Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

Exercise 2

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Wenqi Liu (Teaching assistant)
Rongfei Juan (Teaching assistant)

Outline

- Introduction
  - Microstructure modeling
  - Tasks
- Software operations
  - DREAM.3D
  - ParaView
- Feedback on Assignment
- Feedback & Questions

Microstructure modeling

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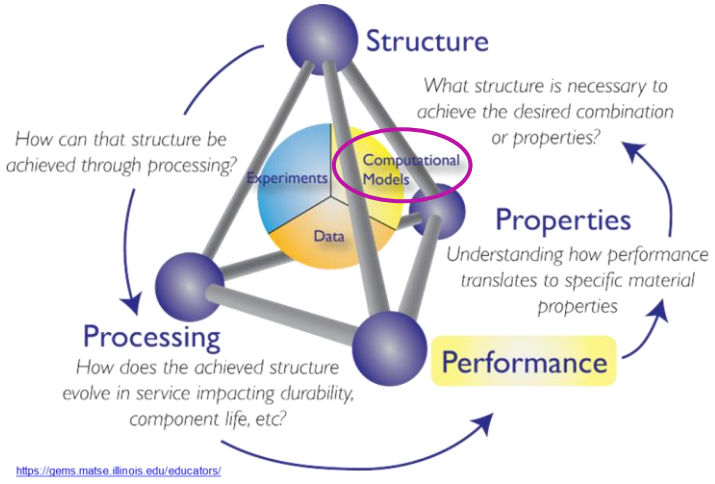
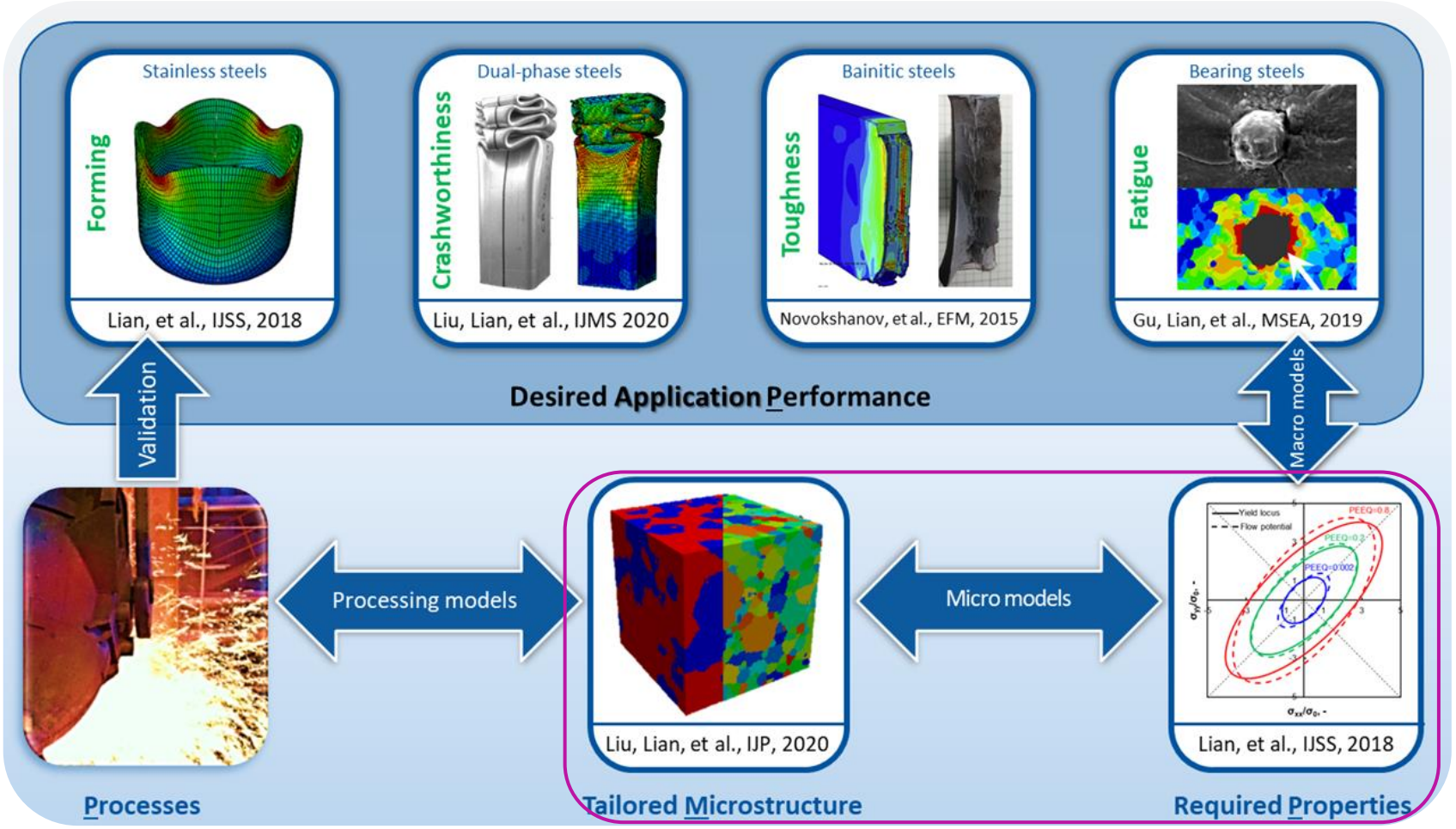
Integrated computational materials engineering (ICME)

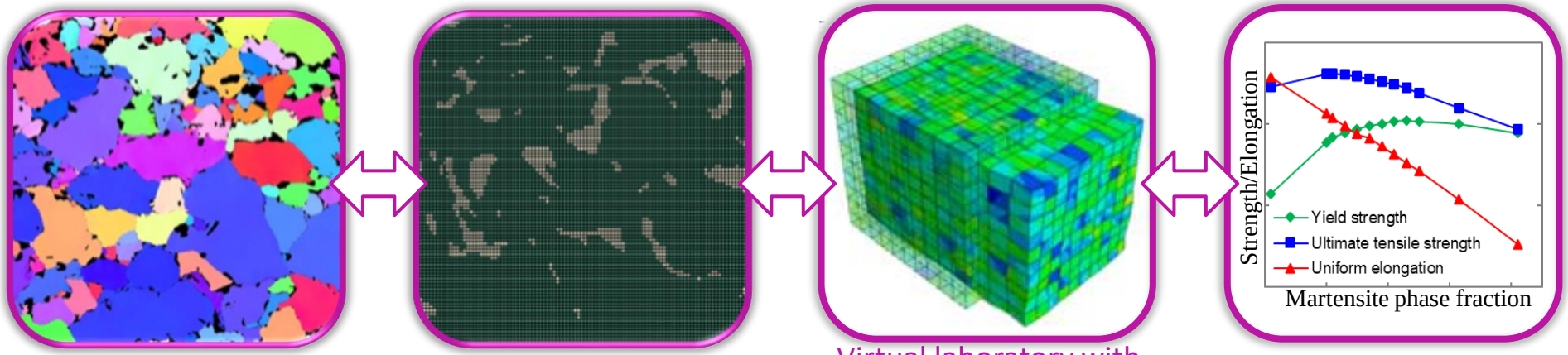




https://www.researchgate.net/lab/Junhe-Lian-Lab

Micromechanics modeling

Microstructure - property relation & microstructure-based material design



Microstructure measurement

e.g. EBSD

Microstructure modeling

e.g. Representative volume element (RVE)

Virtual laboratory with materials behavior models

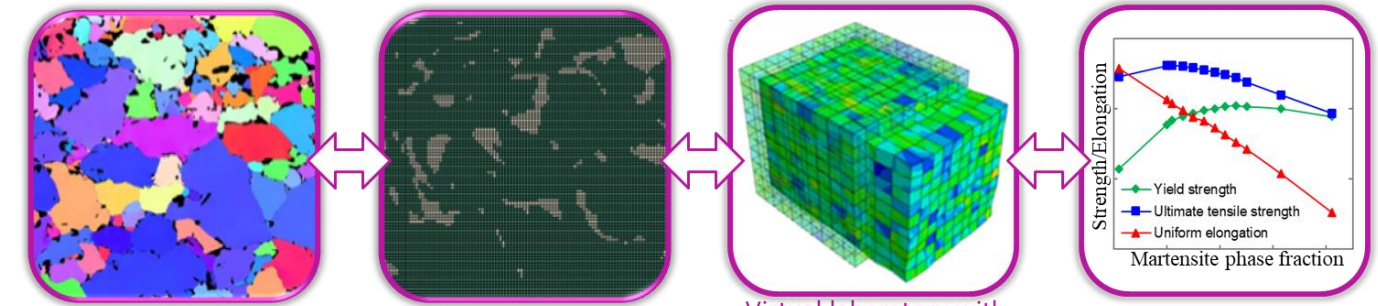
e.g. von Mises stress–strain relation; Crystal plasticity

Mechanical properties

e.g. Force–displacement response; Flow curve

Microstructure modeling - RVE

Microstructure - property relation & microstructure -based material design



Microstructure measurement | Microstructure modeling | Virtual laboratory with materials behavior models | Mechanical properties

***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

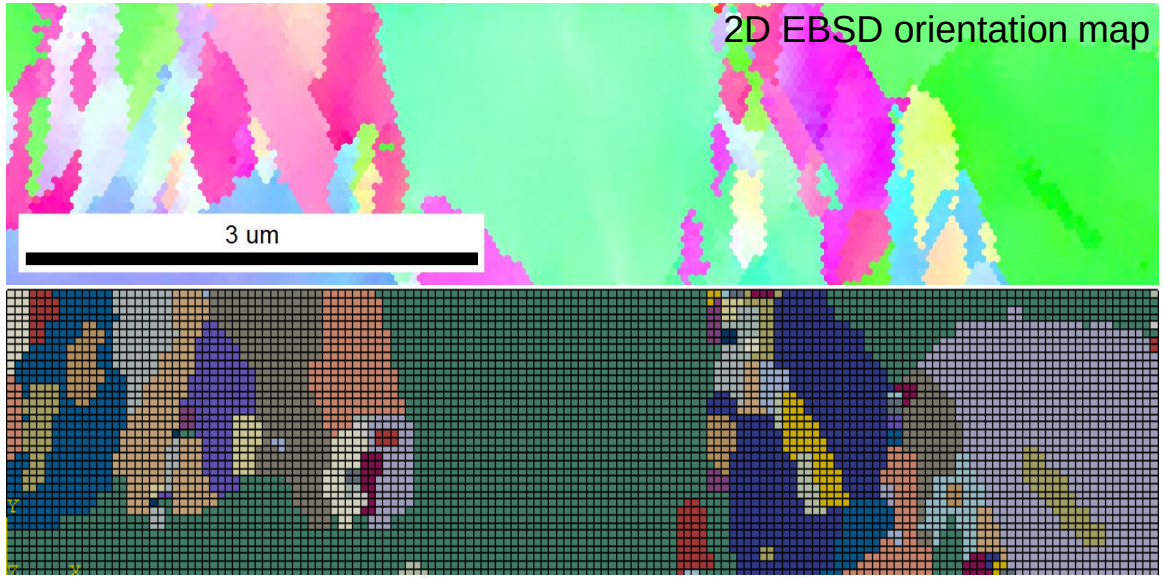
$$\Rightarrow \quad L^M \gg L^{RVE} \gg L^\mu$$

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.)

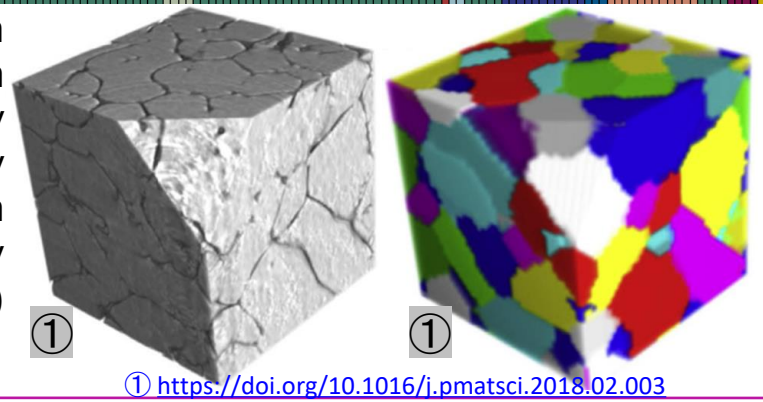
[1] https://doi.org/10.1016/j.pmatsci.2018.02.003

Microstructure modeling - RVE

- *Real microstructure RVE*

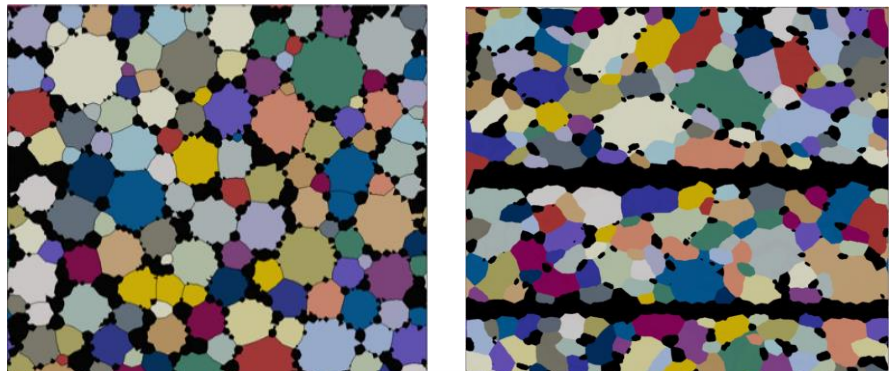


Grain reconstruction by high-energy X-ray diffraction microscopy (3DXRD)

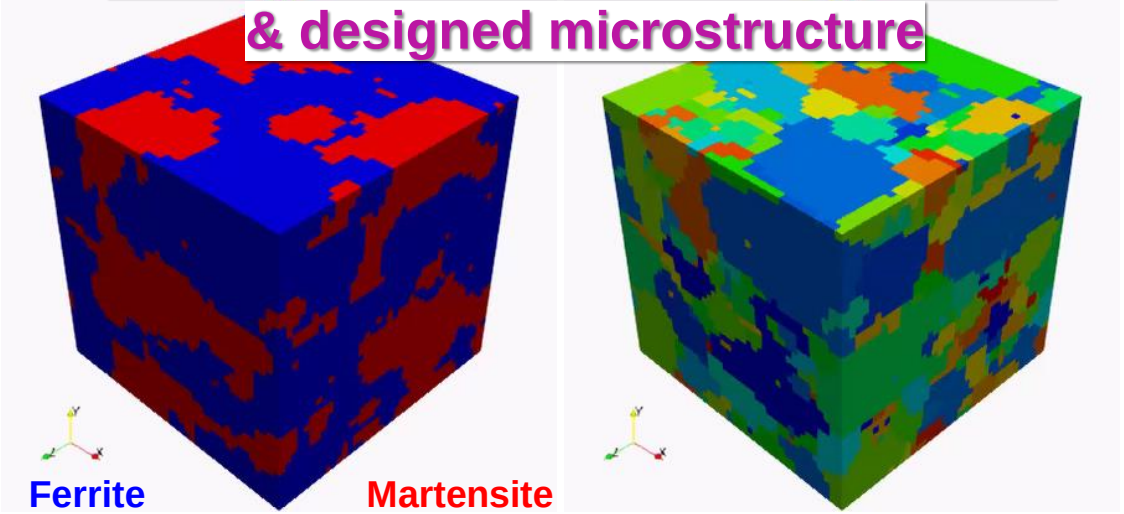


① https://doi.org/10.1016/j.pmatsci.2018.02.003

- *Artificial/synthetic microstructure RVE*



Statistical microstructure information & designed microstructure

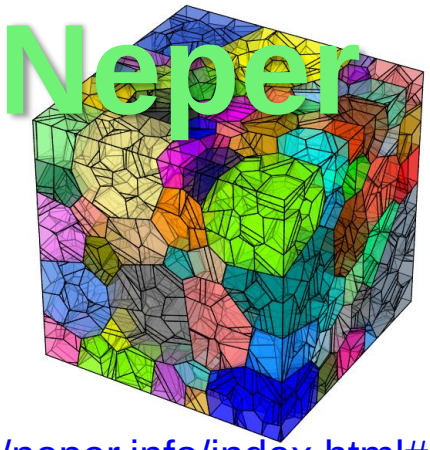


Microstructure modeling - RVE

- 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

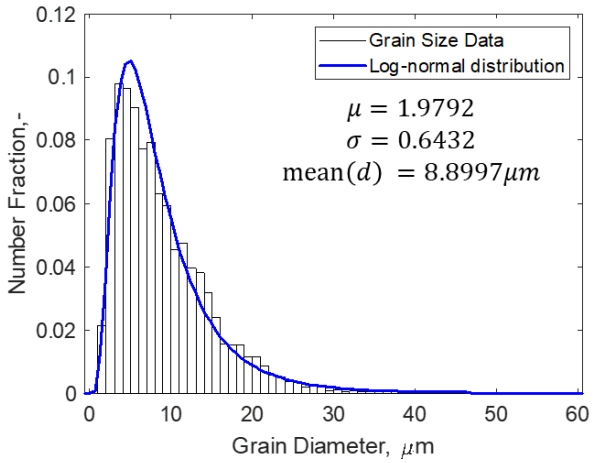
https://www.paraview.org

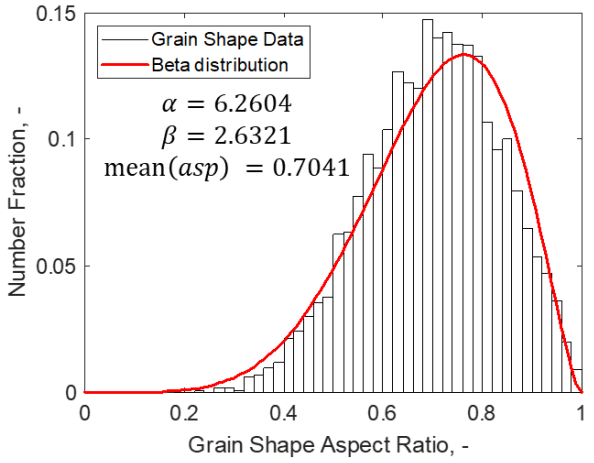
micress®

https://micress.rwth-aachen.de/index.html [2]

Tasks

Tasks





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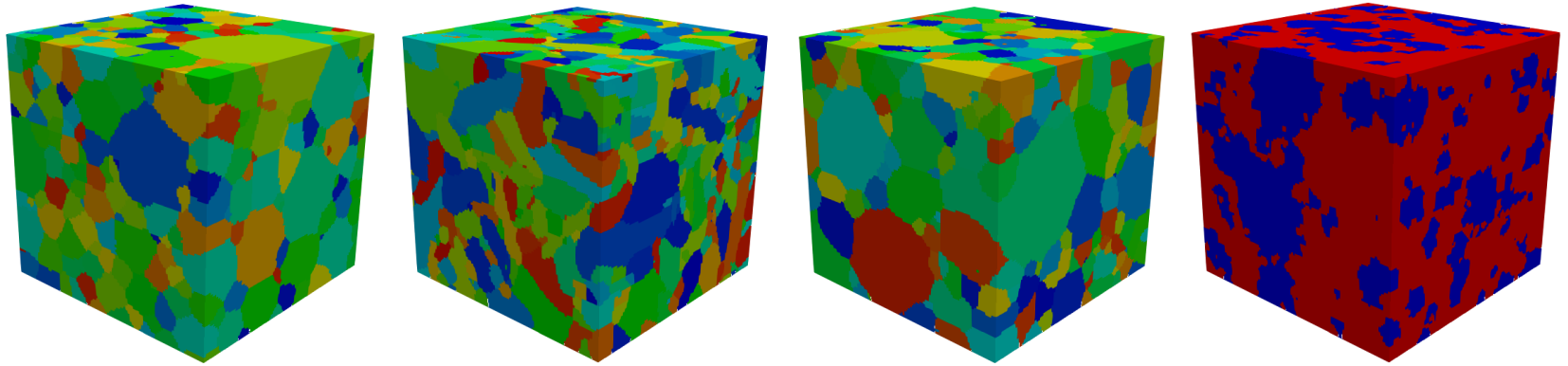

1-Grain Map | 2-Grain Map | 3-Grain Map | 4-Phase Map

Tasks:

1. Single-phase structure with equiaxed grains and pre-defined grain size distribution.
2. Single-phase structure with elongated grains and pre-defined grain size distribution.
3. Single-phase structure with pre-defined grain size and shape distribution.
4. Dual-phase structure with pre-defined grain size and shape distribution.

DREAM.3D & ParaView preparation

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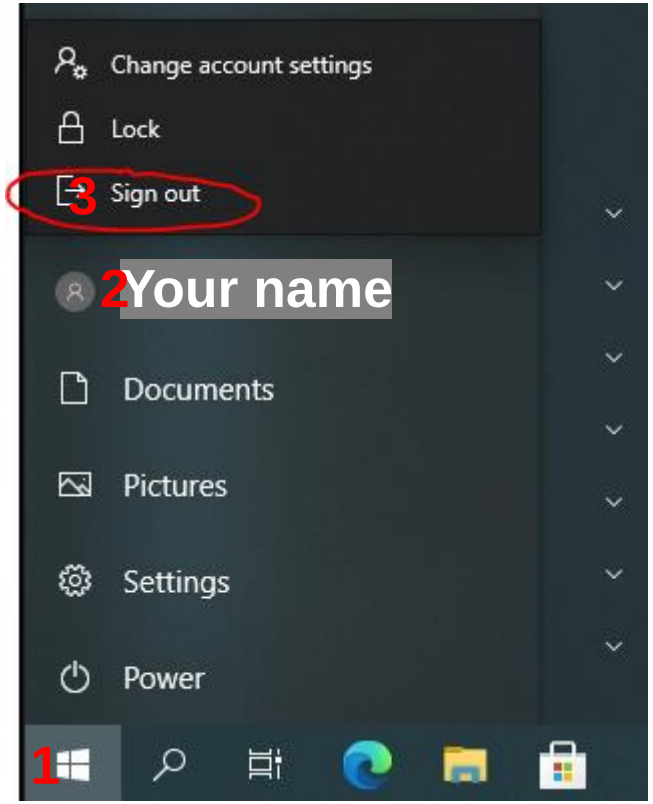
Software preparation

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 DOT as the decimal separator, NO COMMA!



Please download and extract the zip file of DREAM.3D and ParaView, and copy it to your work folder. It might take 1-2 h for download/unzip/ installation.
For DREAM.3D, no installation is needed, just unzip package and start.
For ParaView, you can choose the package or installation version.

Not secure | dream3d.bluequartz.net/Download/

http://dream3d.bluequartz.net

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DREAM3D In Use

Origins of DREAM3D

Download

Choose the version according to your operating system.

Prebuilt Binaries

The current version is 6.5.160 and is available in prebuilt binaries for MacOS, Windows and Linux operating systems:

Operating System	Notes
MacOS - DREAM3D-6.5.160-OSX.dmg	MacOS 10.14 and greater required, including macOS 11.0. Download is a Disk Image
MacOS - DREAM3D-6.5.160-OSX.zip	MacOS 10.14 and greater required, including macOS 11.0. Download is a Zip file
Windows - DREAM3D-6.5.160-Win64.zip	Windows version 8 or 10
Linux - DREAM3D-6.5.160-Linux-x86_64.tar.gz	Ubuntu 18.04 or Equivelant. Self contained tar archive.

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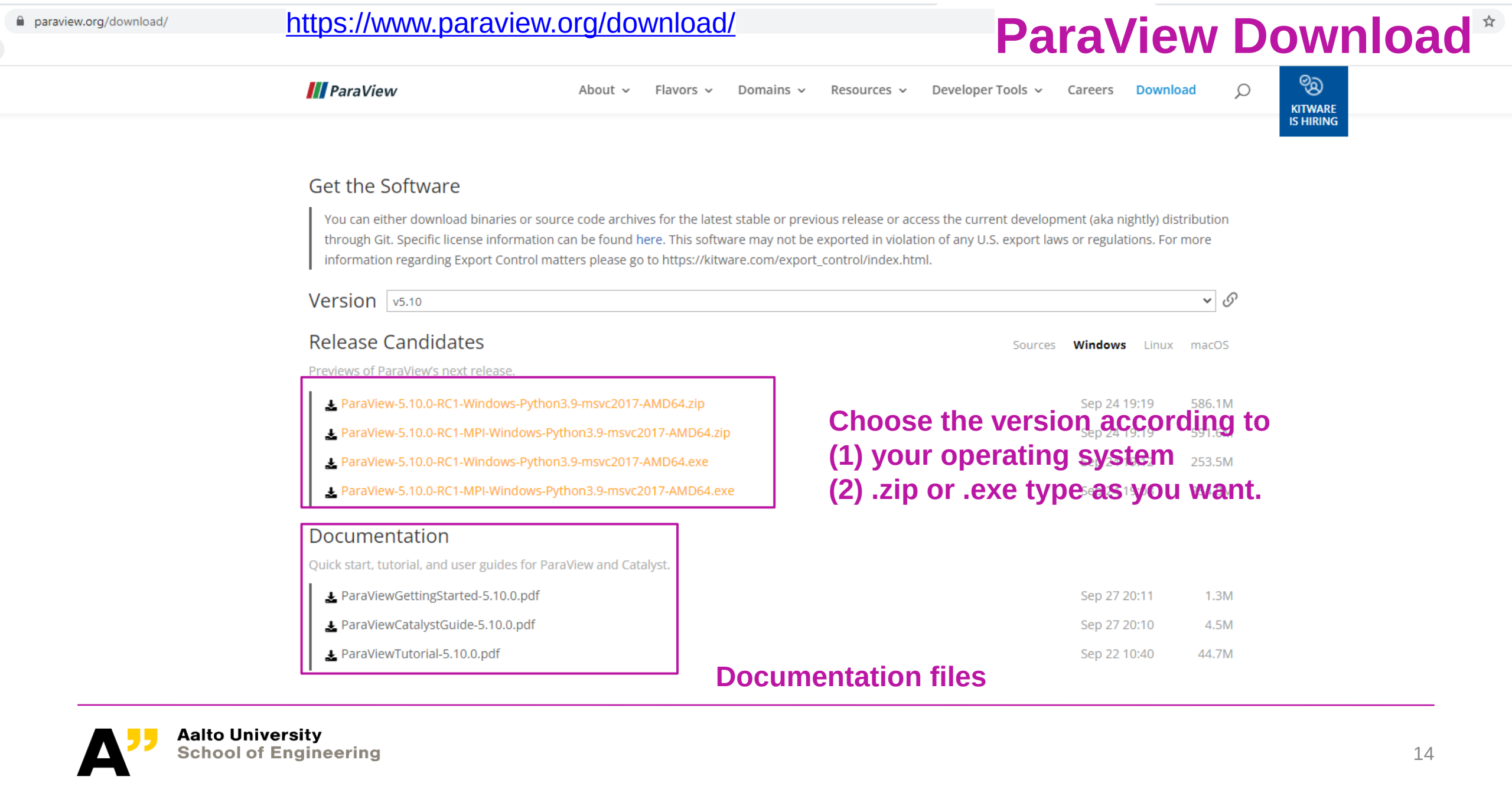
Prebuilt Binaries

ParaView Download

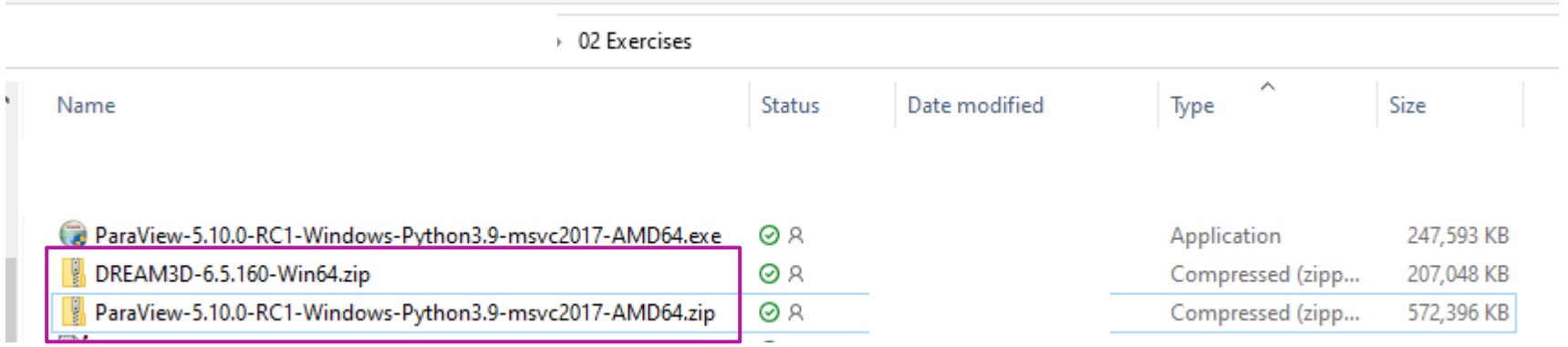
https://www.paraview.org/download/



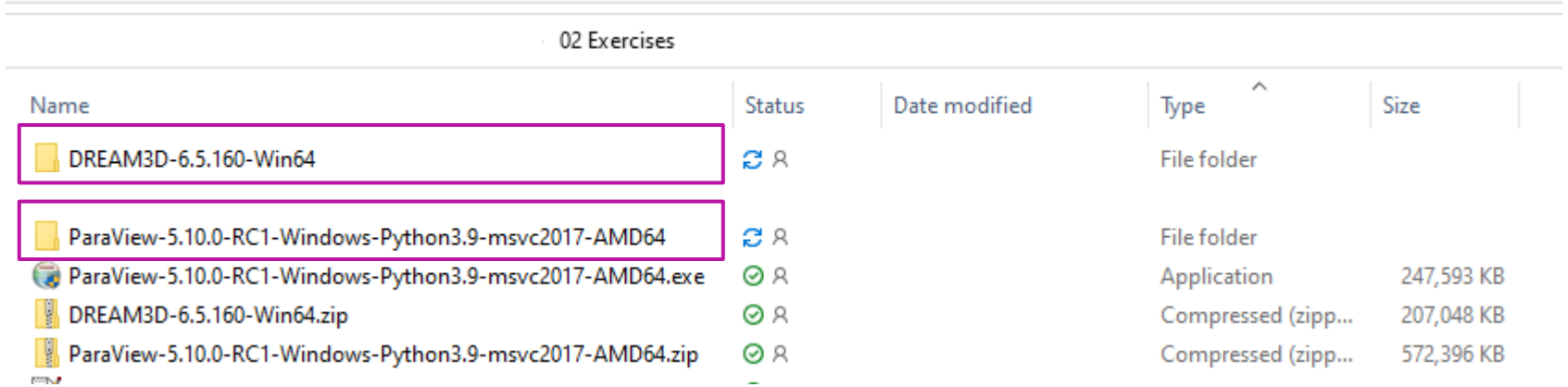
Choose the version according to
(1) your operating system
(2) .zip or .exe type as you want.

Documentation files

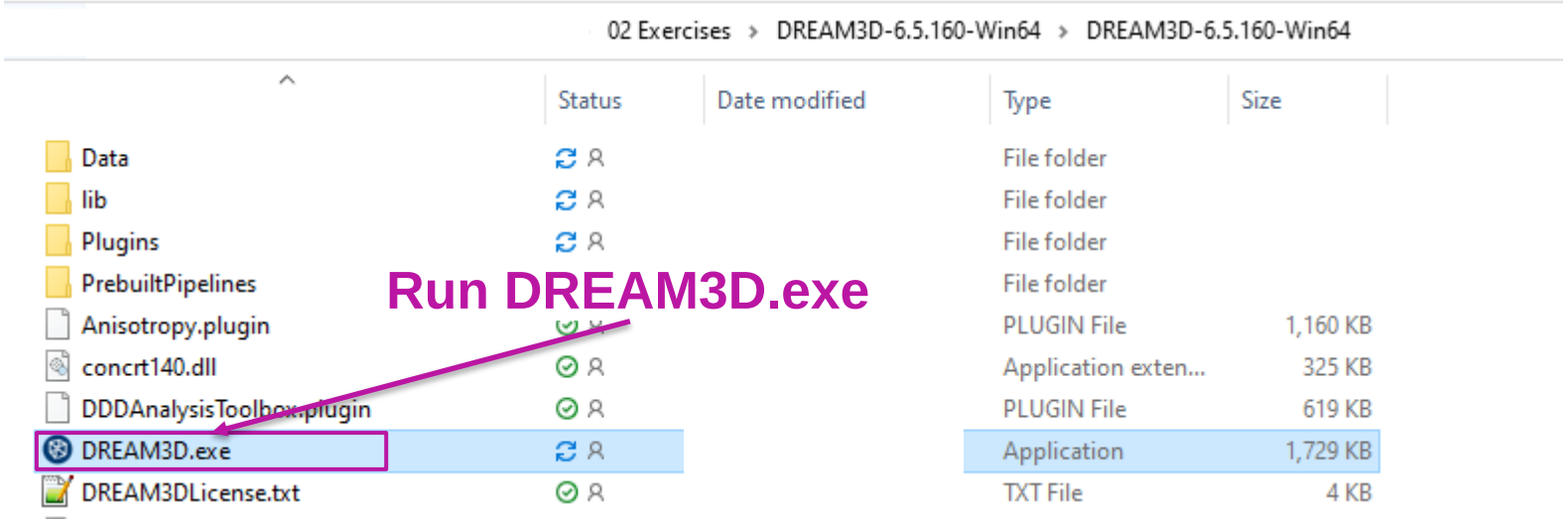
DREAM.3D & ParaView Extraction

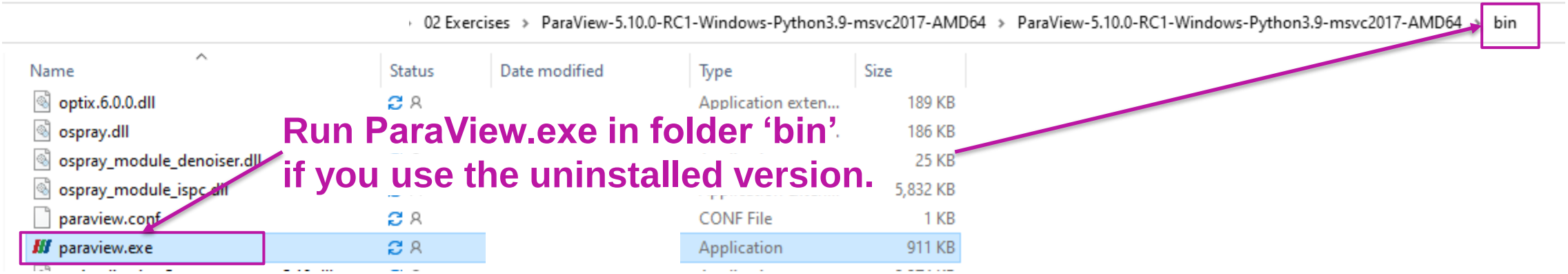


Extract the DREAM.3D/ParaView .zip file

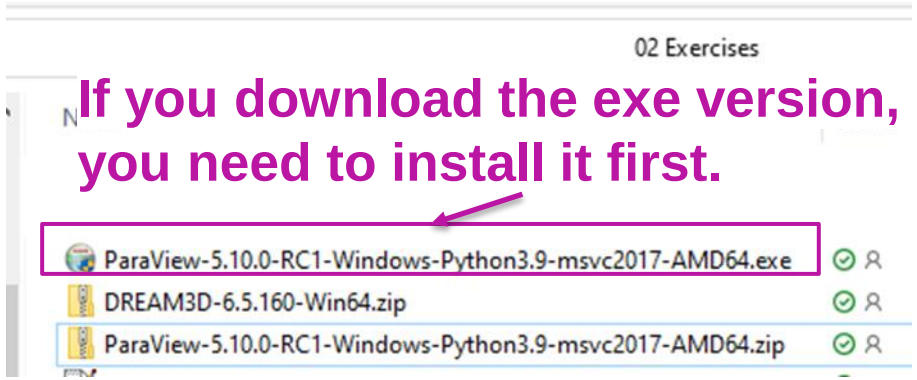


DREAM.3D & ParaView running





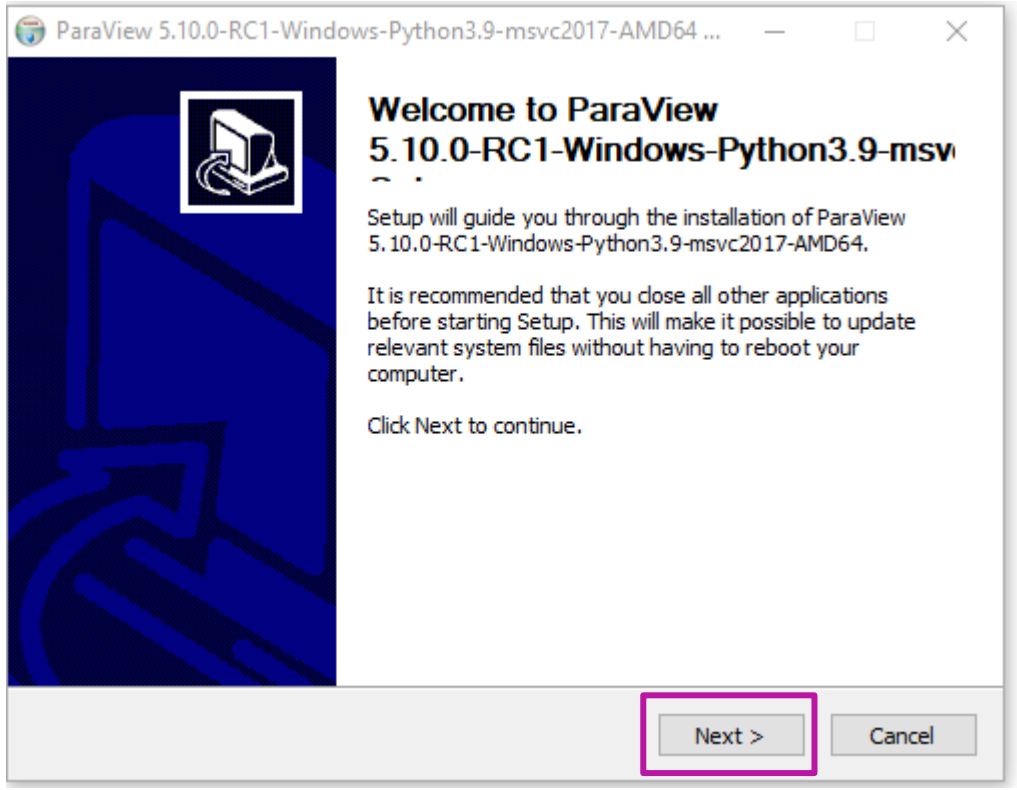
ParaView installation

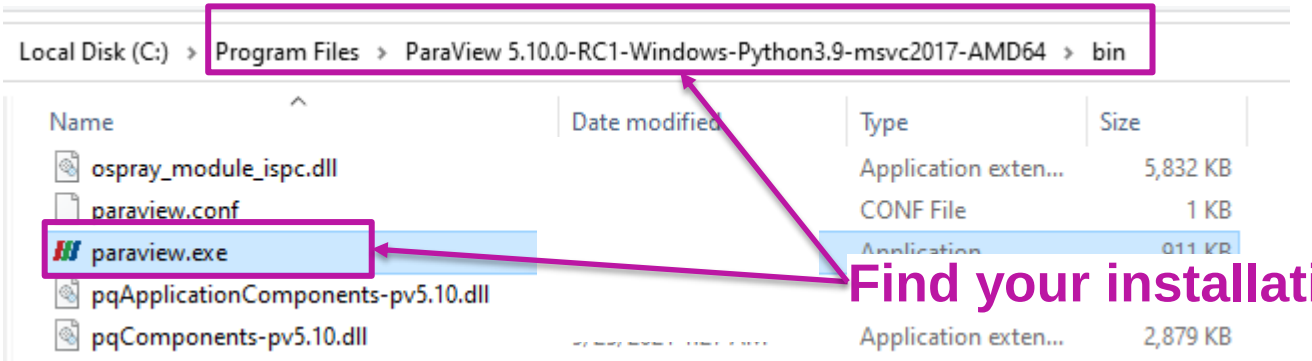


If you download the exe version, you need to install it first.

You are probably asked for the confirmation to run an .exe application in windows system.

Click ‘Yes’, then step by step to install ParaView on your computer.





Find your installation folder and run ParaView.exe

Basic DREAM.3D operation (1. Equiaxed single phase)

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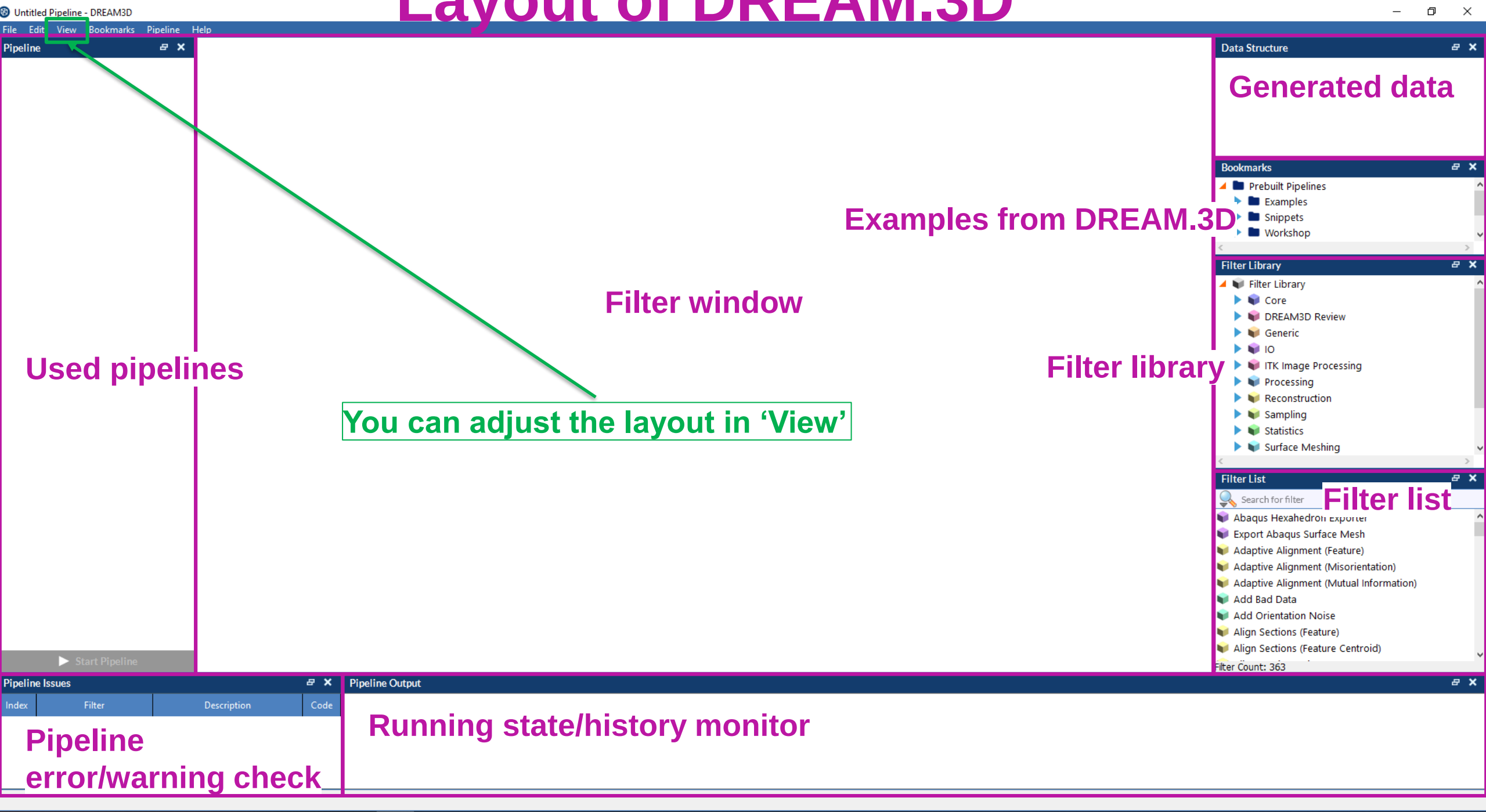
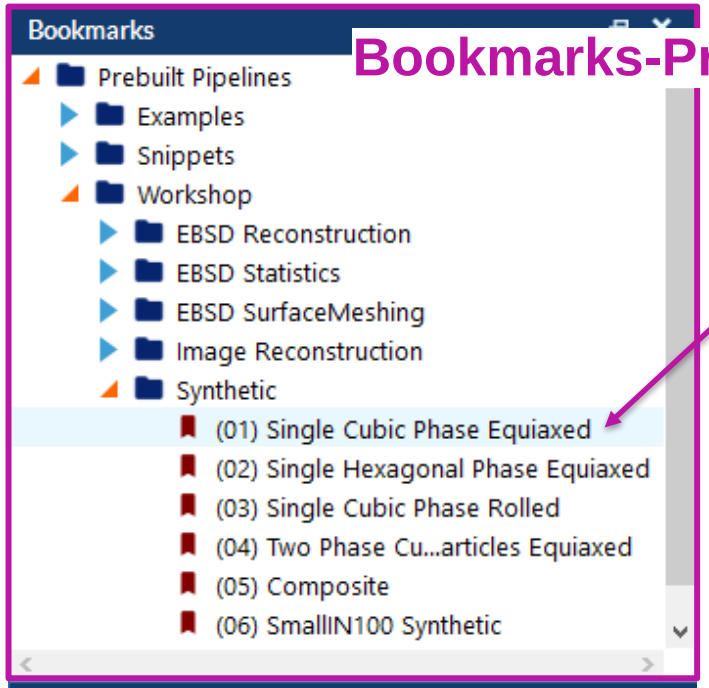
Layout of DREAM.3D

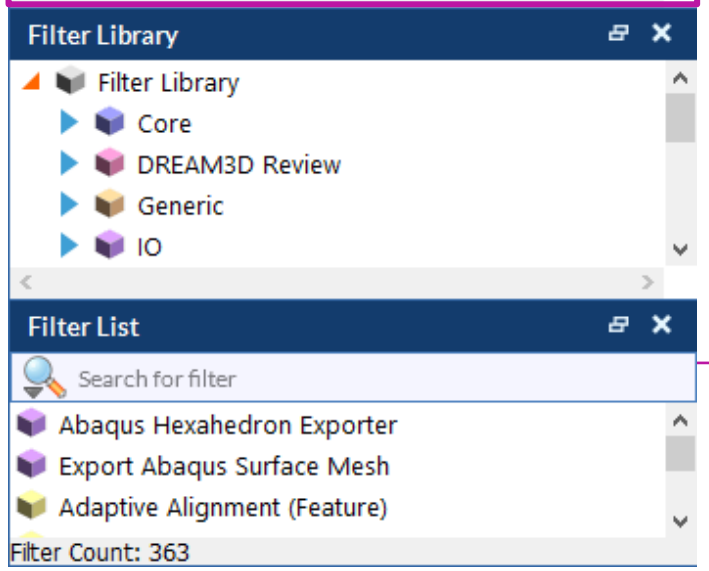


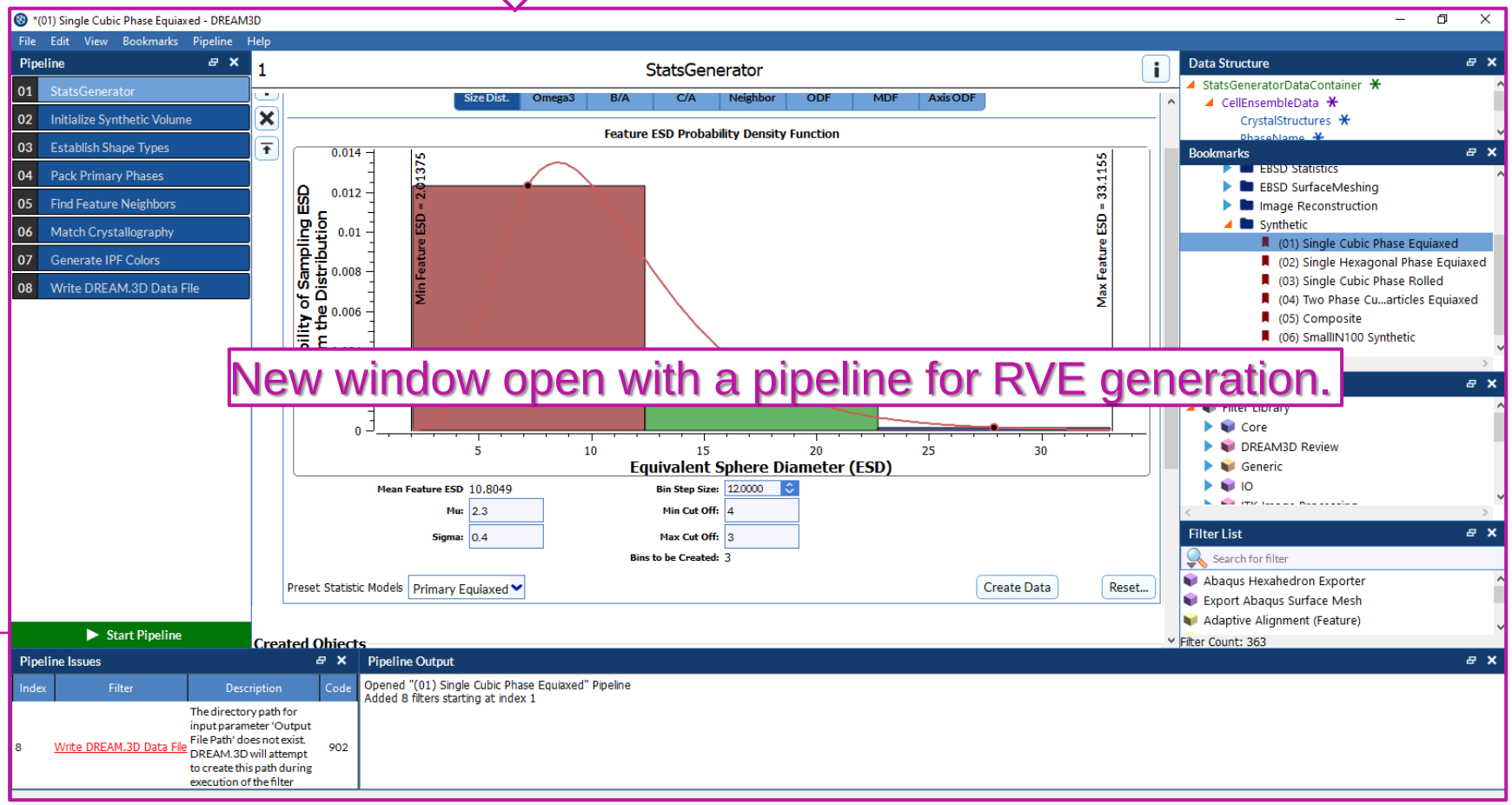
Build up a pipeline

Bookmarks-Prebuilt pipelines: Examples from DREAM.3D

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

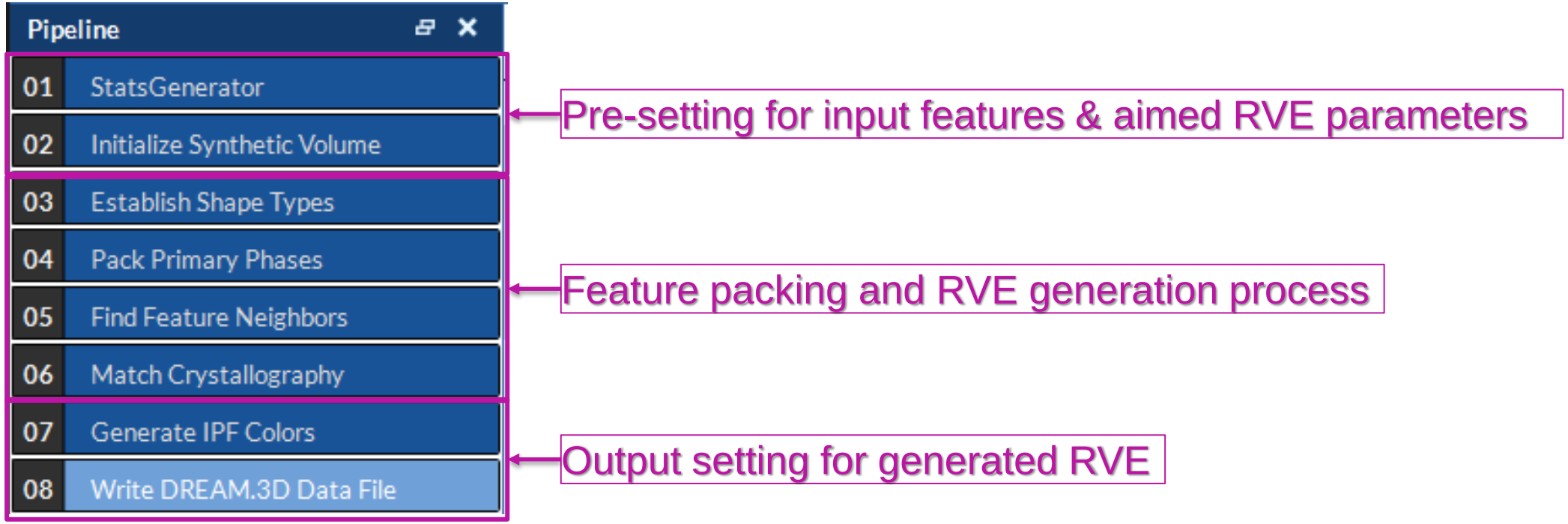






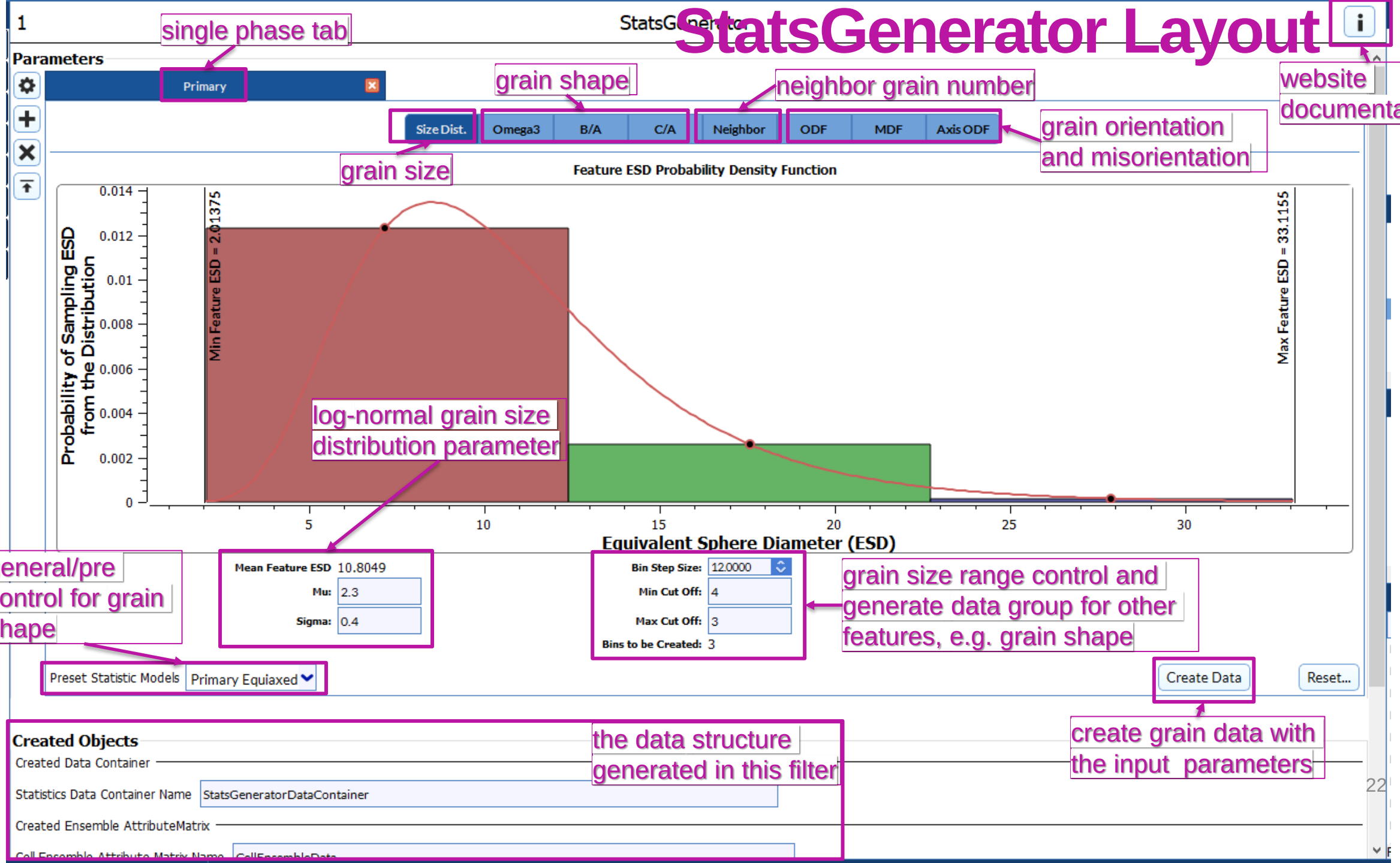
New window open with a pipeline for RVE generation.

DREAM.3D pipelines

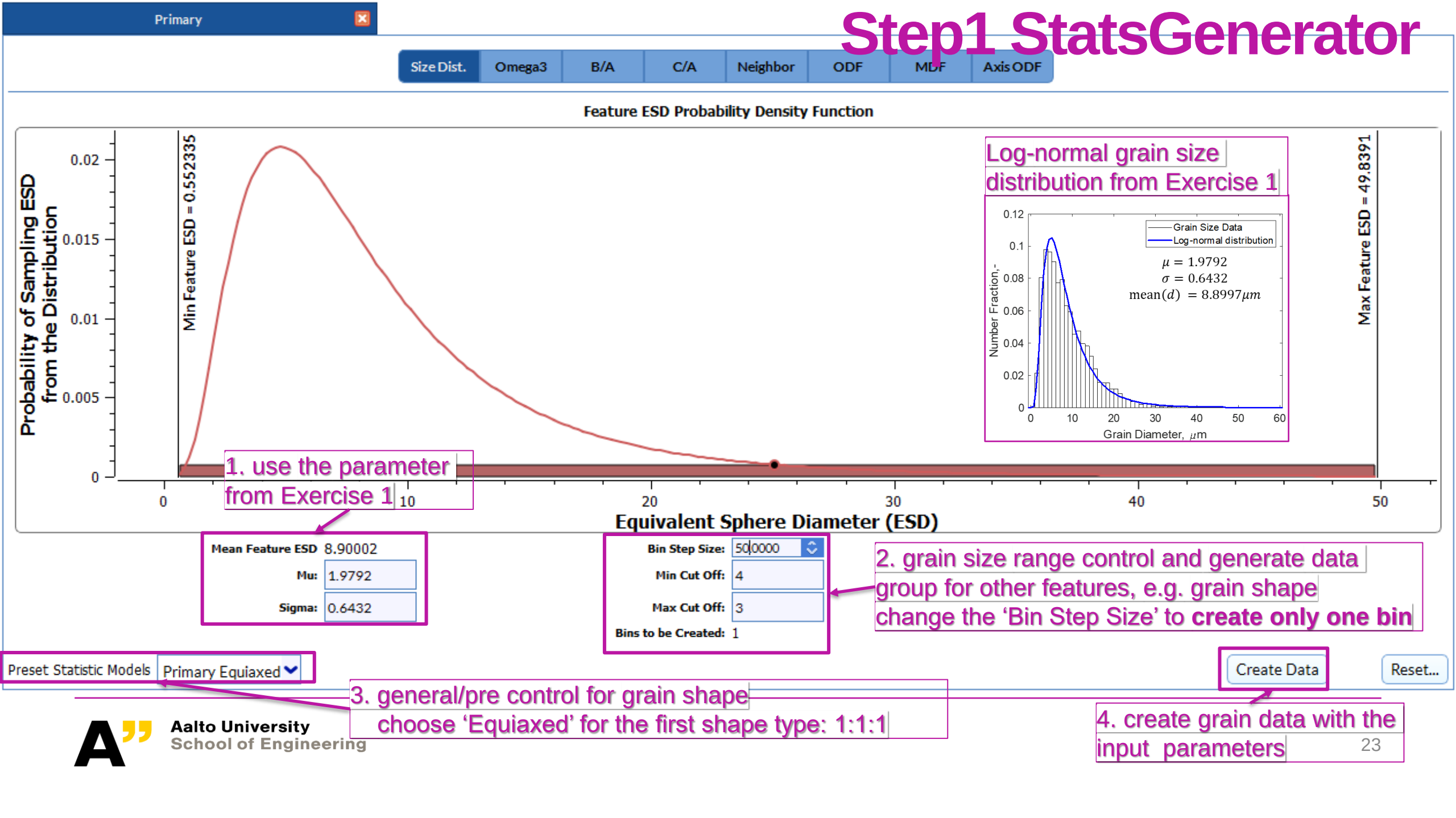


In DREAM.3D, the pipeline is used to achieve a specific function, composed of different filters.
E.g., filters 01-08 are combined here to generate a RVE with single phase, pre-defined grain size distribution, and the equiaxed grain shape.

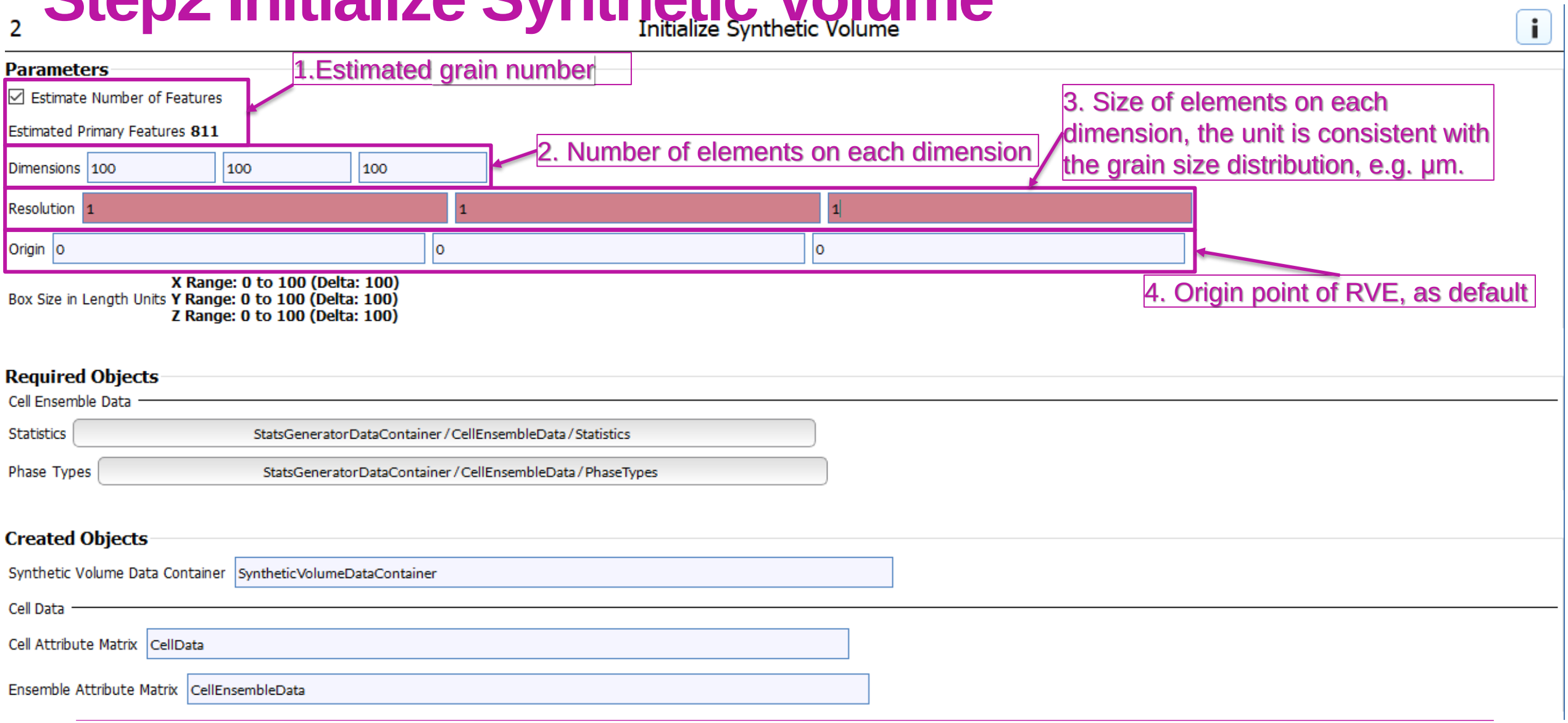
StatsGenerator Layout



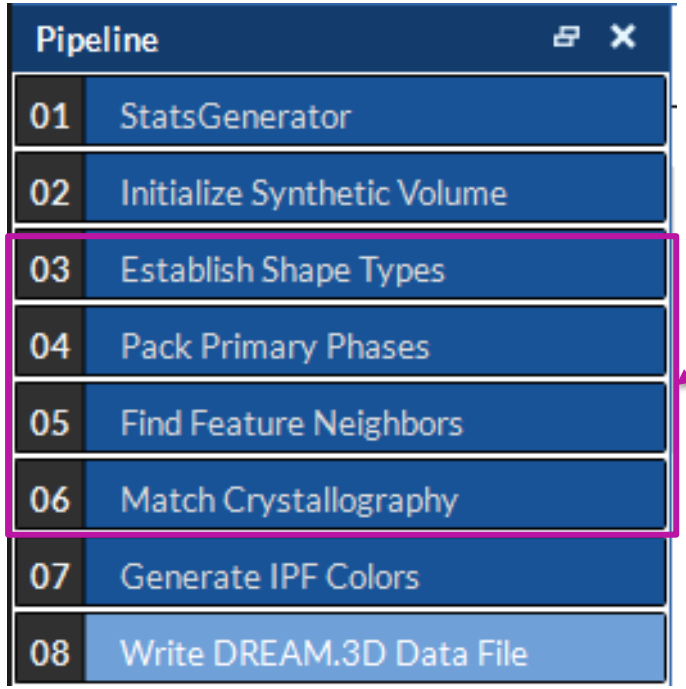
Step1 StatsGenerator



Step2 Initialize Synthetic Volume



DREAM.3D - Generation process



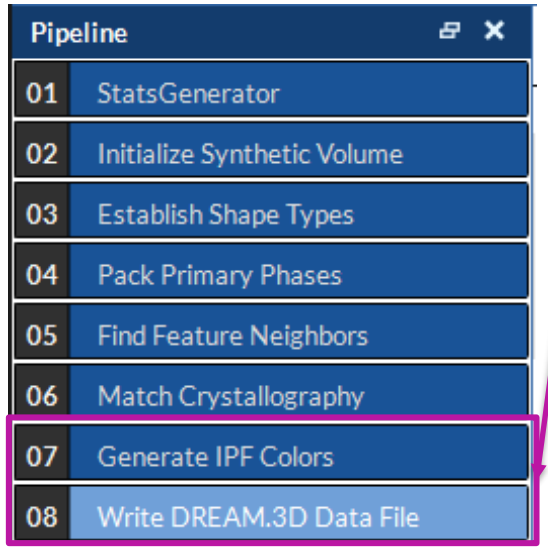
Feature packing and RVE generation process:

- 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://www.dream3d.io/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'.

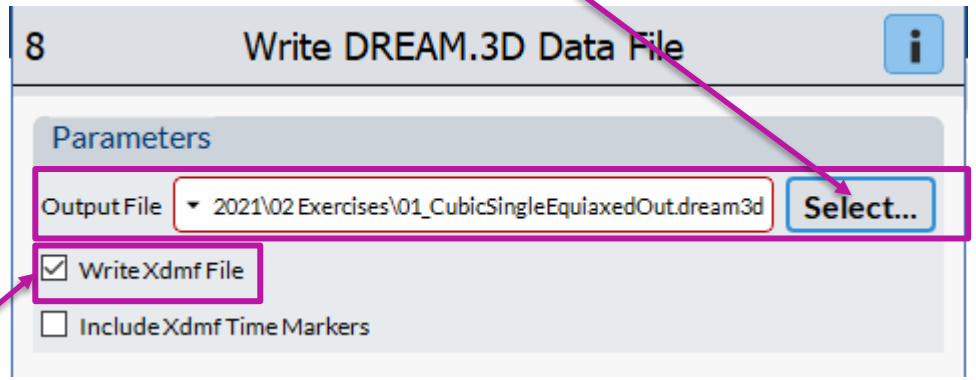
DREAM.3D - RVE output



Step4 Output setting for generated RVE

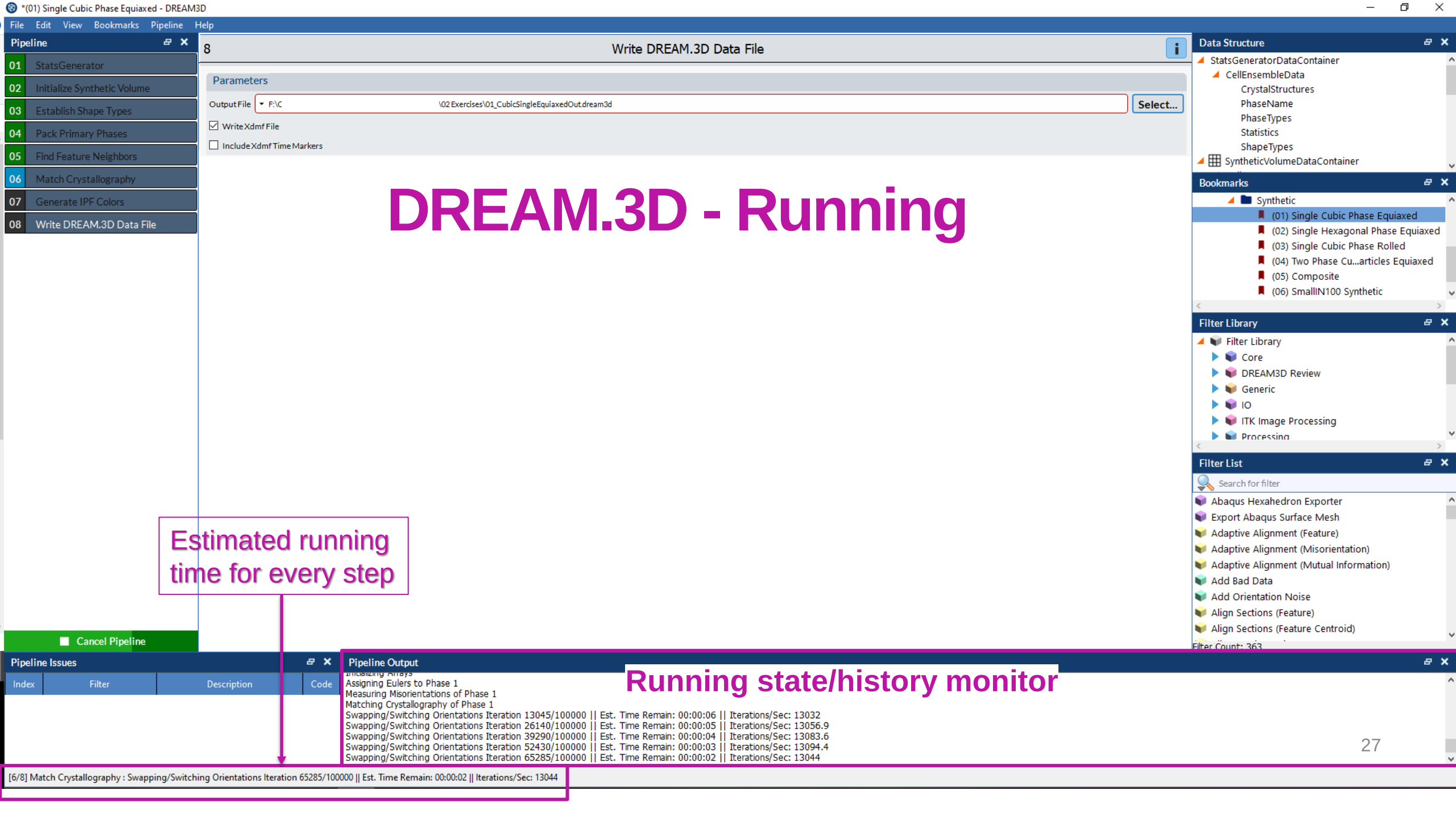
- 'Generate IPF Colors' is set for the grain orientation distribution. Use the default setting.

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

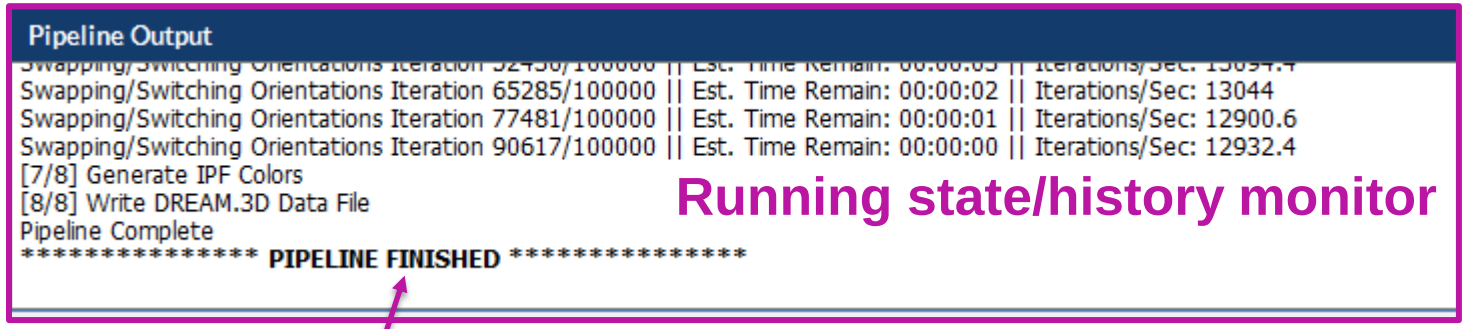


4.2. Choose the 'Write Xdmf File' option, which is used for the visualization of 3D RVE in ParaView.

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 F:\C \02 Exercises\01_CubicSingleEquiaxedOut.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
Running state/history monitor
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
[6/8] Match Crystallography : Swapping/Switching Orientations Iteration 65285/100000 || Est. Time Remain: 00:00:02 || Iterations/Sec: 13044

DREAM.3D - Data files

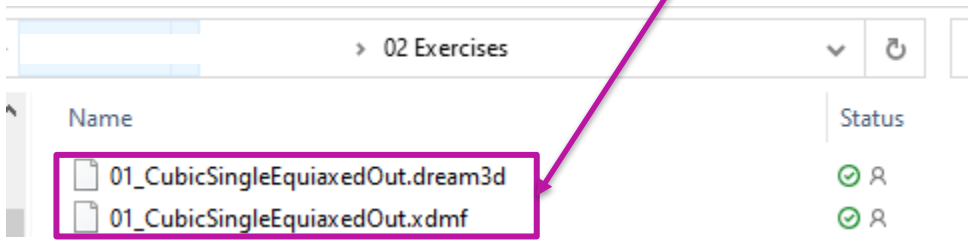


Running state/history monitor

Successfully finished

Check your DREAM.3D output folder:

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



ParaView operation

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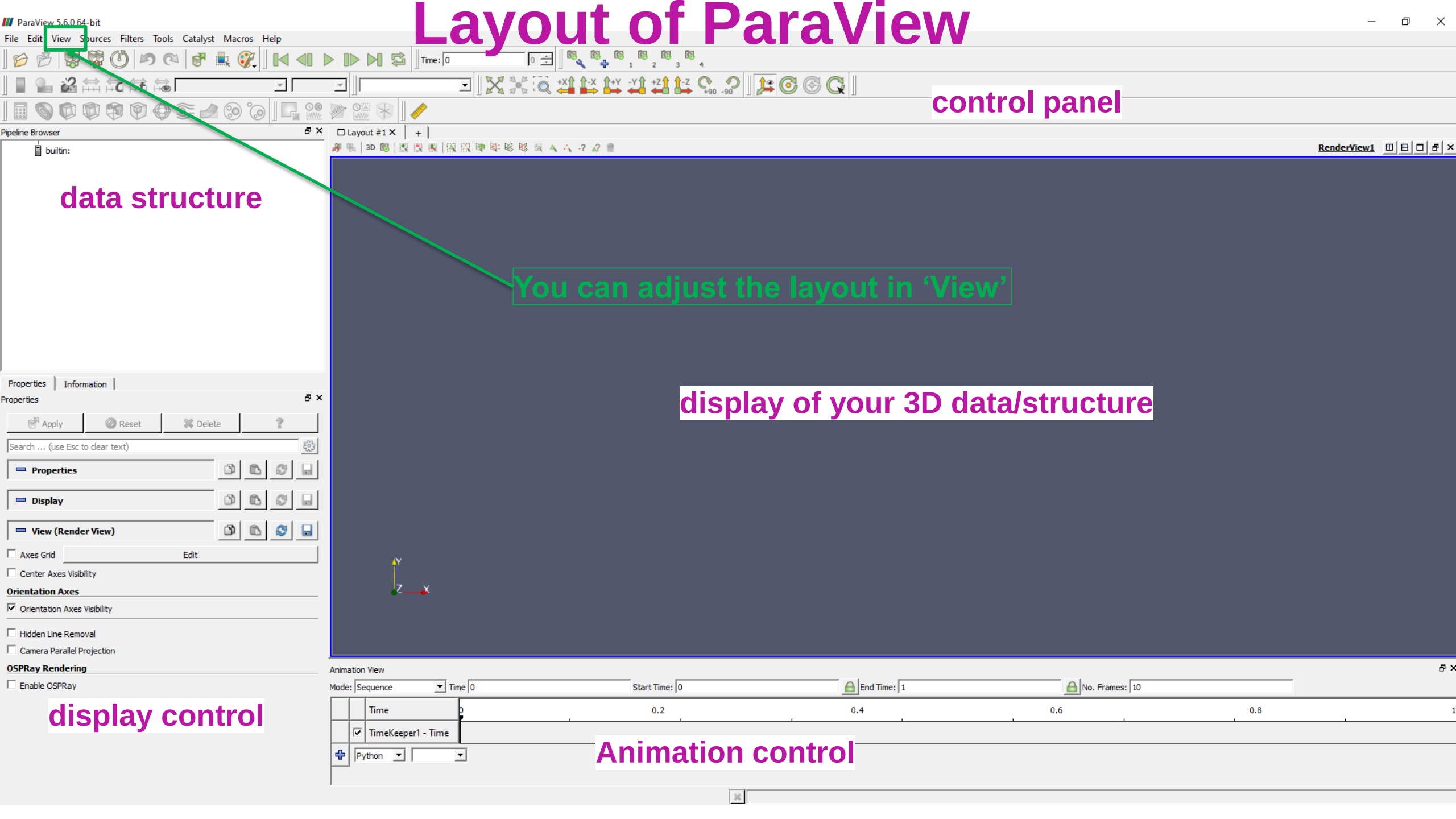
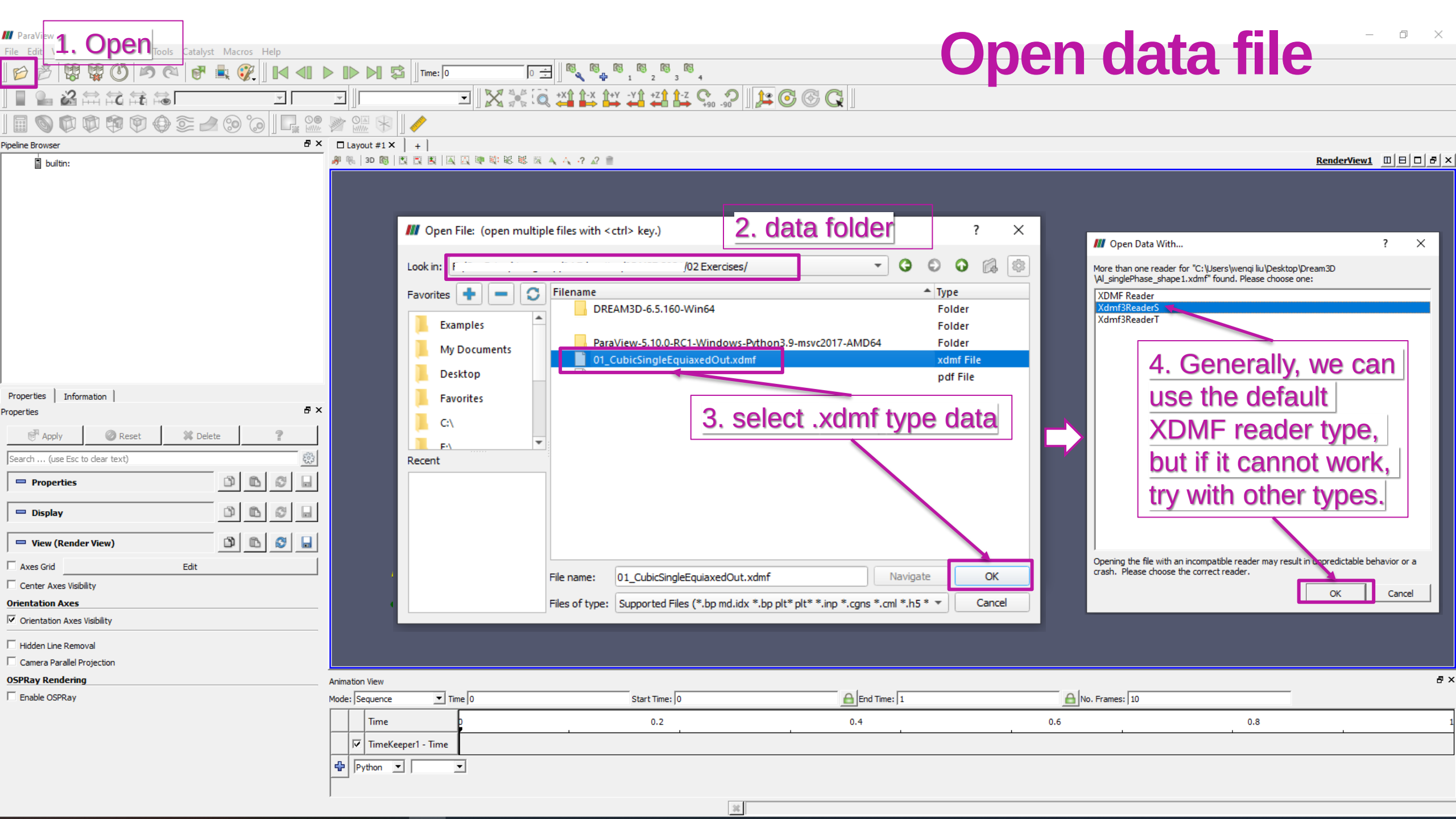
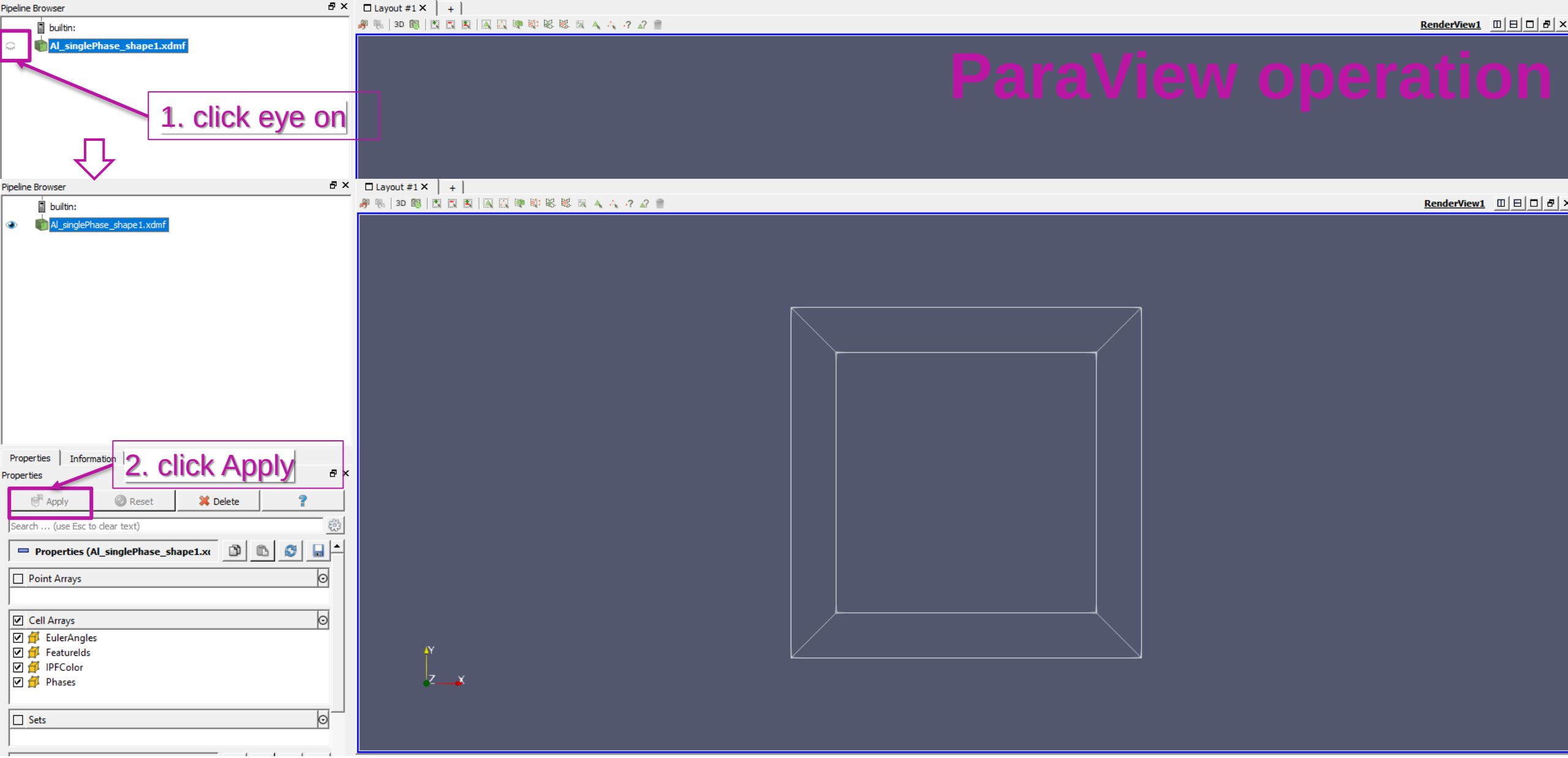
Layout of ParaView

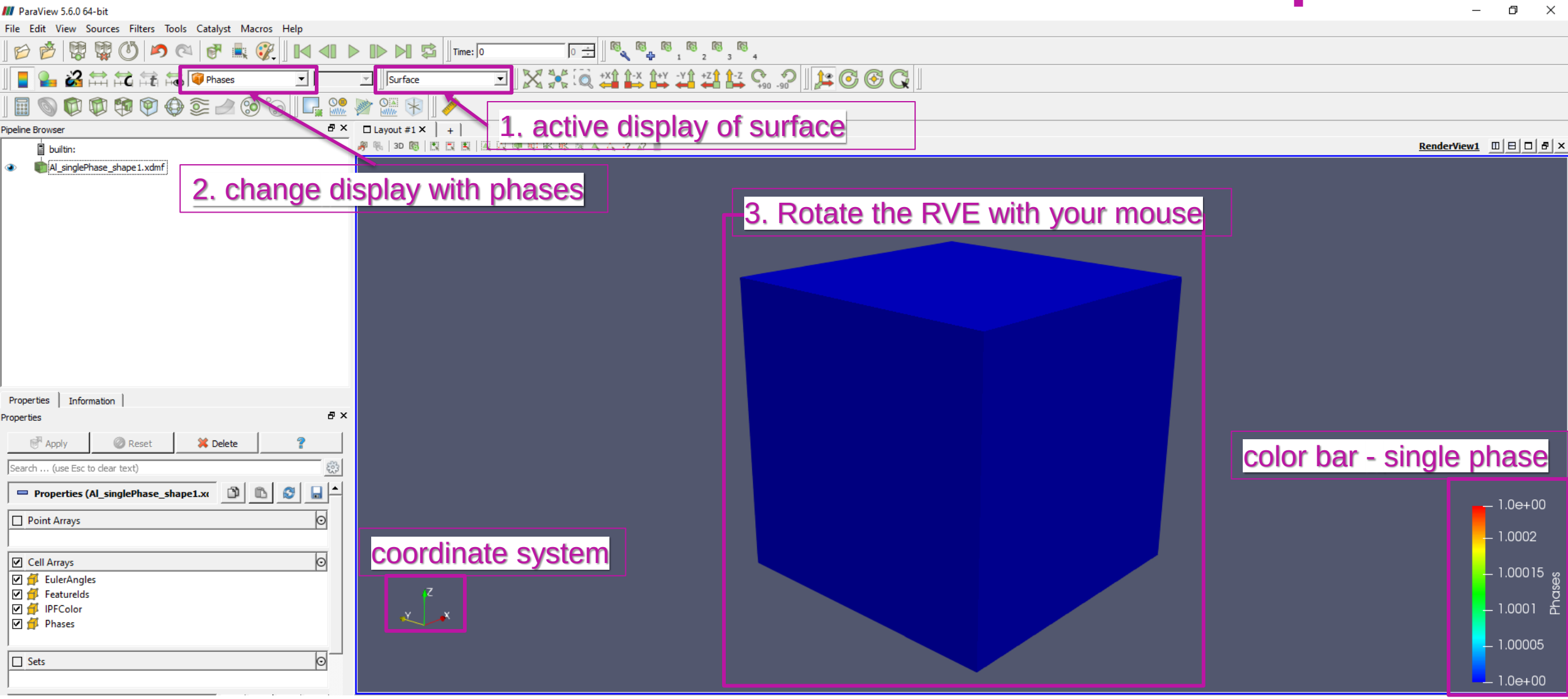


Open data file

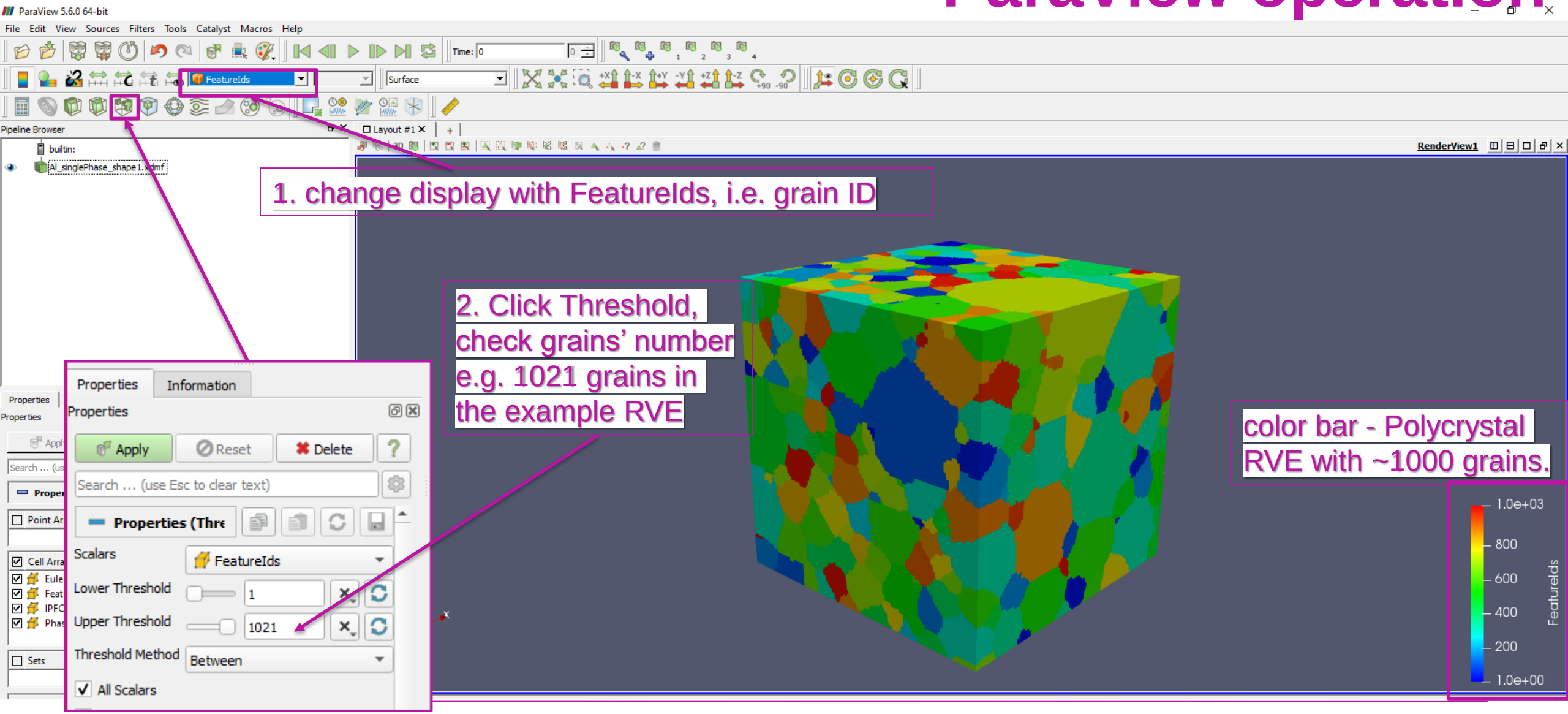



Pipeline Browser
builtin:
Al_singlePhase_shape1.xdmf
1. click eye on
ParaView operation
Layout #1
RenderView1
Pipeline Browser
builtin:
Al_singlePhase_shape1.xdmf
Layout #1
RenderView1
Properties
Information
2. click Apply
Properties
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties (Al_singlePhase_shape1.x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

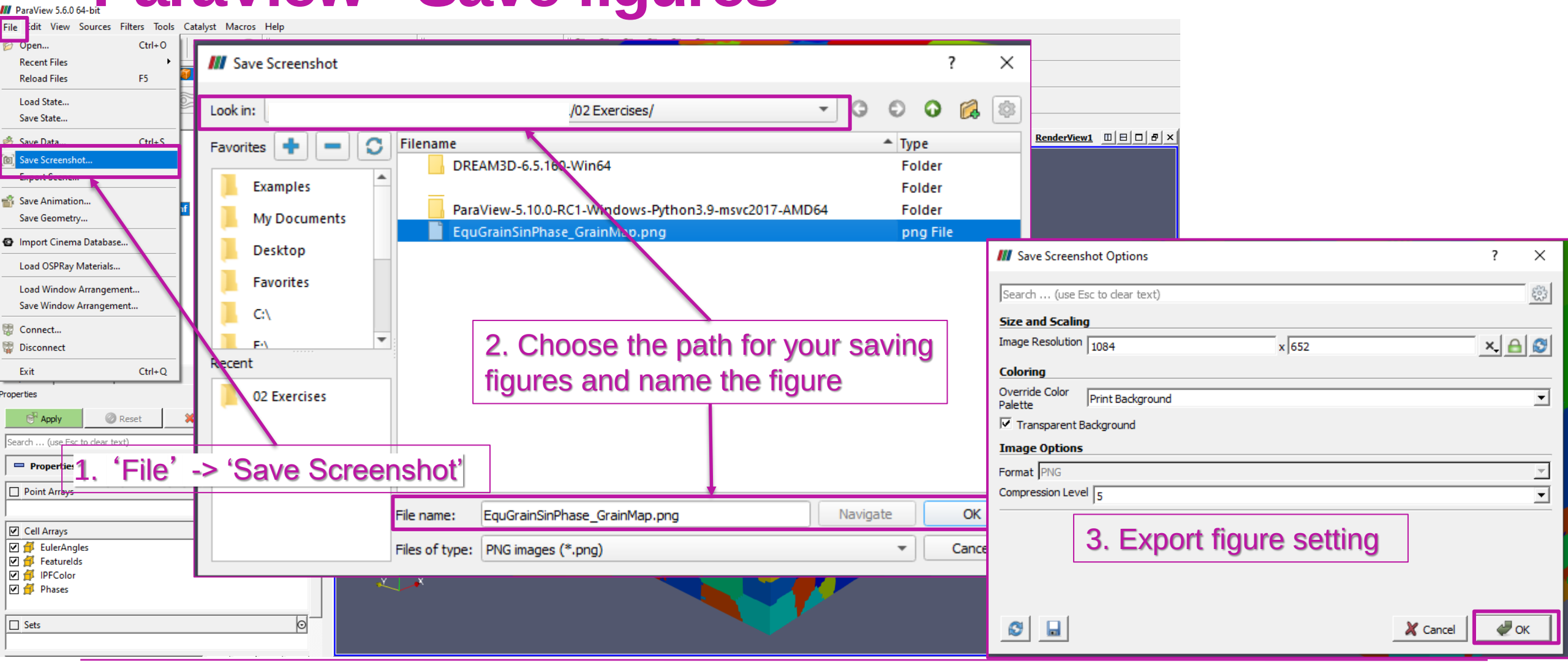
ParaView operation



ParaView operation



ParaView - Save figures



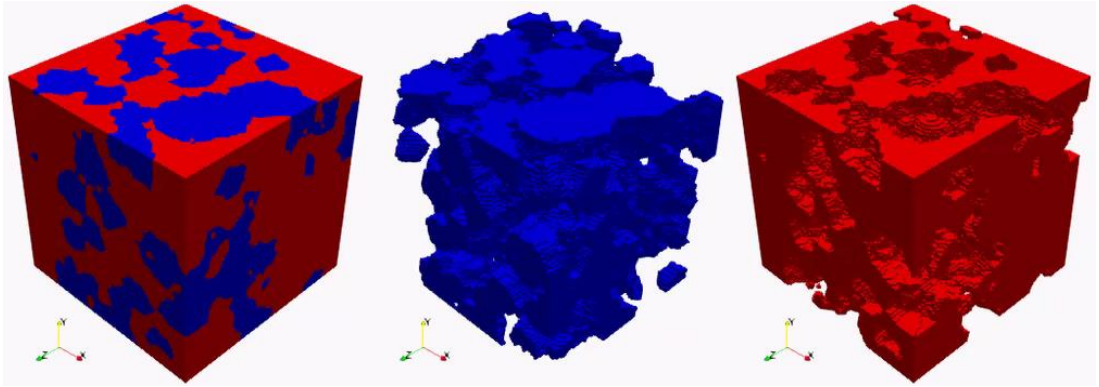
Advanced DREAM.3D operation

Aalto University
School of Engineering

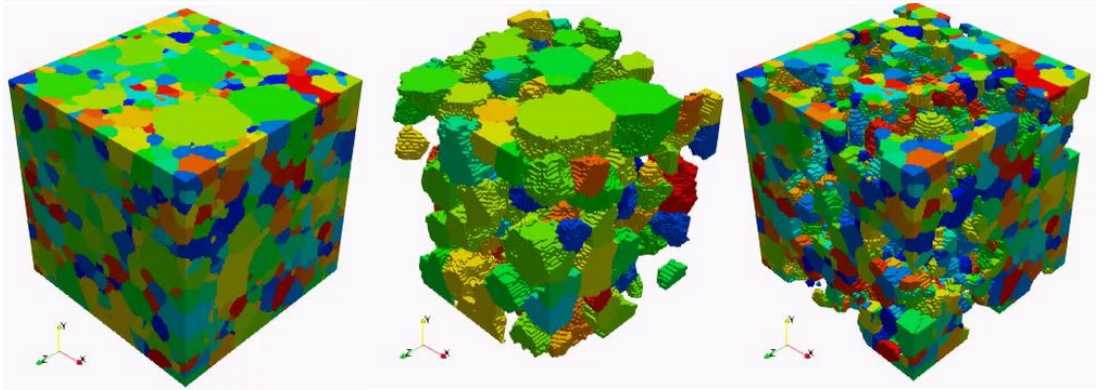
DREAM.3D For more features

2. Elongated/Rolled grain structure
3. Grain shape distribution
4. Dual-/multi-phase structure

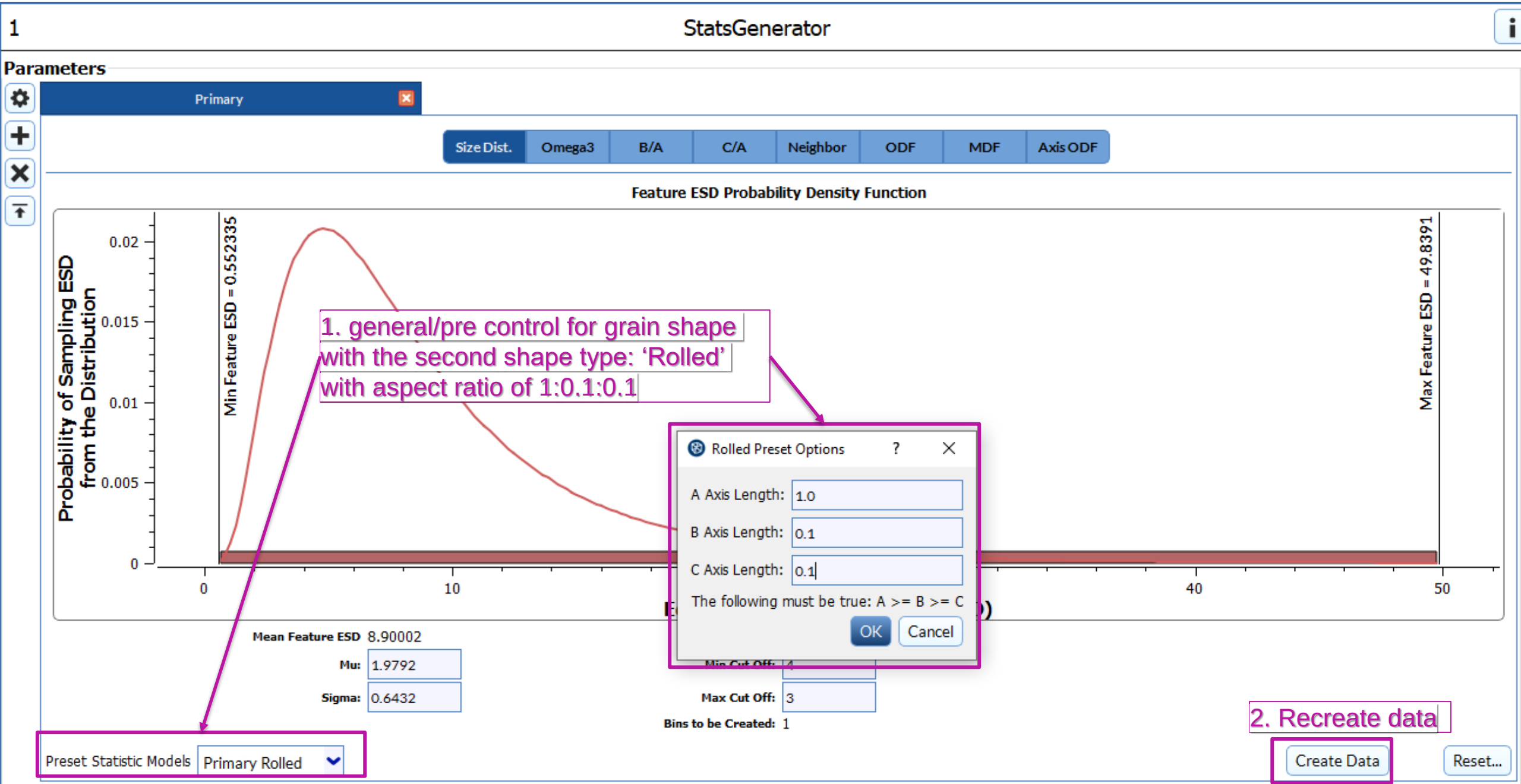
Phase map



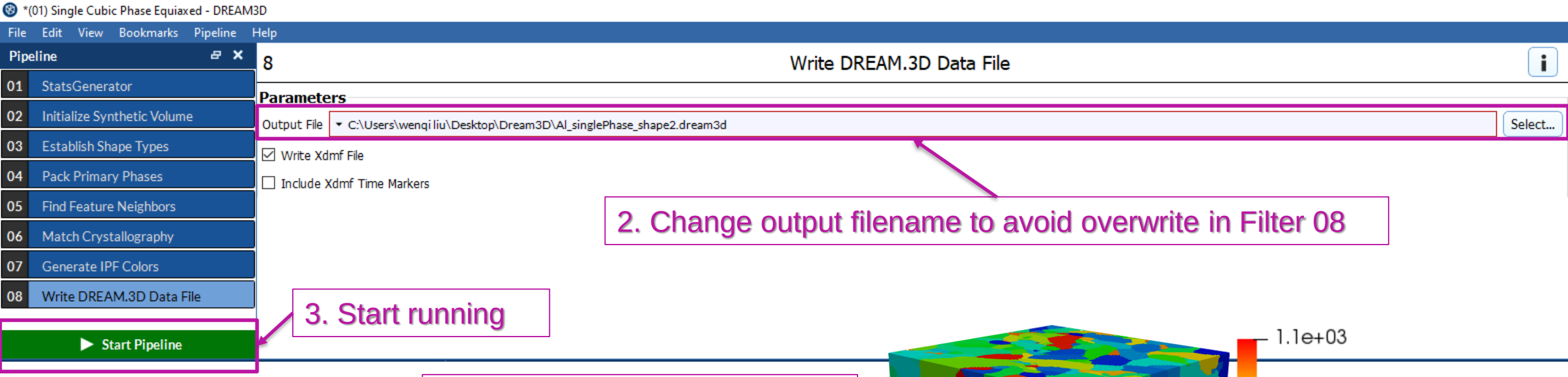
Grain map



2. DREAM.3D - Rolled grain structure



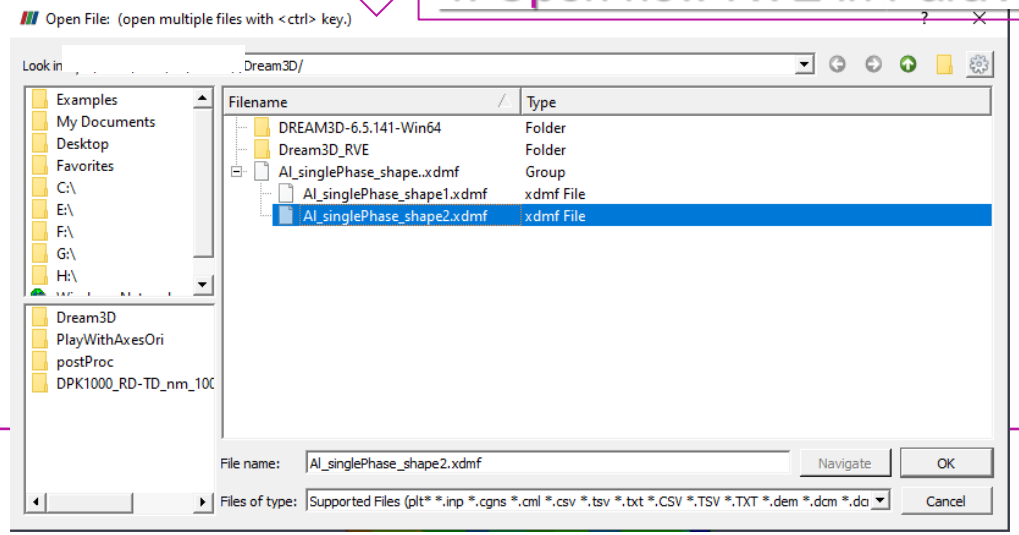
2. DREAM.3D - Rolled grain structure

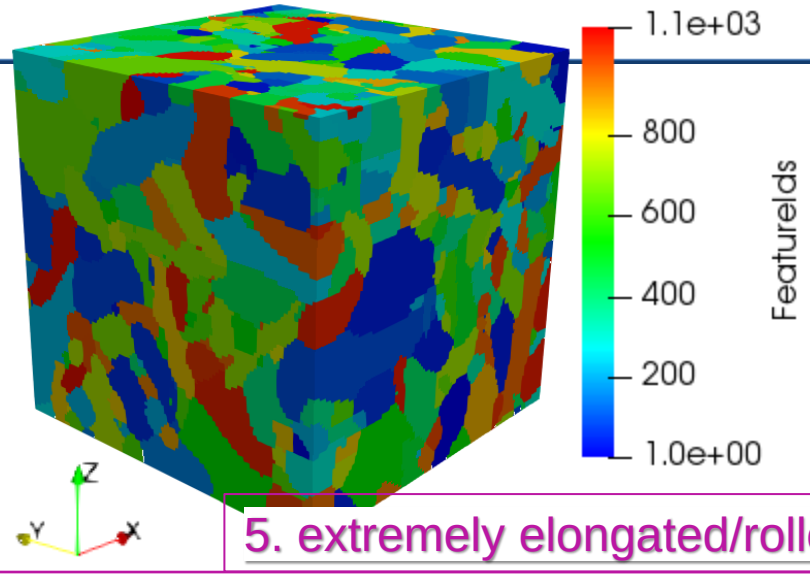


2. Change output filename to avoid overwrite in Filter 08

3. Start running

4. Open new RVE in ParaView

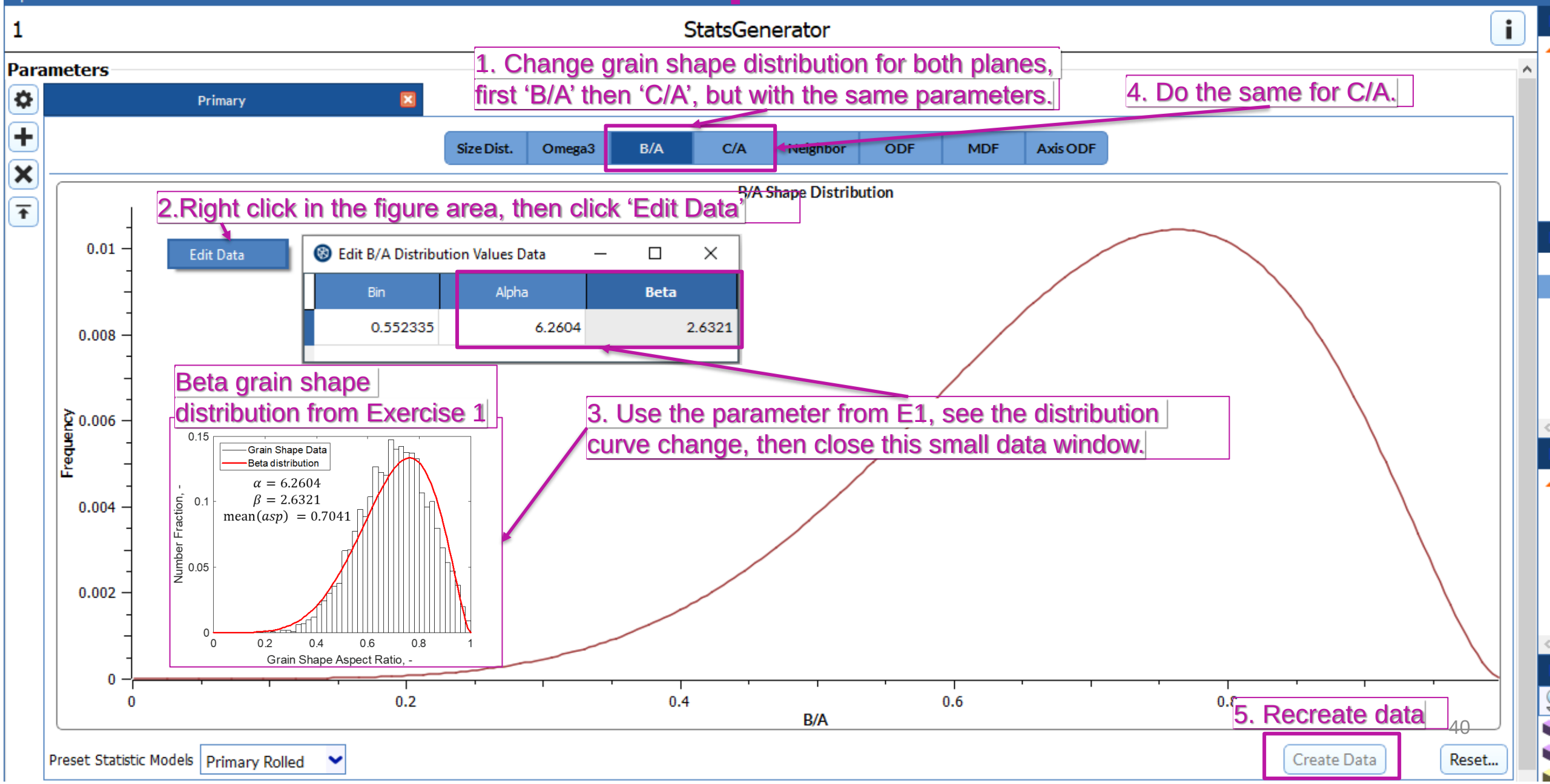




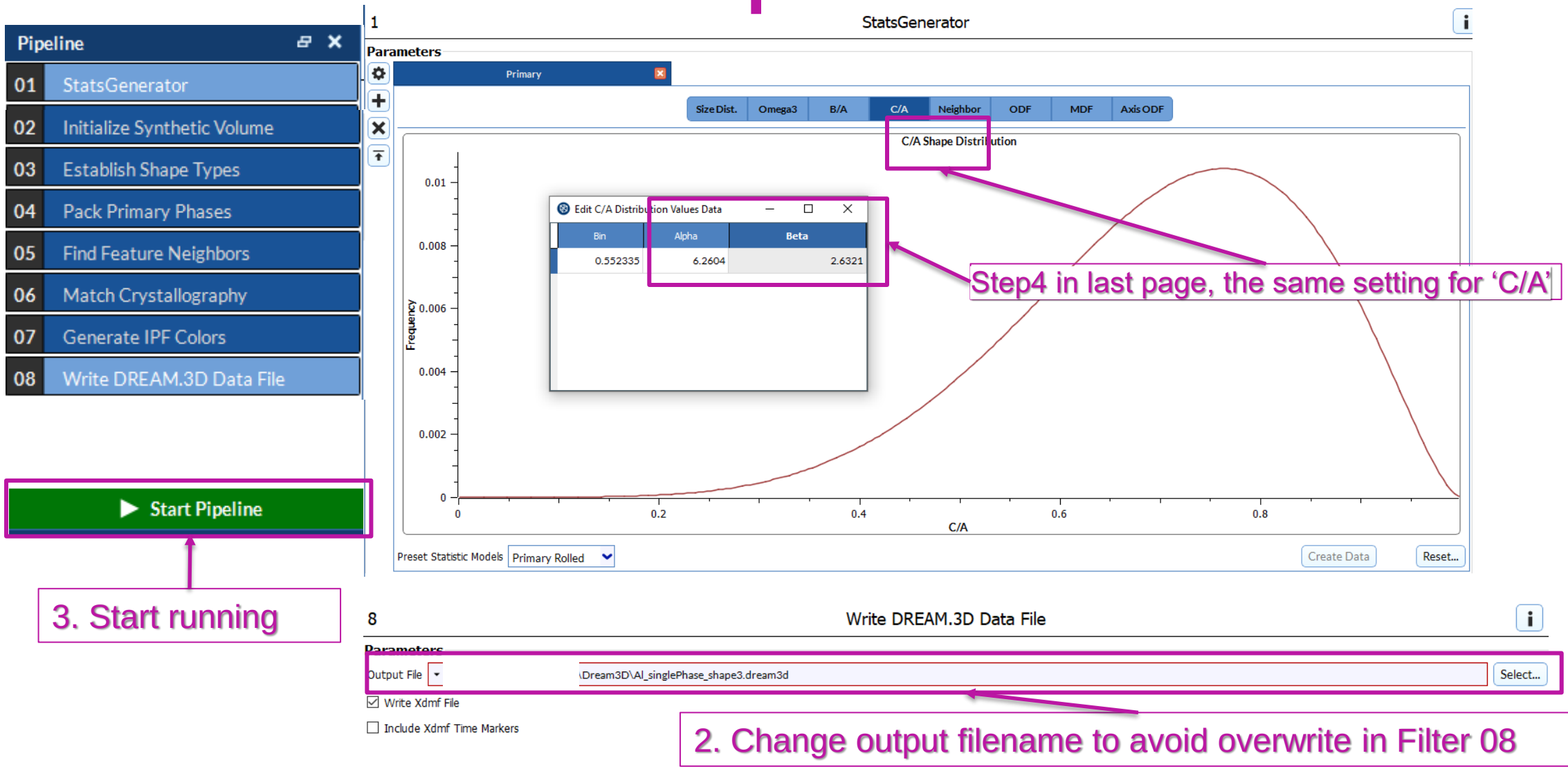
5. extremely elongated/rolled grains

1. Keep the same settings for filters 2-7 as before.

3. DREAM.3D - Grain shape distribution

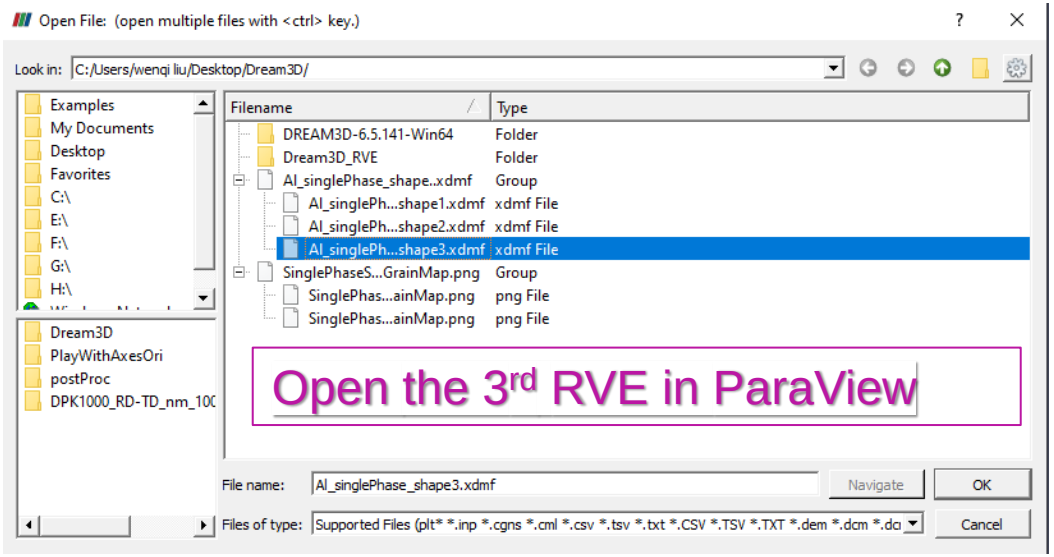


3. DREAM.3D - Grain shape distribution

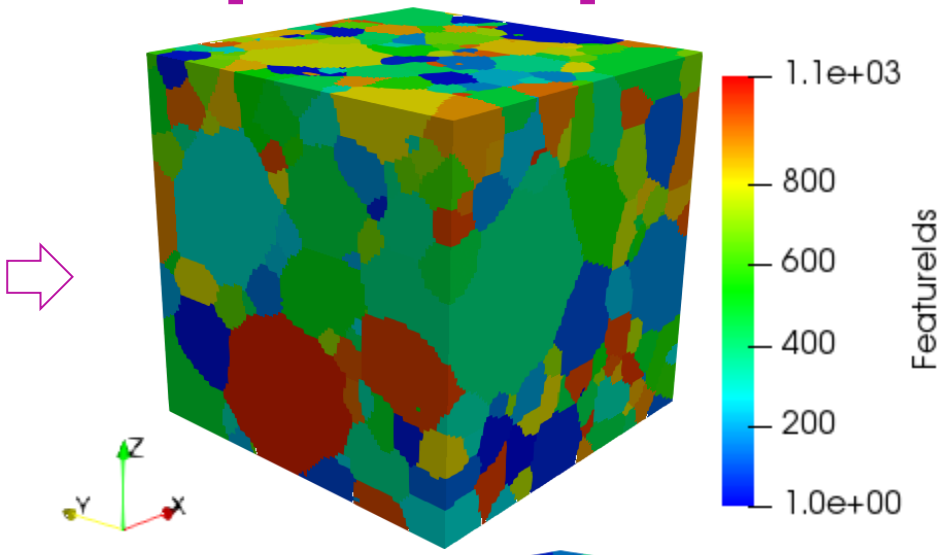


1. Keep the same settings for filters 2-7 as before.

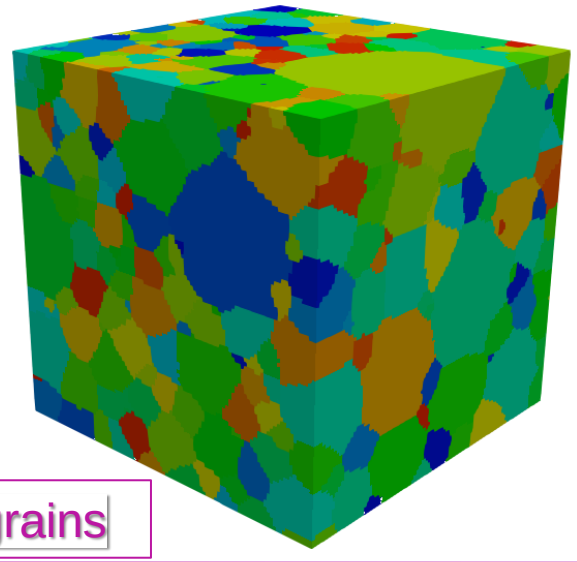
1-3. DREAM.3D - Grain shape comparison



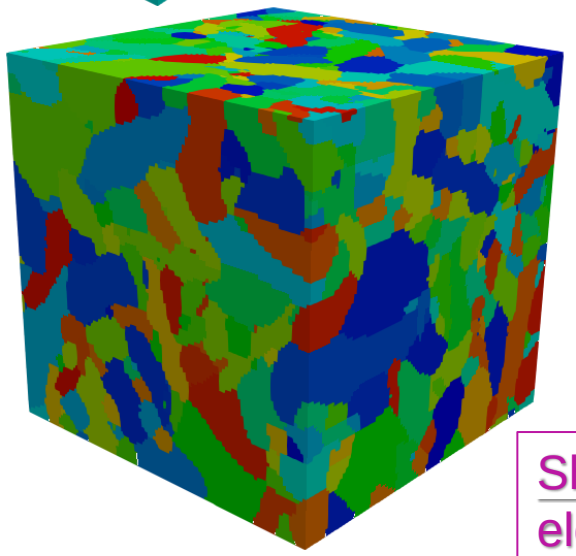
Open the 3rd RVE in ParaView



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



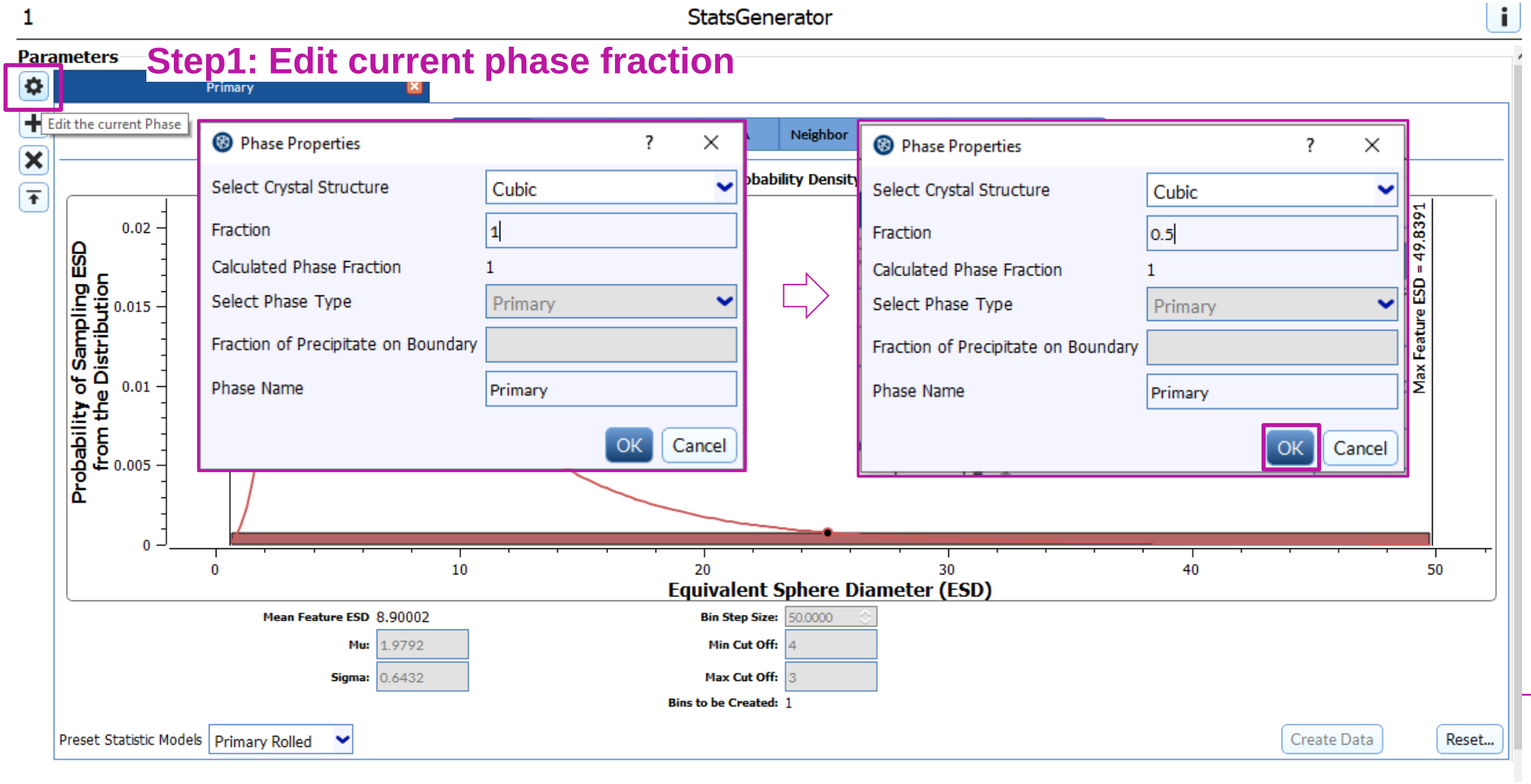
Shape 1: Equiaxed grains



Shape 2: Extremely elongated/rolled grains

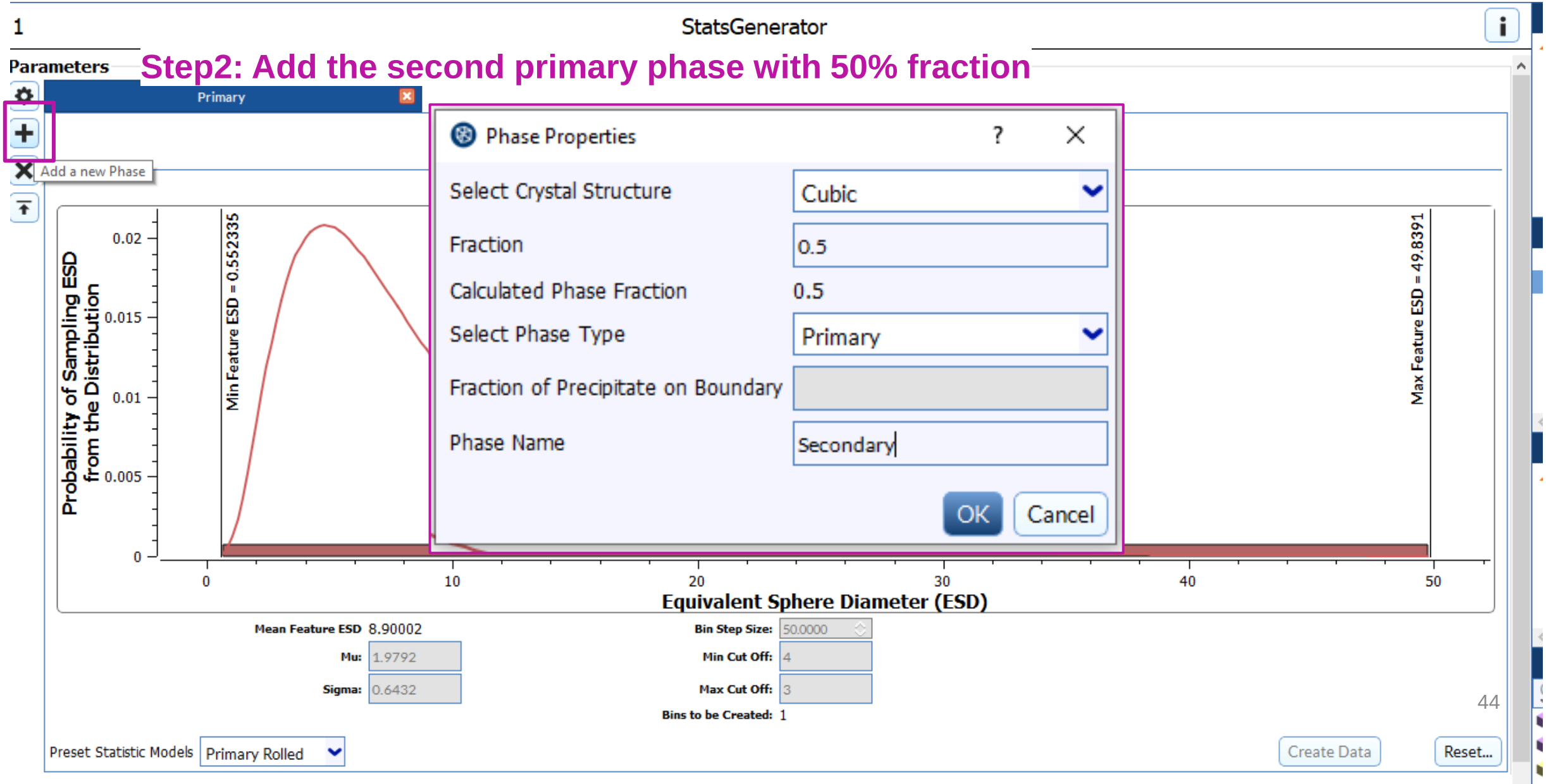
4. DREAM.3D - Dual-phase structure

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

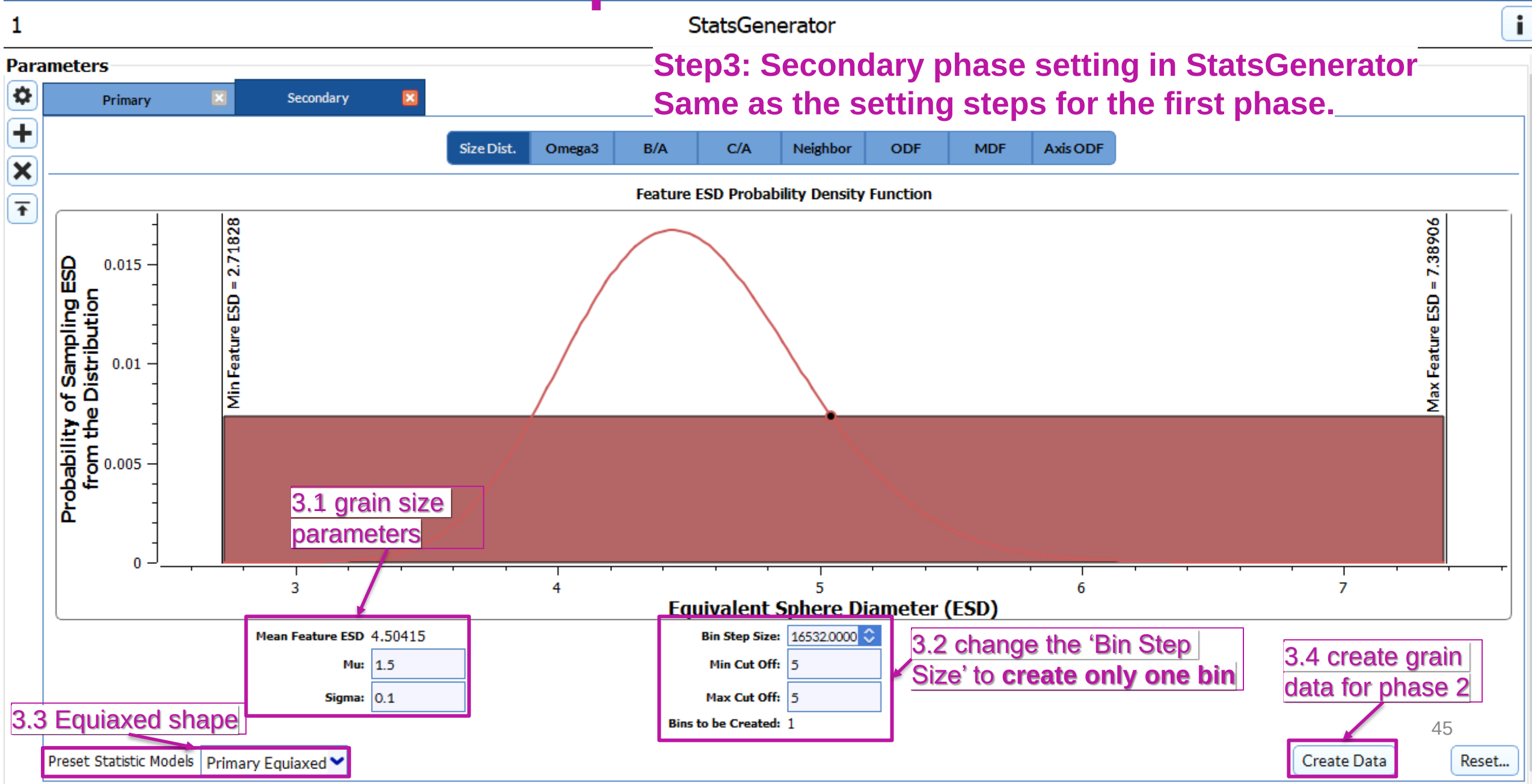


4. DREAM.3D - Dual-phase structure

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



4. DREAM.3D - Dual-phase structure



4. 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 in Filter 08

Step4: Check every filter to solve errors/warnings.

Keep the same settings for filters 2-7 as before.

Step6: Start running

Step7: Waiting a while for running

Data Structure

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

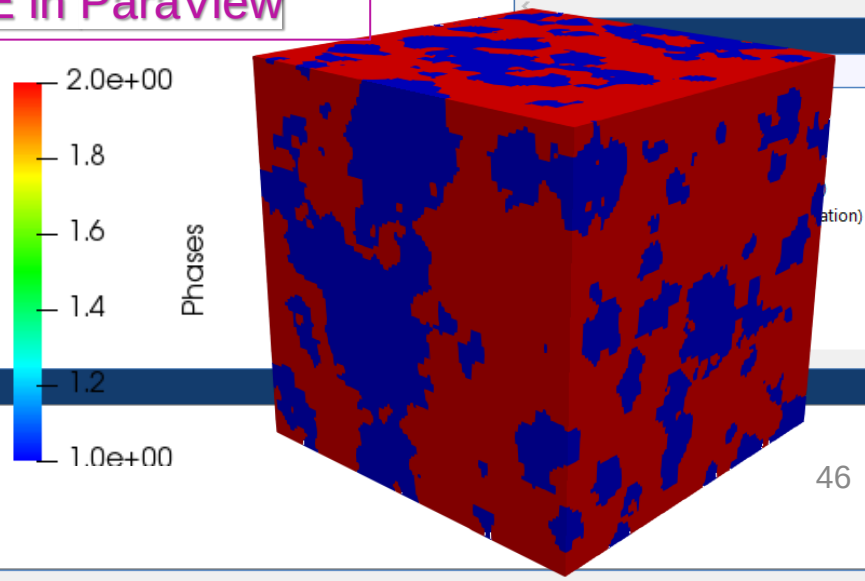
Bookmarks

- 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

Step8: Open new RVE in ParaView



Pipeline Issues

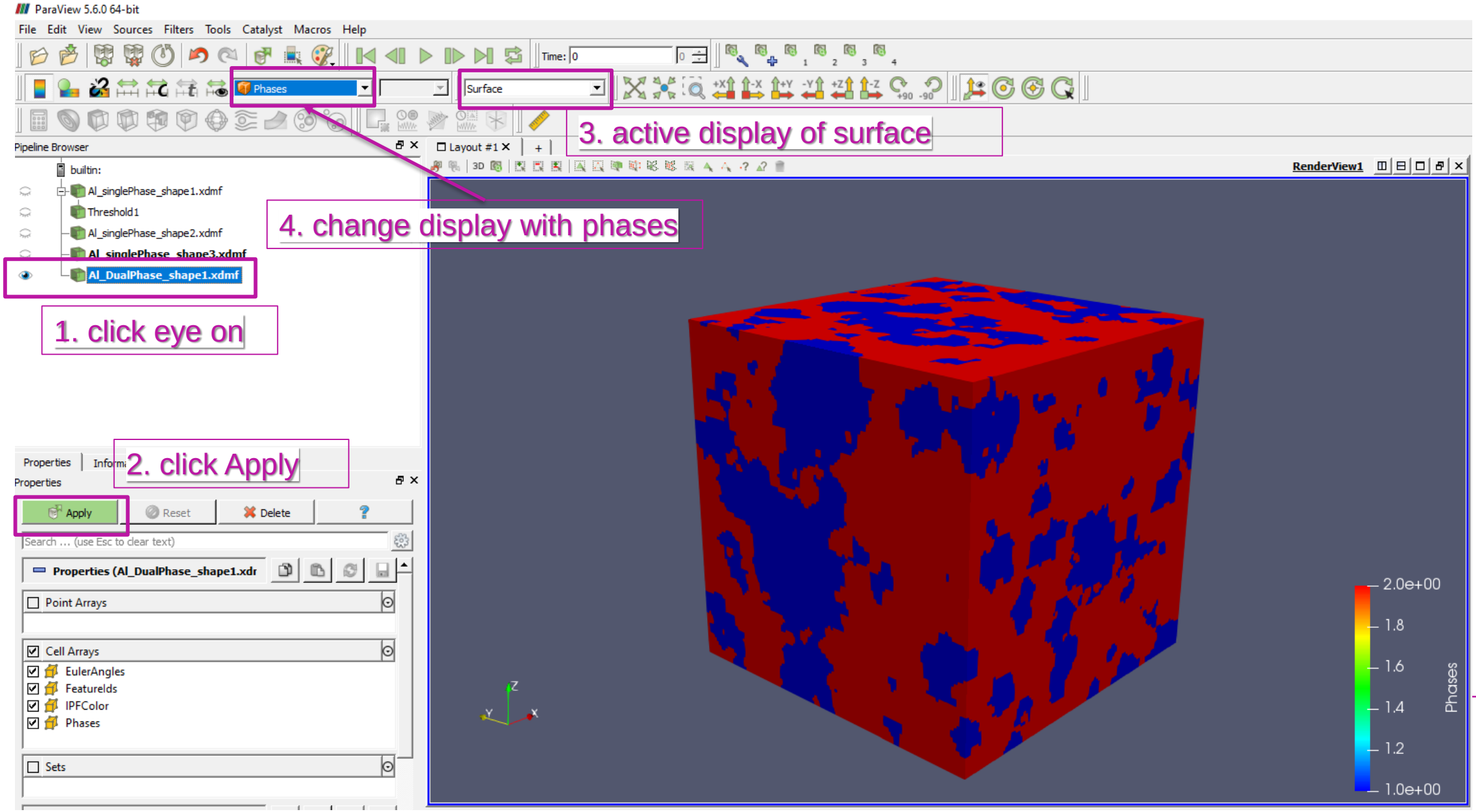
Index	Filter	Description	Code

Pipeline Output

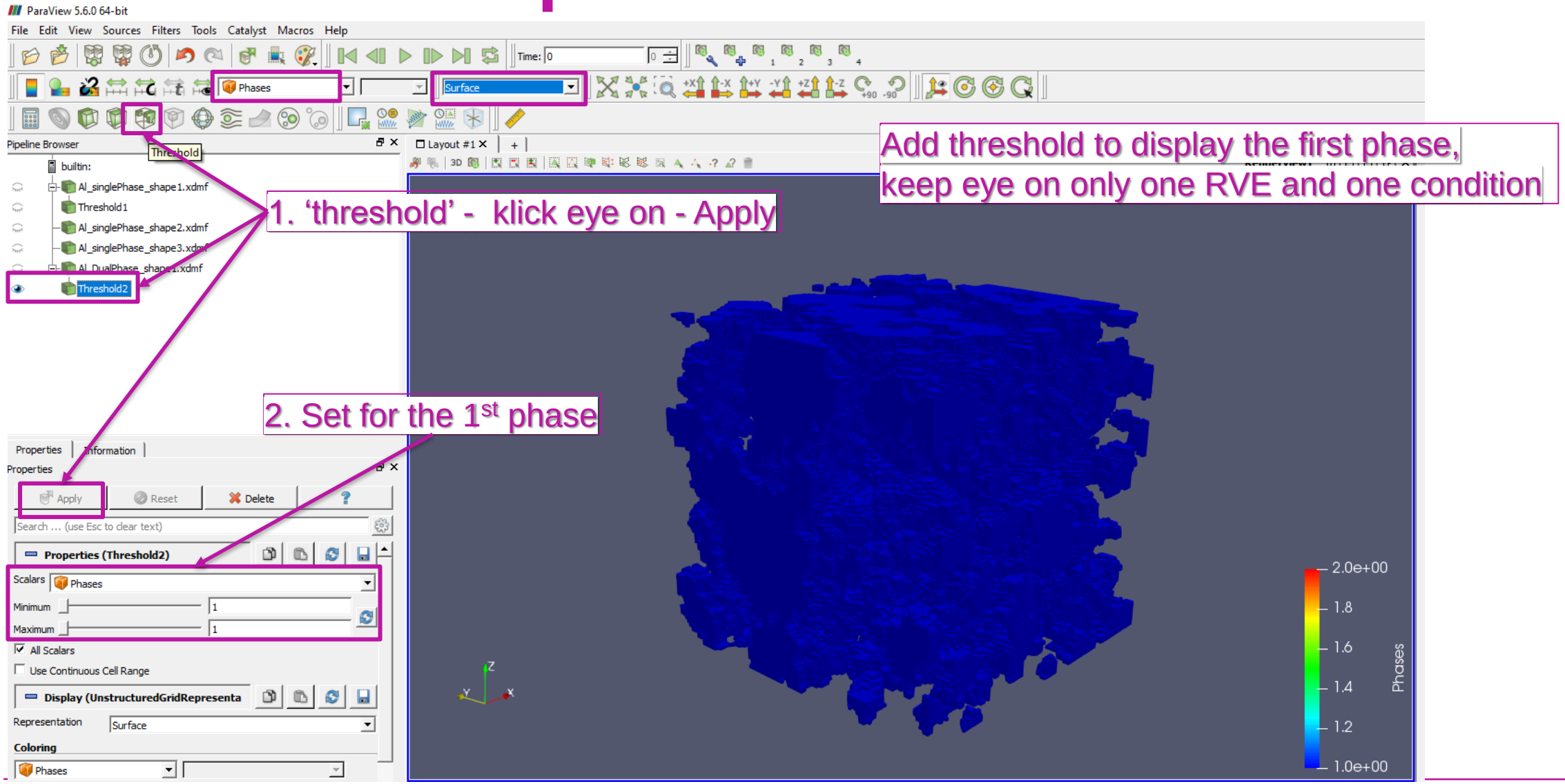
Swapping/Switching Orientations Iteration 36678/100000 || Est. Time Remain: 00:00:05 || Iterations/Sec: 12213.8
Swapping/Switching Orientations Iteration 49003/100000 || Est. Time Remain: 00:00:04 || Iterations/Sec: 12238.5
Swapping/Switching Orientations Iteration 60509/100000 || Est. Time Remain: 00:00:03 || 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

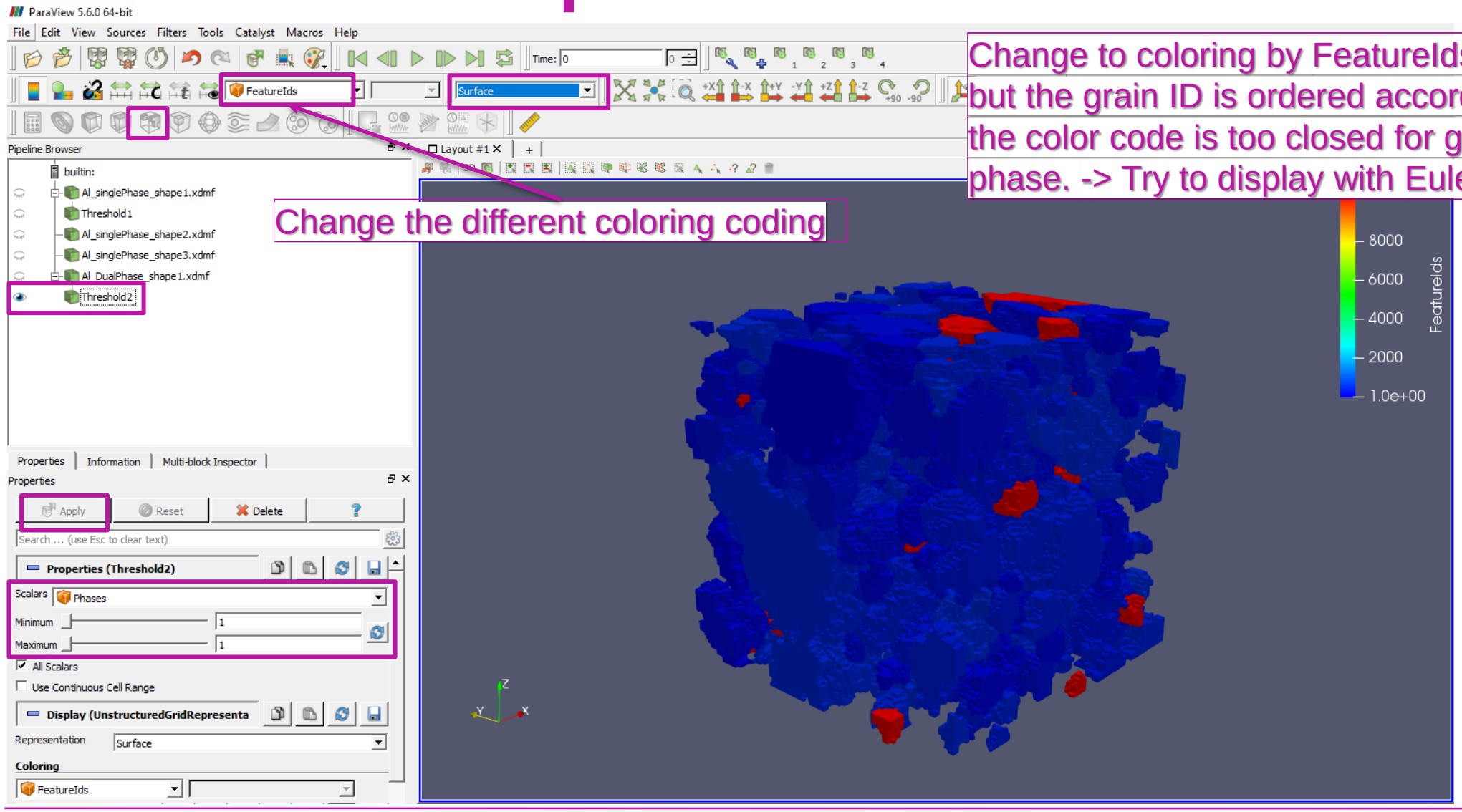
4. ParaView - Dual-phase structure



4. ParaView - Dual-phase structure



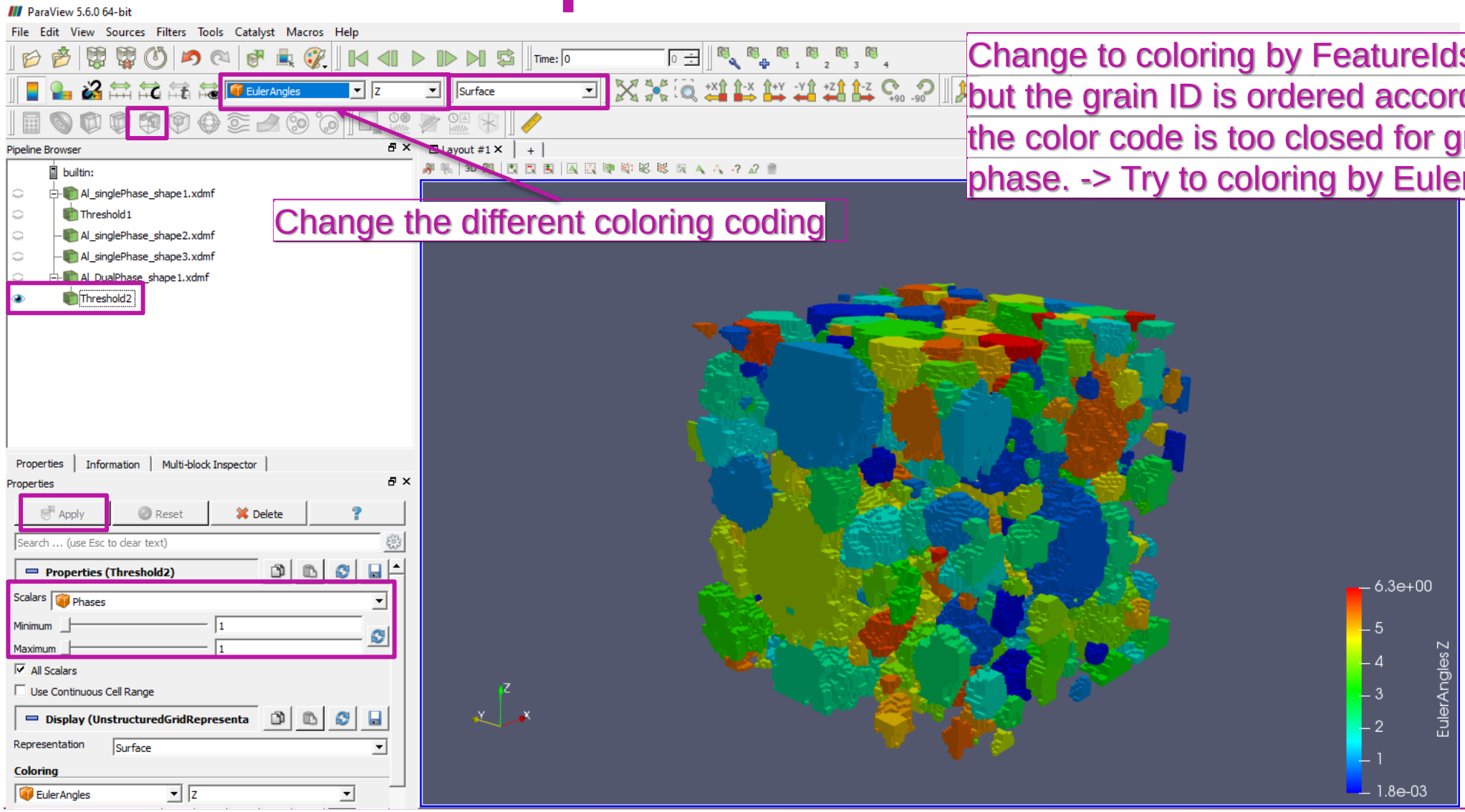
4. ParaView - Dual-phase structure



Change the different coloring coding

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

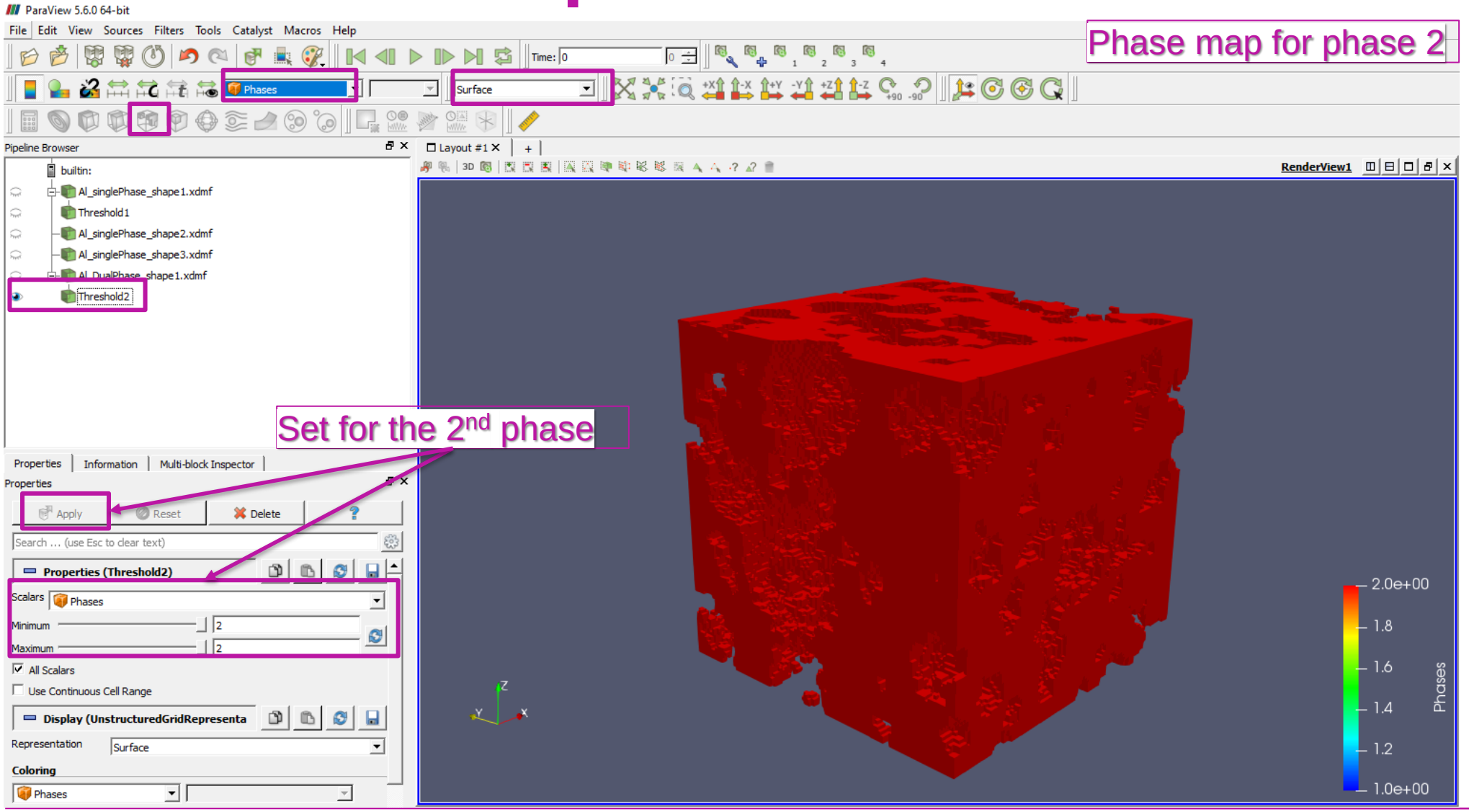
4. ParaView - Dual-phase structure



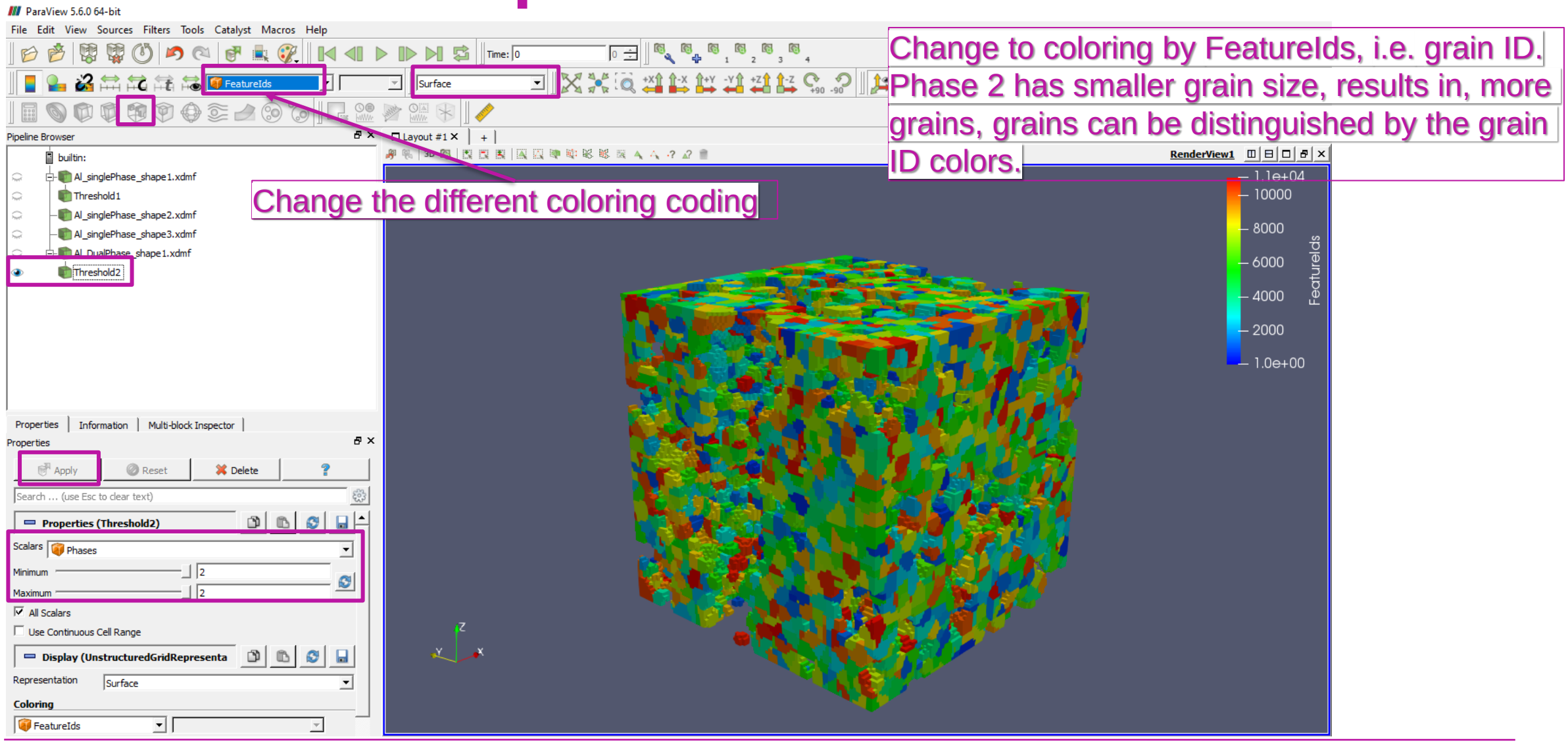
Change the different coloring coding

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-Z

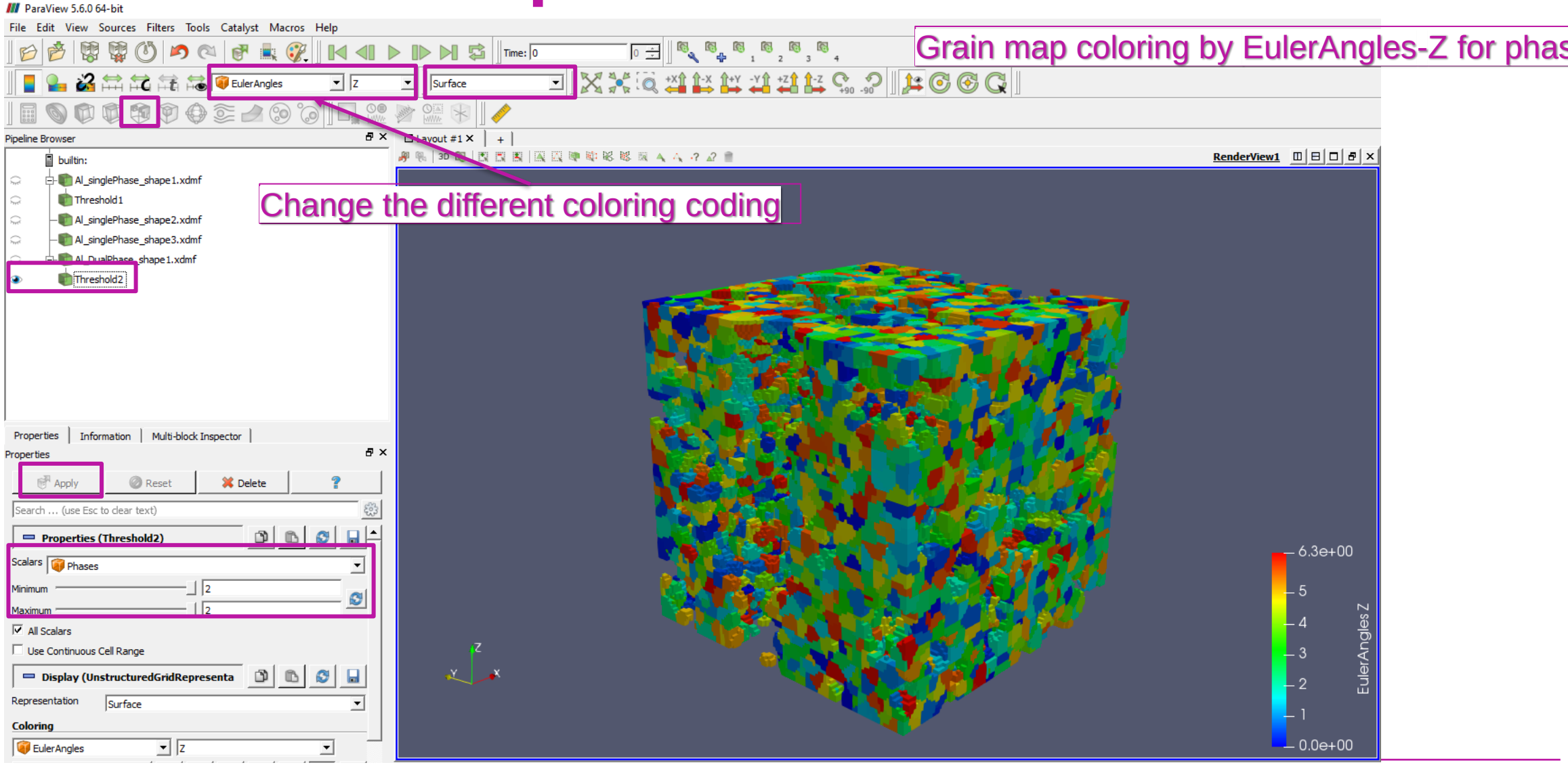
4. ParaView - Dual-phase structure



4. ParaView - Dual-phase structure

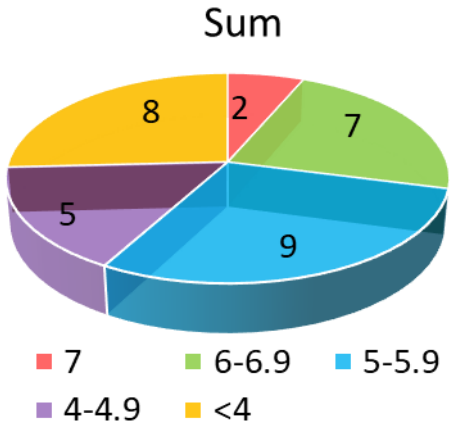


4. ParaView - Dual-phase structure



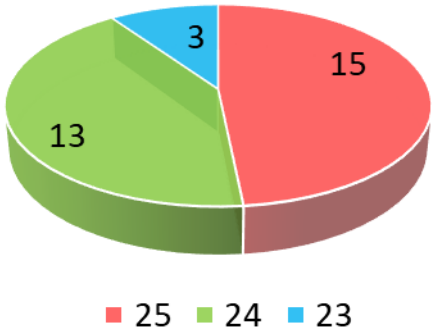
Feedback - Assignment

Assignment 01 - Summary

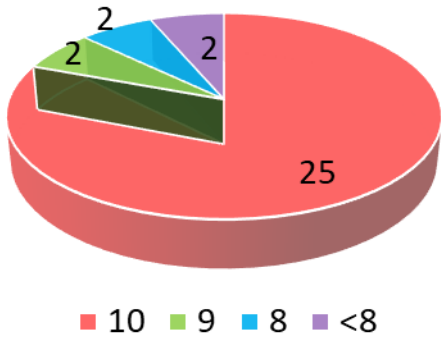


- Submission: 31
- Full points: 100, is calculated as 7 points in the final grade system.
- Due date: 18:00, 07.11.2021 (3 delayed submission)
- Grading criteria are listed in the assignment solution.
- Tolerant grading, high points ≠ exactly accurate answers!
- Check the assignment solution carefully! This is the only standard answer (for calculations, equations, derivations, definitions) if there are similar questions in the exam.

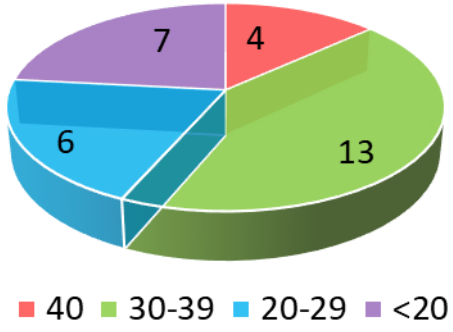
Task 1: 31, 25 points



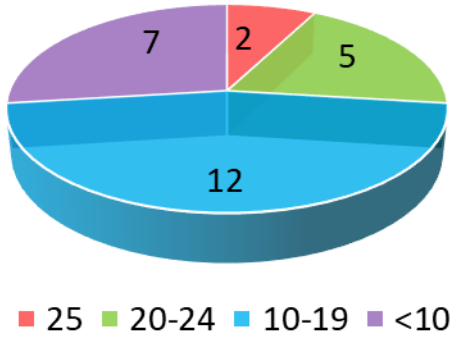
Task 2: 31, 10 points



Task 3: 30, 40 points



Task 4: 26, 25 points



Atomic structure and interatomic bonding

2.1 Calculate the energy (in J) and force (in N) of attraction between a cation with a valence of +2 and an anion with a valence of –1, the centers of which are separated by a distance of 5.3 nm. (Please give the detailed calculation process, and explain your choices or equations and numbers.) (6 points)

The attractive energy between positive and negative ions can be calculated using: $E_A = -\frac{A}{r}$ (Eq. 1) (0.5 points)

Herein, r = 5.3 nm = 5.3×10^{-9} m, and A represents lattice energy and its value could be calculated as: $A = \frac{1}{4\pi\epsilon_0}(|Z_1 e|)(|Z_2 e|)$ (Eq. 2) (0.5 points)

where ϵ_0 is the vacuum permittivity constant ($8.85 \times 10^{-12}\ F/m$), e is the elementary charge ($1.602 \times 10^{-19}\ C$), Z is the chemical valence of ion. Combining Eq. 1 and Eq. 2:

$$E_A = -\frac{1}{4\pi\left(8.85\times10^{-12}\frac{C^2}{N\cdot m^2}\right)(5.3\times10^{-9}m)}[|+2|(1.602\times10^{-19}\ C)][|-1|(1.602\times10^{-19}\ C)] = -8.7082\times10^{-20}\ J$$ (2 points)

Mathematically, energy (E) and force (F) are related as: $E = \int F\ \mathrm{d}r$ (Eq. 3) (0.5 points)

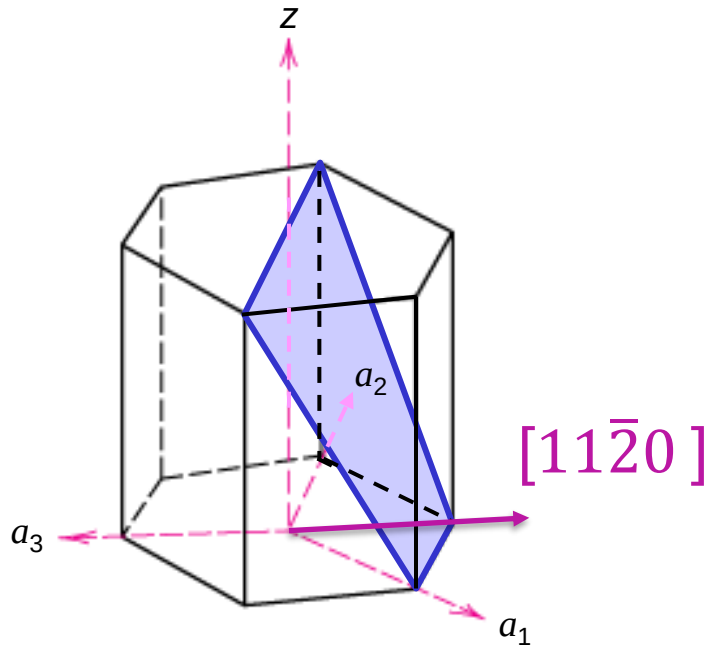
The force of attraction between two ions can be driven as: $F_A = \frac{A}{r^2}$ (Eq. 4) (0.5 points)

If we take ion 1 to be the cation that has a charge of +2 and ion 2 to be the anion with charge –1; also, from the problem statement. Thus, we compute the force of attraction between these two ions as follows:

$$F_A = \frac{A}{r^2} = \frac{1}{4\pi\left(8.85\times10^{-12}\frac{C^2}{N\cdot m^2}\right)(5.3\times10^{-9}m)^2}[|+2|(1.602\times10^{-19}\ C)][|-1|(1.602\times10^{-19}\ C)] = 1.6430\times10^{-11}N$$ (2 points)

Crystallographic Planes (HCP)

- For hexagonal unit cells a similar procedure is used
  - Determine the intercepts with the a_1, a_2, and z axes, then determine the Miller-Bravais Indices h, k, i, and l (hkil)



example	a_1	a_2	c
1. Relocate origin – not needed			
2. Intercepts	a	∞a	c
3. Reciprocals	$1/a$	$1/\infty a$	$1/c$
4. Normalize	a/a	$a/\infty a$	c/c
	1	0	1
5. Reduction	$h = 1$	$k = 0$	$l = 1$
6. Determine index	$i = -(h + k)$	$i = -(1 + 0) = -1$	
7. Miller-Bravais Indices	$(10\bar{1}1)$		

$a_1+a_2+a_3=0$ h+k+i=0

u+v+t=0

Crystal structure

Miller indices - Cube

Miller-Bravais indices - HCP

Crystal plane: (hkl) (hkil)

Crystal plane family: {hkl} {hkil}

Crystal direction: [uvw] [uvtw]

Crystal direction family: <uvw> <uvtw>

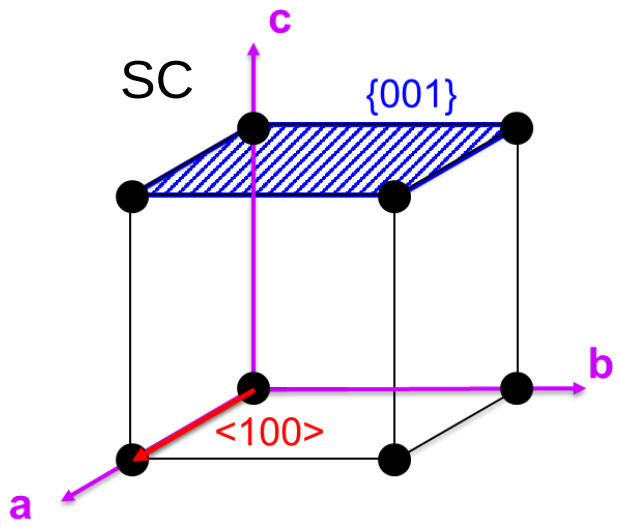
minus value: $\bar{1}$ instead of -1

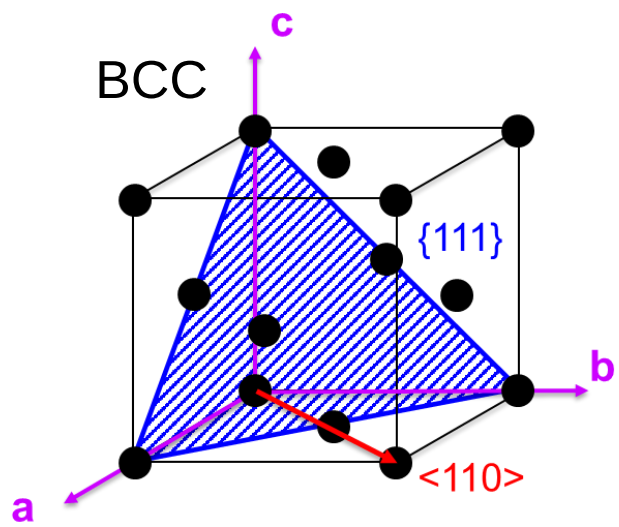
e.g. for HCP most closed packet planes:

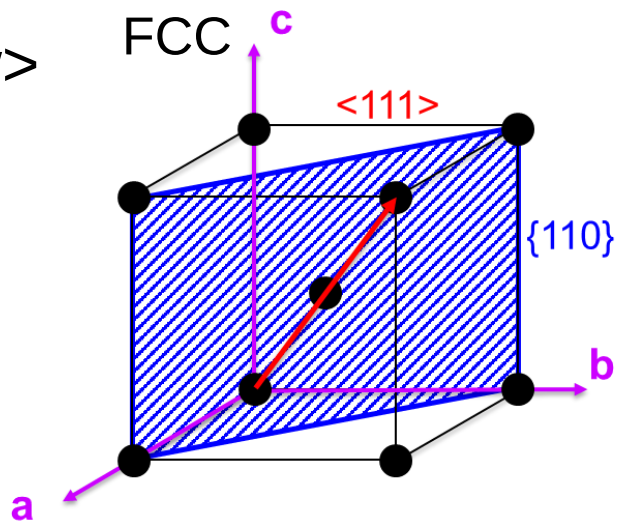
$< 11\bar{2}0 >$ ✓

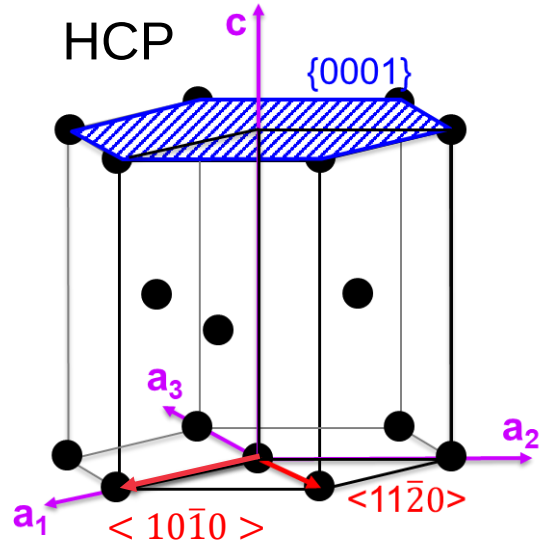
$< 11-20 >$ ✗

$< 110 >$ ✗

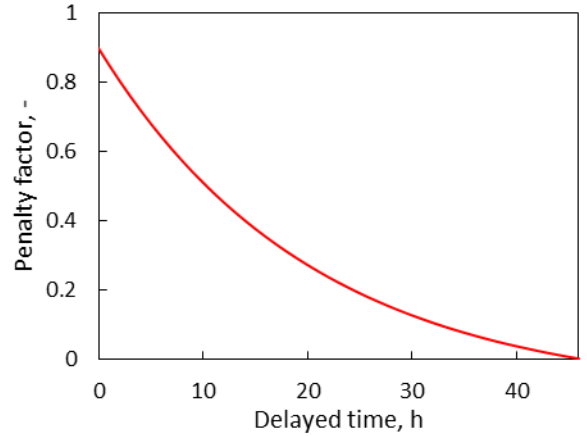








Assignment - General rules



Timelines

- Open on MyCourses: every Monday before 18:00.
- Deadline: every Sunday at 18:00 to MyCourses.
- Cut-off deadline: every Tuesday at 16:00 to MyCourses.
- Solution open on MyCourses: every Tuesday at 16:30.
- Q&A time: every Tuesday at 16:30-18:00 (via Zoom: https://aalto.zoom.us/j/62428835336).
- For the last assignment (A6), no extension and later submission allowed, solution will be given on MyCourses before 18:30, 12.12.2021.

Grades

- Delayed submission will be subjected to a penalty function in an exponential relation with time.
- Full points: 100 for every assignment, which will be calculated as 5-7 points in the final grade system. The weighted pointes will be indicated in each assignment.
- In total, 40 points for 6 assignments.

Assignment - General rules

Submission rules

- Only PDF type file is accepted for submission, please summarize all your answers/solutions in **one PDF file for every assignment**.
- Please name your assignment files with the assignment number and your first name and surname, and link them with short underlines: '**ANr_Firstname_Surname.pdf**', e.g. for the first Assignment 'A1_Wenqi_Liu.pdf'.
- It is appreciated to **sort the PDF pages in the TaskNr order**, which is helpful to speed up the evaluation process.
- Learning Group work is encouraged for this course. You could form a group with **max one additional peer** to review the lecture/exercise content and discuss the tasks in the assignment. After discussion, please **finish your assignment independently** and submit your individual report. Please note the **duplicate report is not accepted!** If you have a learning group, please **indicate who your group member is** in the submitted report. In addition, clearly state the individual contributions of each group member.

Assignment - General rules

- When required, always show the step-by-step derivation or calculation processes, without which hinting the number does not qualify for grades.
- When required, always give a brief and concise explanation or description, without which hinting the right choice or answer does not qualify for grades.
- **Citation is necessary** if you are using any figures/data that are not generated by yourself.
- Handwriting/plotting is acceptable, just **make sure that your handwriting/final photo in the system is clear enough, otherwise it may affect the grading for details/calculation process.**

- Tolerant grading, high points ≠ exactly accurate answers!
- Check the assignment solution carefully! This is the only standard answer (for calculations, equations, derivations, definitions) if there are similar questions in the exam.

If you have further questions, please use the 'General discussion' channel in MyCourses.
=> 1 points for forum activities.

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 **18:00 on 14.11.2020.**
- Use the Zoom Chat function or raise your hands!
- Please avoid emails and use the “General discussion” on MyCourses!

Slides will be uploaded after Exercise.