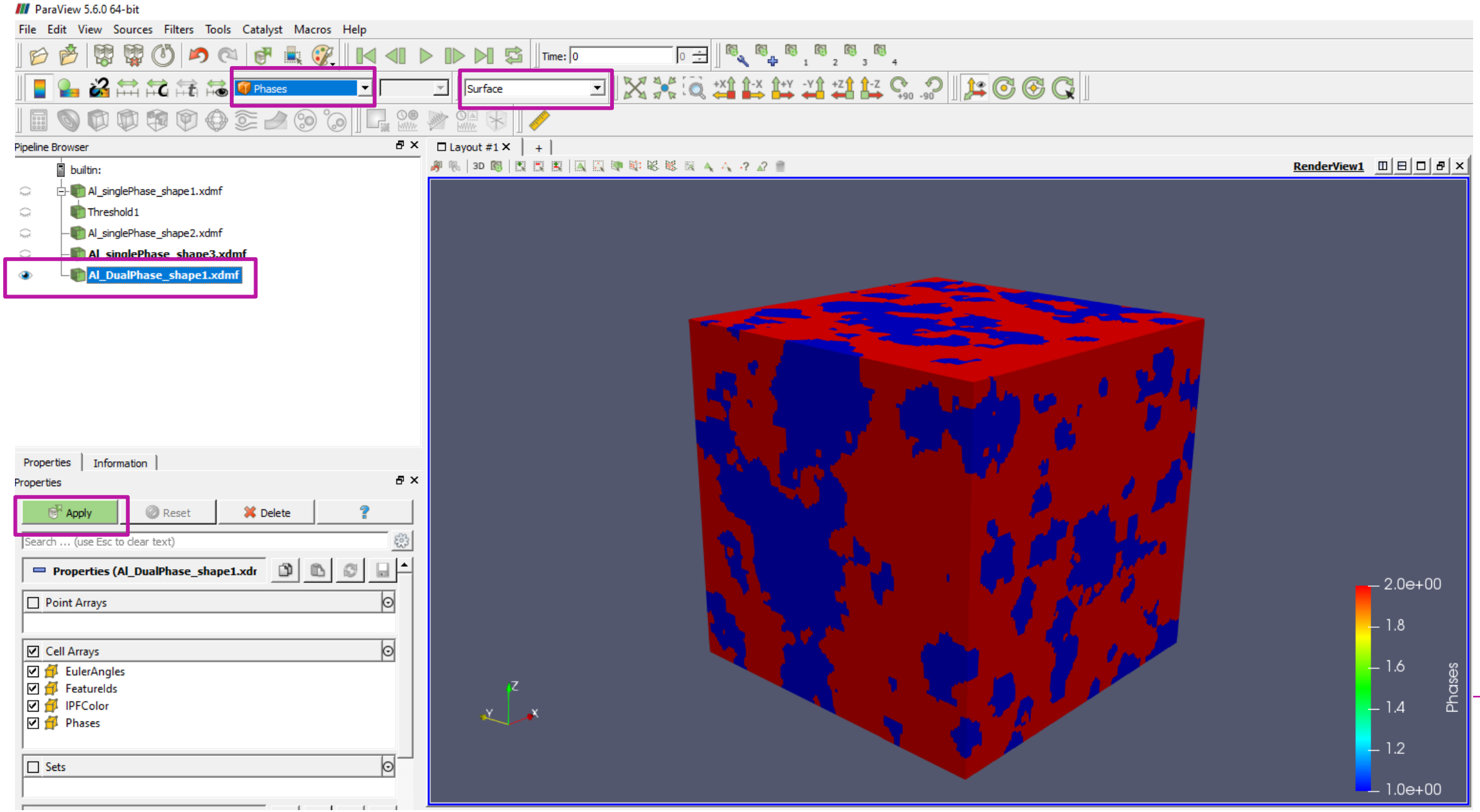
Index	Filter	Description	Code

Pipeline Output

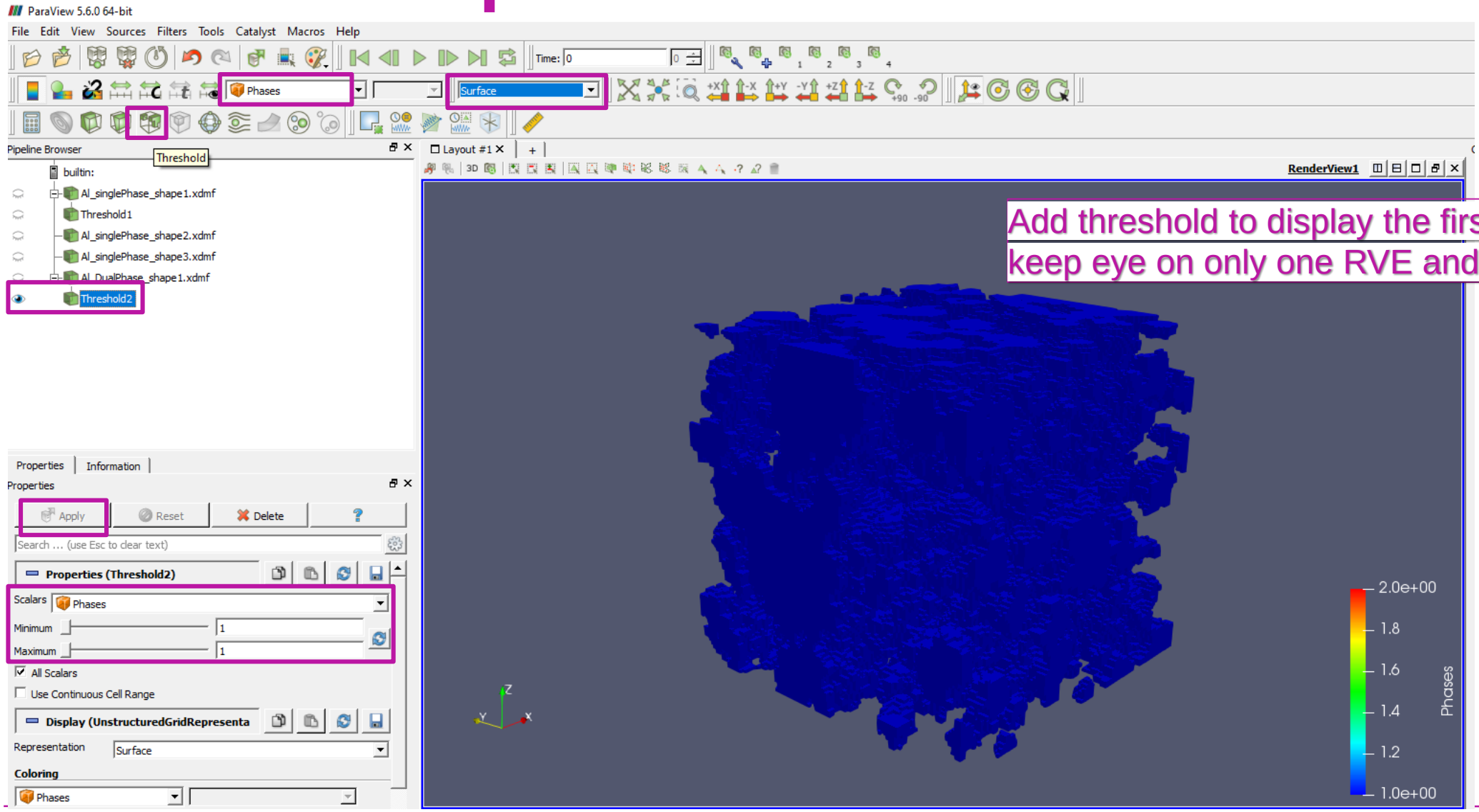
Swapping/Switching Orientations Iteration 36678/100000 || Est. Time Remain: 00:00:05 || Iterations/Sec: 12213.8
Swapping/Switching Orientations Iteration 49003/100000 || Est. Time Remain: 00:00:04 || Iterations/Sec: 12238.5
Swapping/Switching Orientations Iteration 60509/100000 || Est. Time Remain: 00:00:03 || Iterations/Sec: 12089.7
[7/8] Generate IPF Colors
[8/8] Write DREAM.3D Data File
Pipeline Complete
********** PIPELINE FINISHED **********

[4/8] Pack Primary Phases : Swapping/Moving/Adding/Removing Features Iteration 32794/1129200 || Est. Time Remain: 00:07:15 || Iterations/Sec: 2519.9

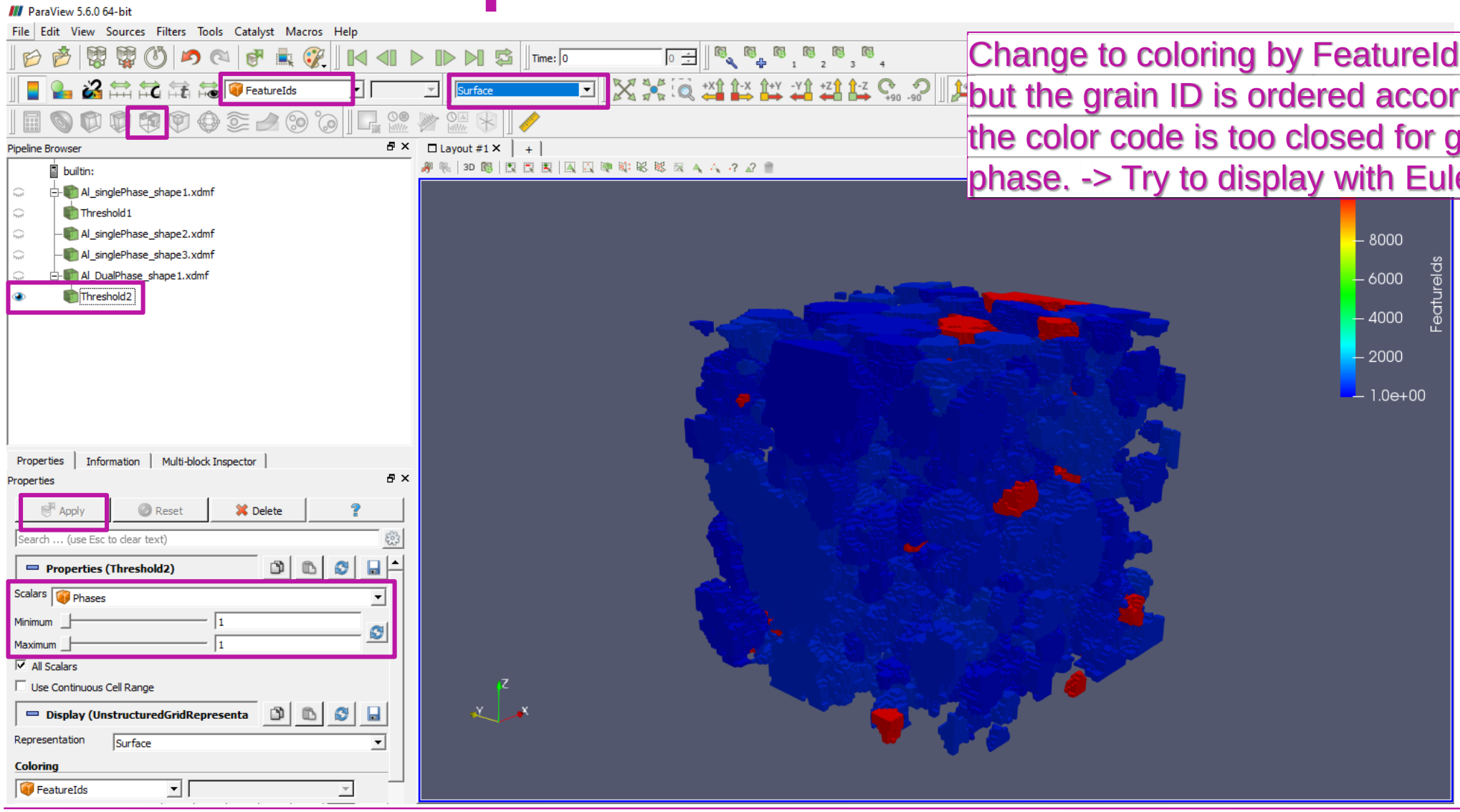
ParaView - Dual-phase structure



ParaView - Dual-phase structure

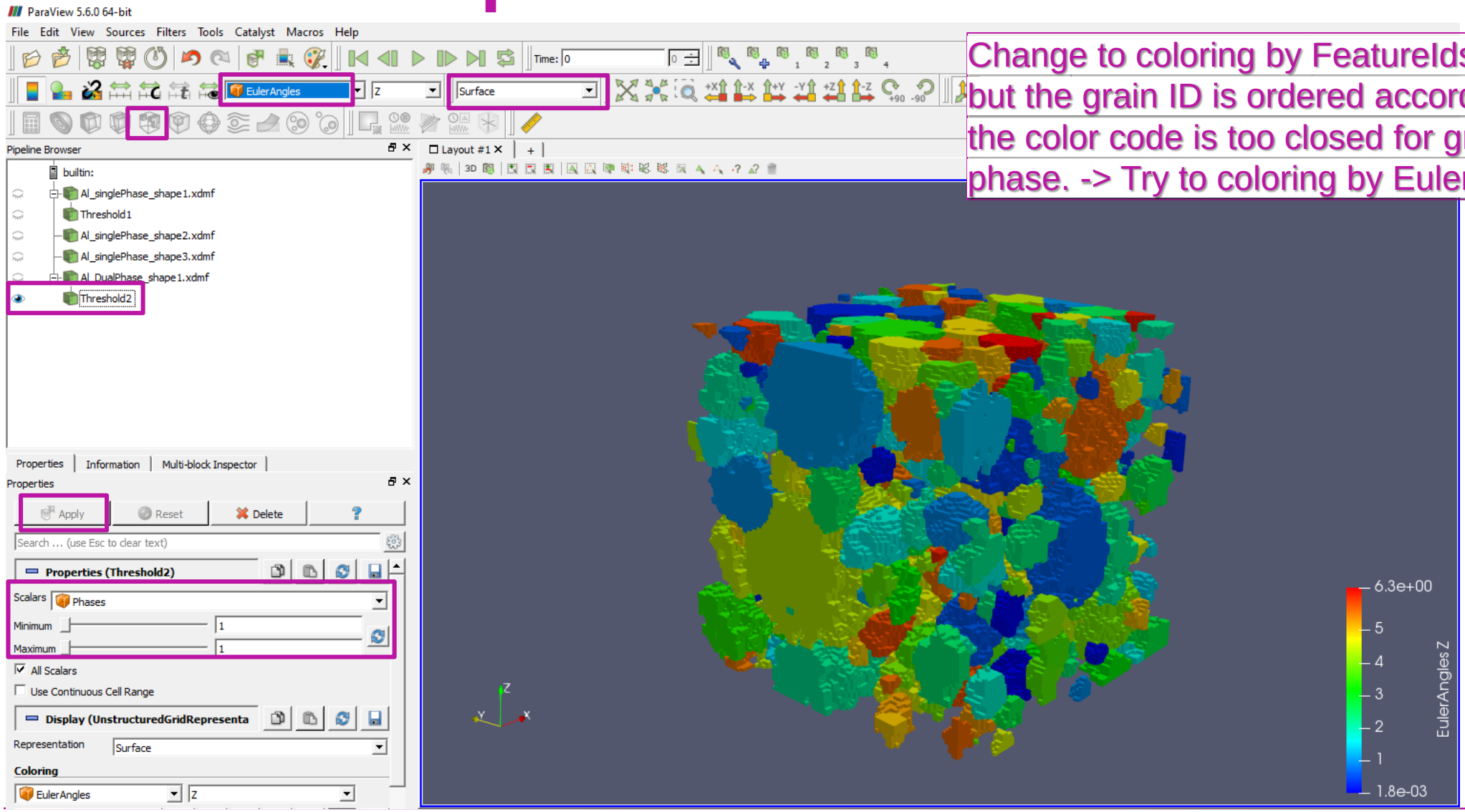


ParaView - Dual-phase structure



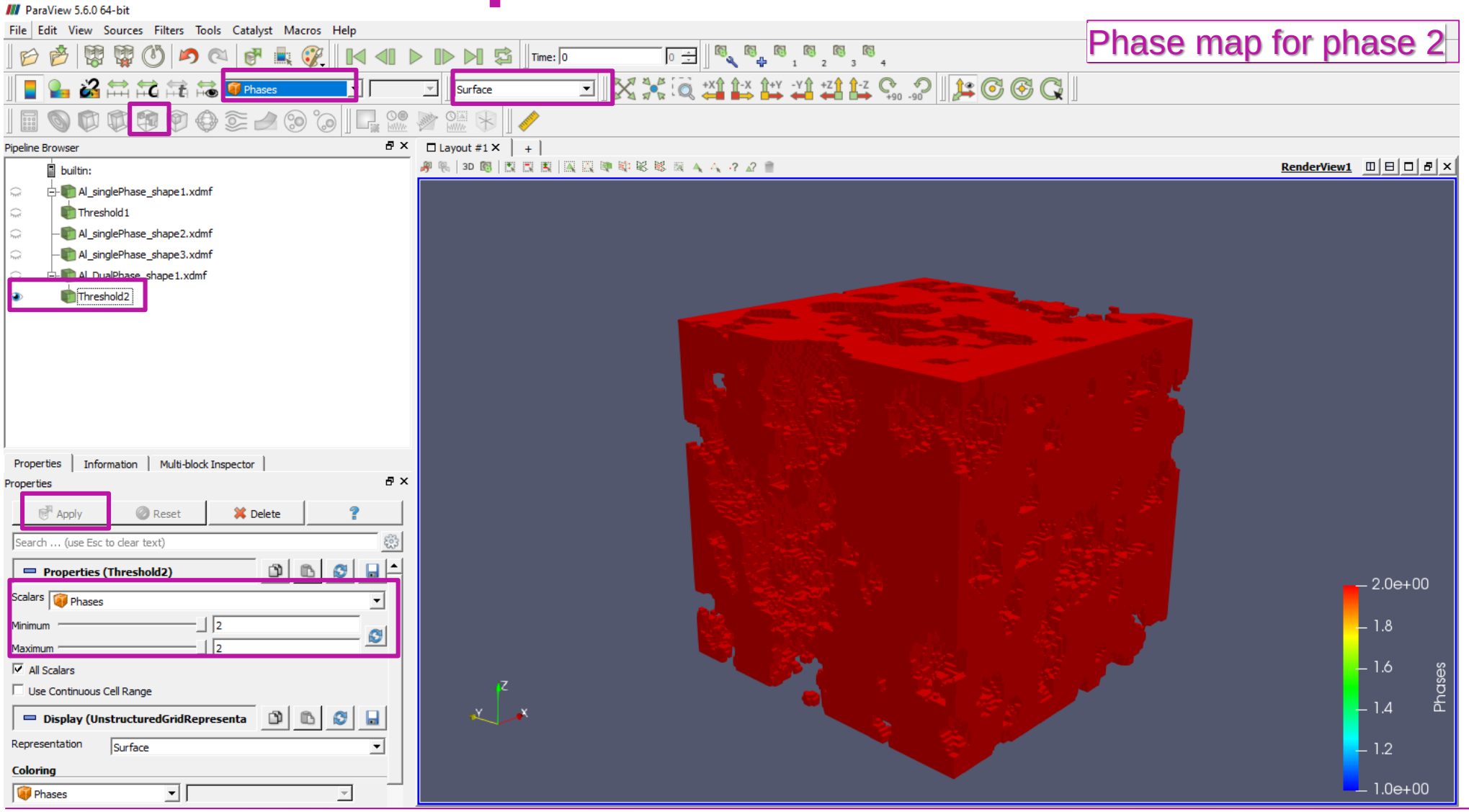
Change to coloring by FeatureIds, i.e. grain ID but the grain ID is ordered according to phase, the color code is too closed for grains in one phase. -> Try to display with EulerAngles

ParaView - Dual-phase structure

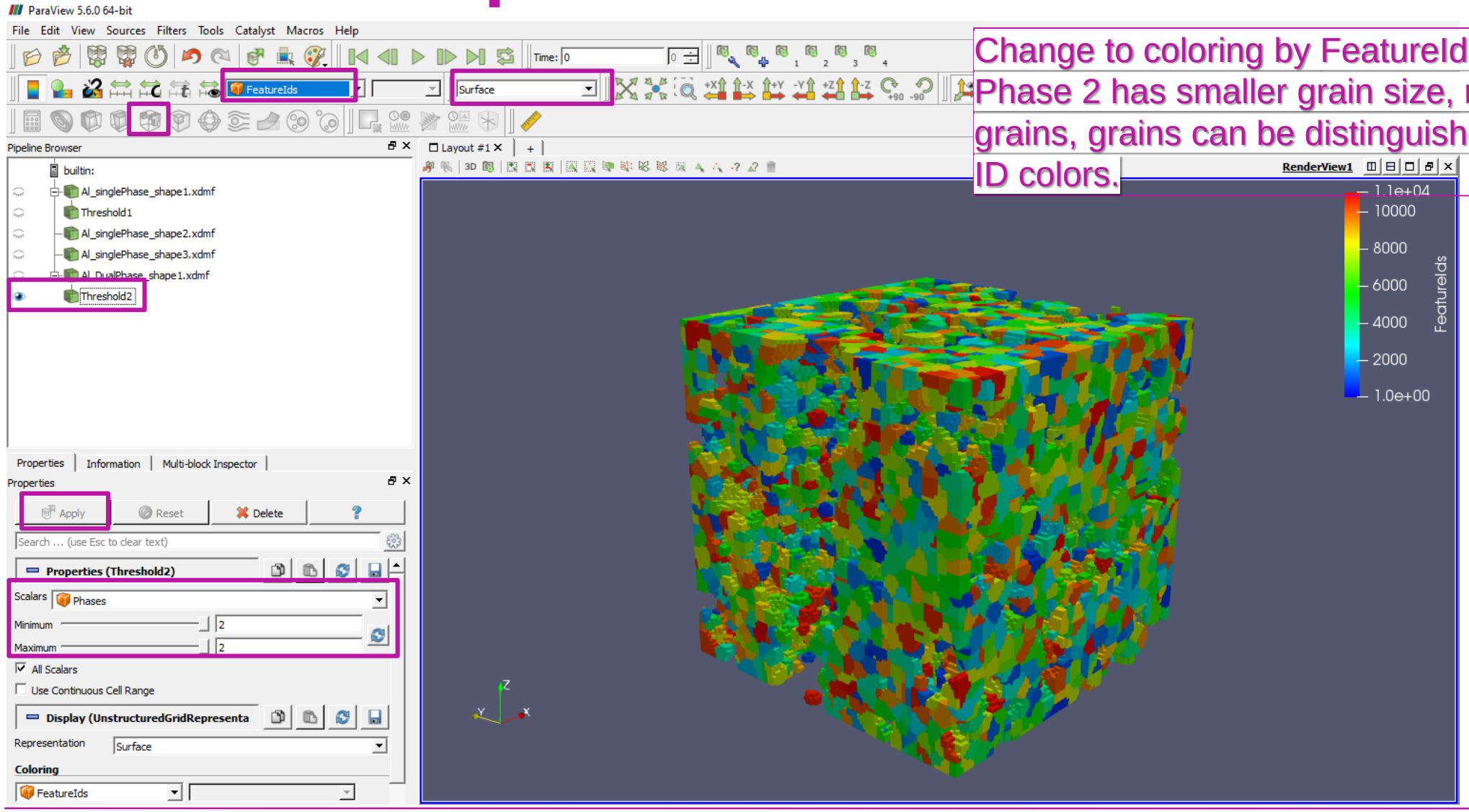


Change to coloring by FeatureIds, i.e. grain ID but the grain ID is ordered according to phase, the color code is too closed for grains in one phase. -> Try to coloring by EulerAngles

ParaView - Dual-phase structure

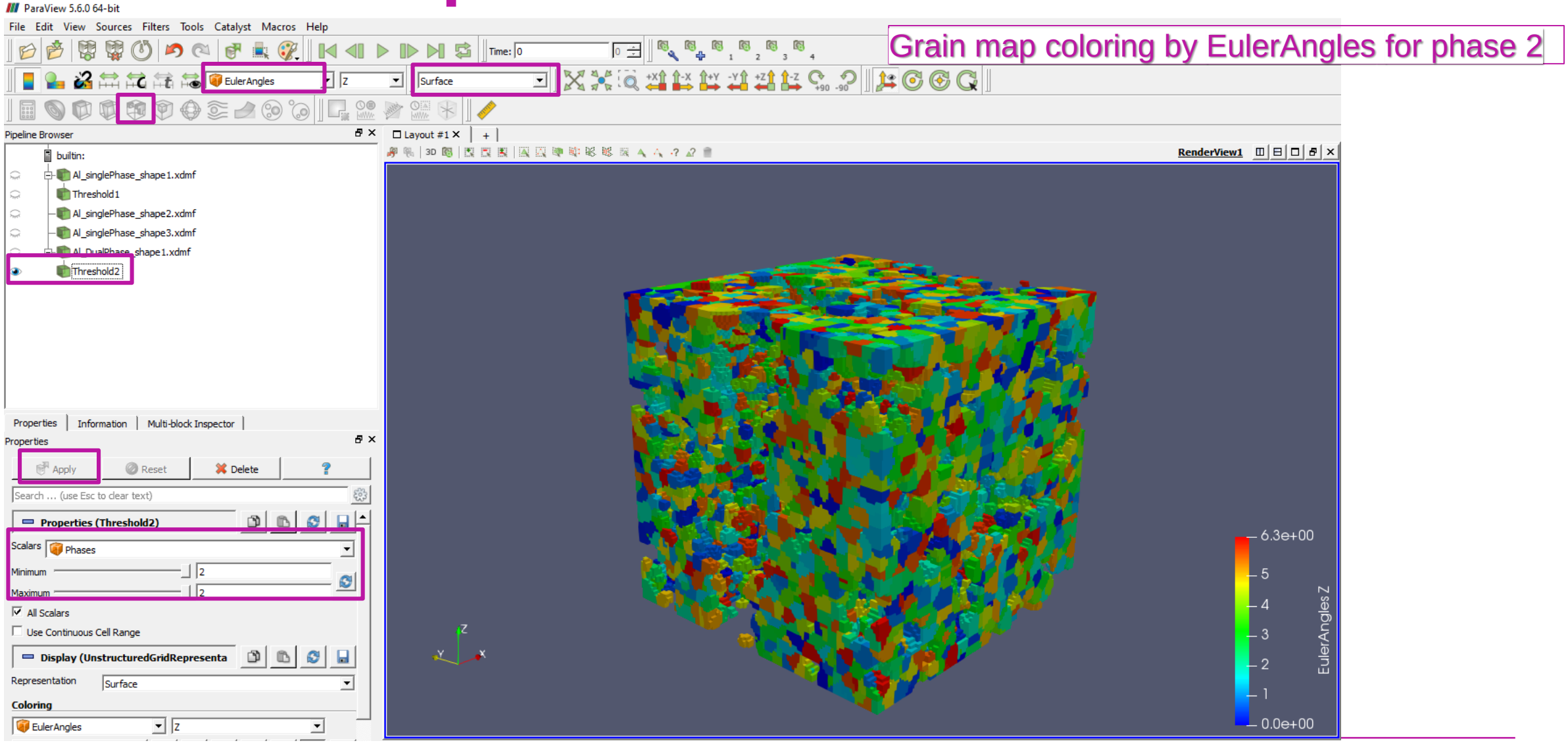


ParaView - Dual-phase structure



Change to coloring by FeatureIds, i.e. grain ID. Phase 2 has smaller grain size, results in, more grains, grains can be distinguished by the grain ID colors.

ParaView - Dual-phase structure



Grain map coloring by EulerAngles for phase 2

Resources

Materials:

- [1] Swantje Bargmann, et al.: Generation of 3D representative volume elements for heterogeneous materials: A review, Progress in Materials Science, 2018, 96:322-384, https://doi.org/10.1016/j.pmatsci.2018.02.003.
- [2] Georg J. Schmitz, Ulrich Prahl, Handbook of Software Solutions for ICME, 2016.

Software:

- Dream3D: http://dream3d.bluequartz.net
- ParaView: https://www.paraview.org/download/

Questions?

- **Assignment** submission DL is **23:00 on 08.11.2020.**
- **Contact: MyCourses 'General discussion' channel,**

  Wenqi Liu, **wenqi.liu@aalto.fi**

Slides will be updated after Exercise.