

A”

Aalto University  
School of Engineering

# COE-C2004 - Materials Science and Engineering

## Exercise 2

*Prof. Junhe Lian*

*Wenqi Liu (Teaching assistant)*

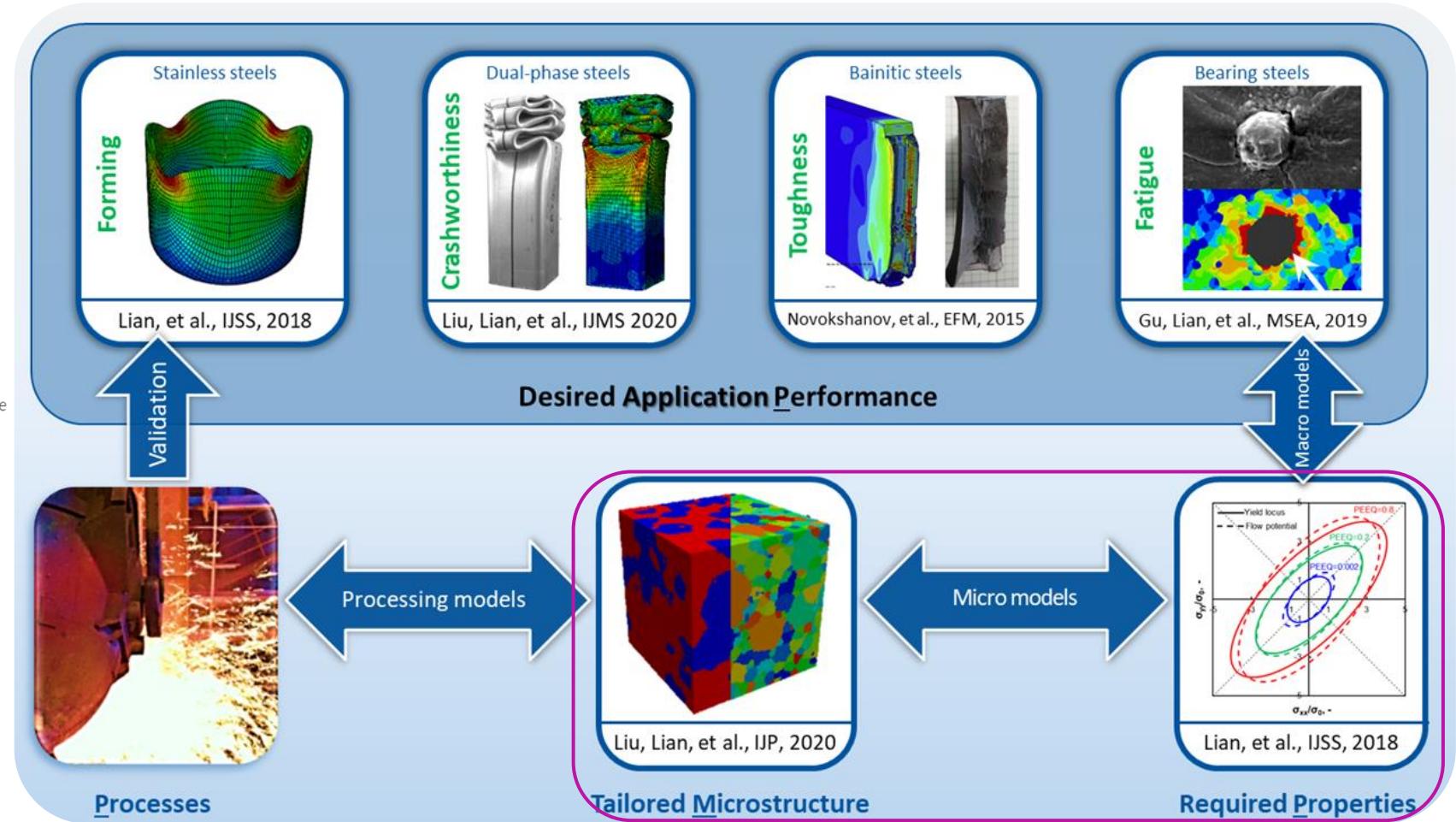
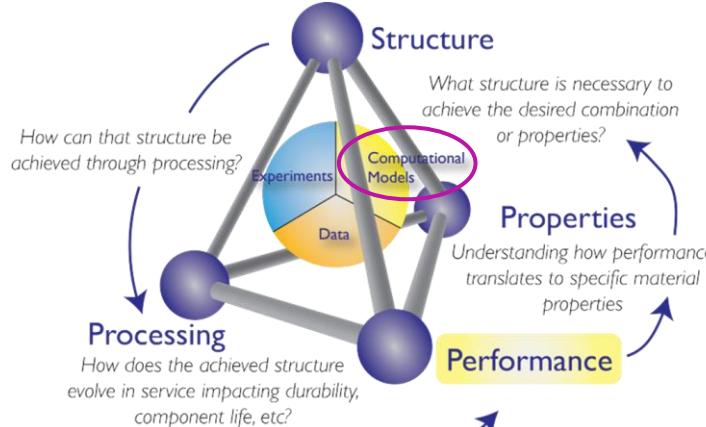
*Rongfei Juan (Teaching assistant)*

# Outline

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

# Microstructure modeling

# Integrated computational materials engineering (ICME)

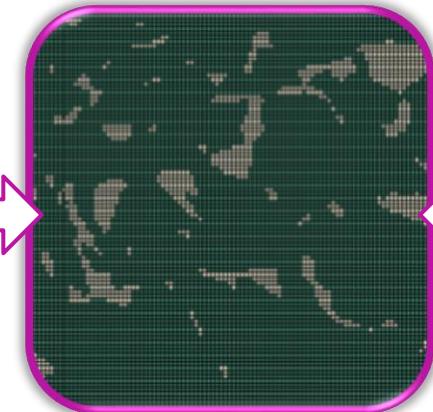


# Micromechanics modeling

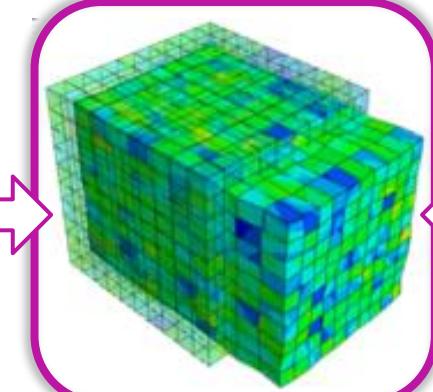
Microstructure - property relation & microstructure-based material design



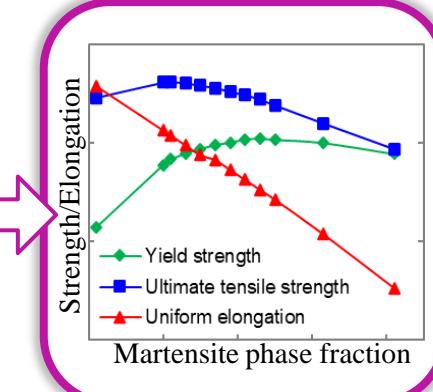
Microstructure measurement



e.g. Representative volume element (RVE)



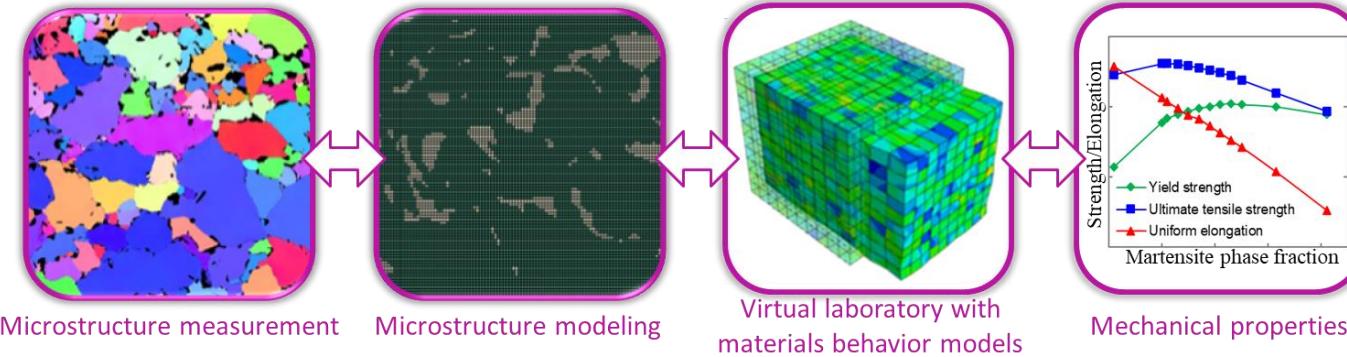
e.g. von Mises stress-strain relation;  
Crystal plasticity



e.g. Force-displacement response;  
Flow curve

# Microstructure modeling - RVE

Microstructure - property relation & microstructure -based material design



**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.

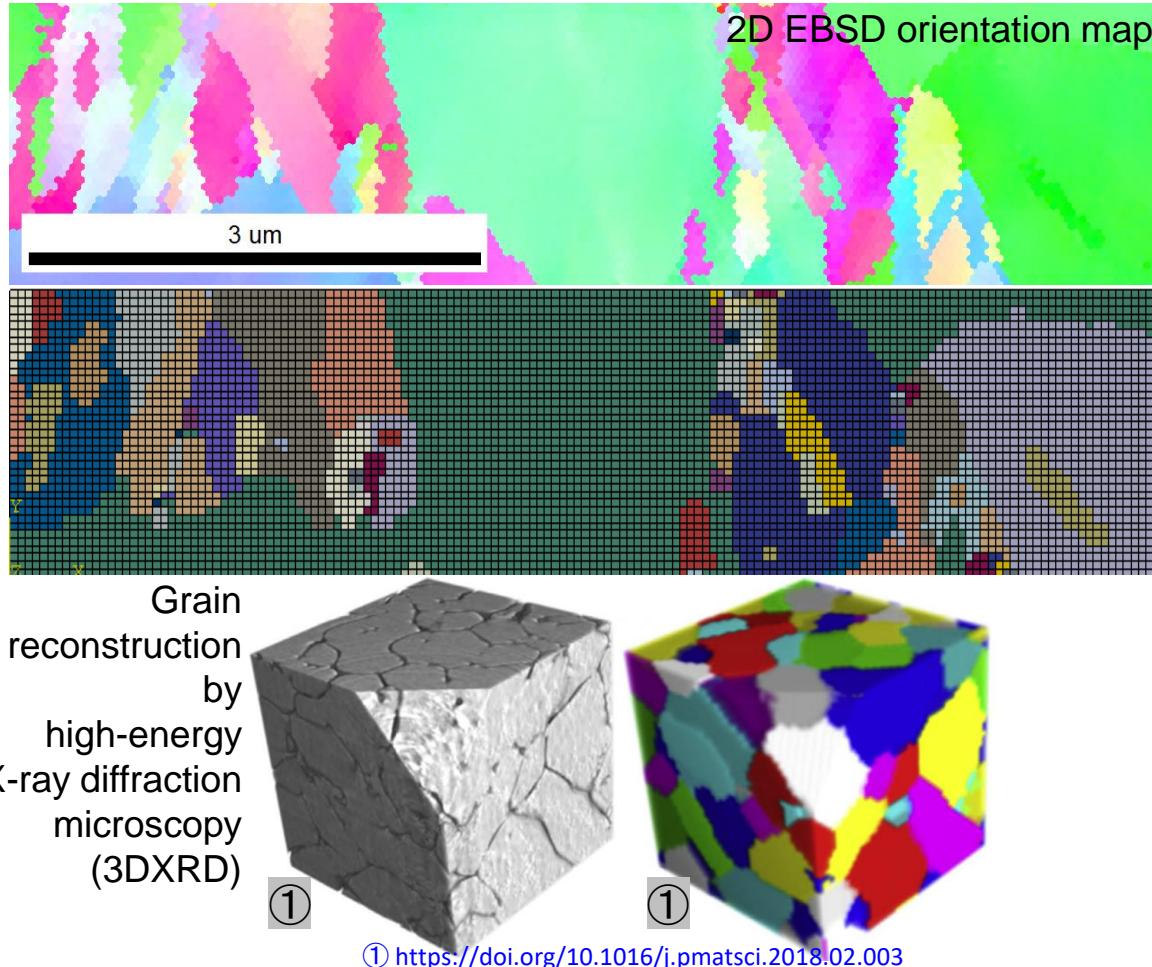
Mesoscale,  $\mu\text{m}$

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

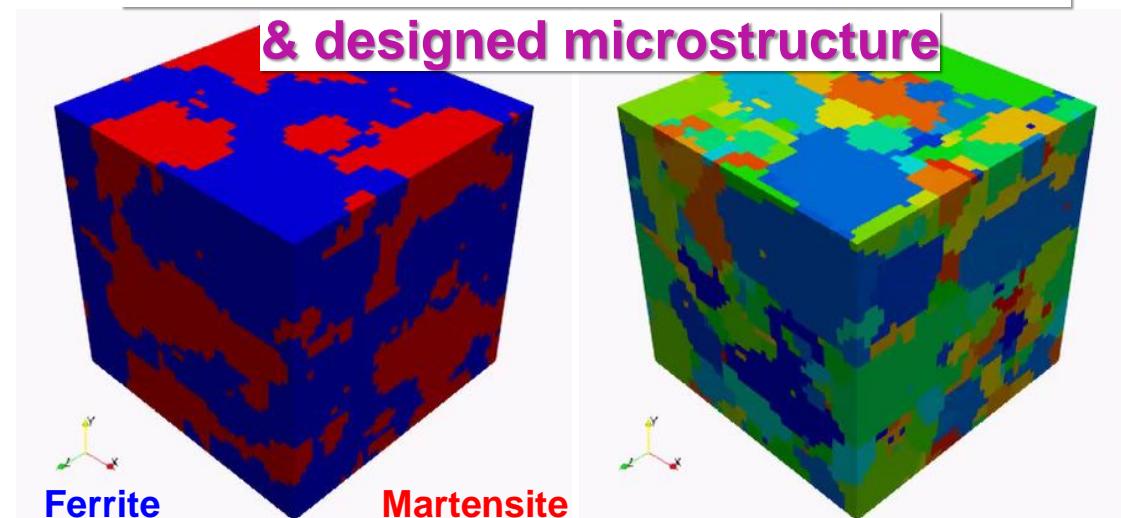
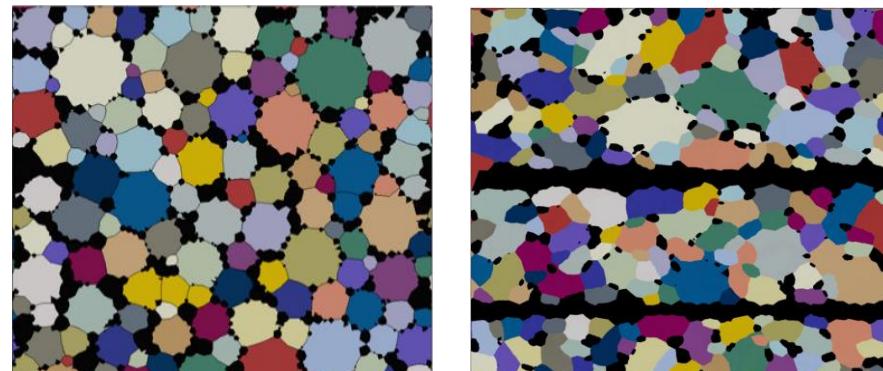
[1] <https://doi.org/10.1016/j.jpmatsci.2018.02.003>

# Microstructure modeling - RVE

- Real microstructure RVE

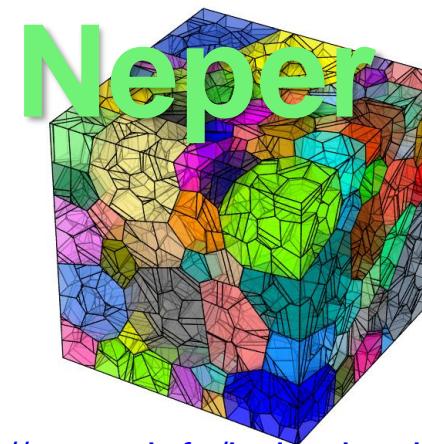


- Artificial/synthetic microstructure RVE



# Microstructure modeling - RVE

- Generation



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



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

- Visualization

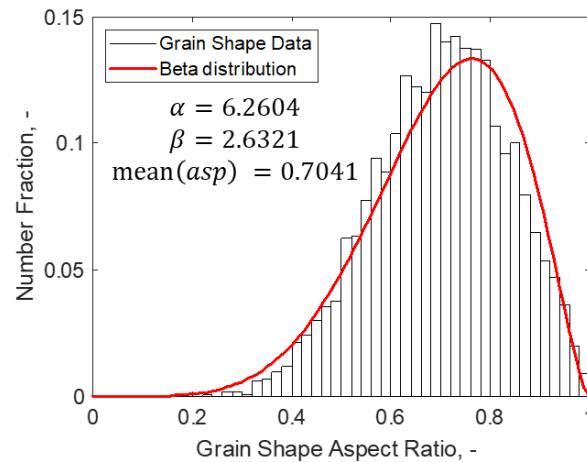
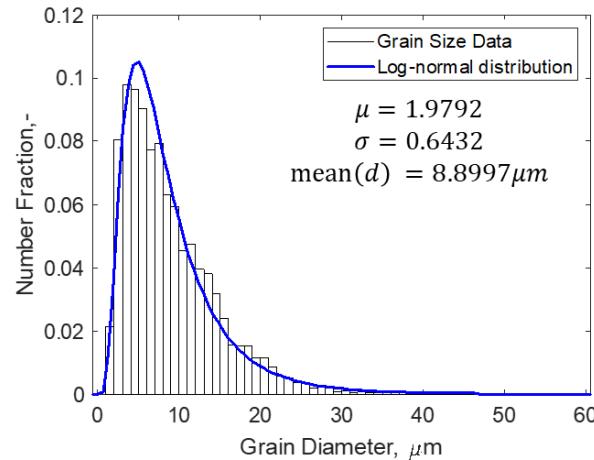


<https://micress.rwth-aachen.de/index.html>

[2]

# Tasks

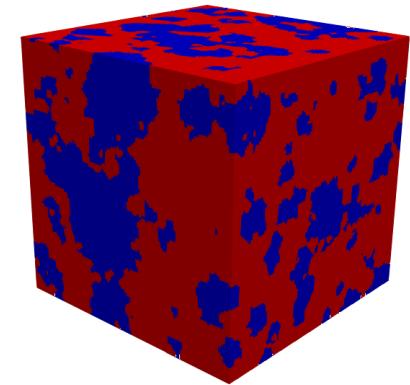
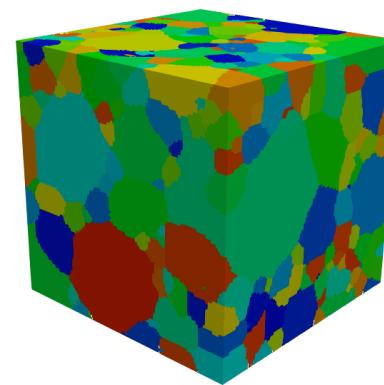
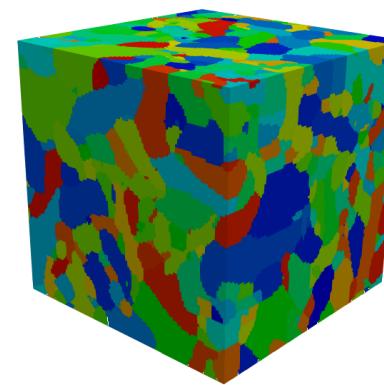
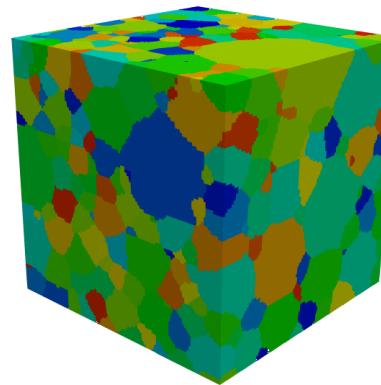
# Tasks



1-Grain 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.



2-Grain Map

3-Grain Map

4-Phase Map

# DREAM.3D & ParaView preparation

# 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](http://mfavdi.aalto.fi), or VMware Horizon Client [vdi.aalto.fi](http://vdi.aalto.fi), for more information, please refer to [Remote access to Windows classroom computers](#).

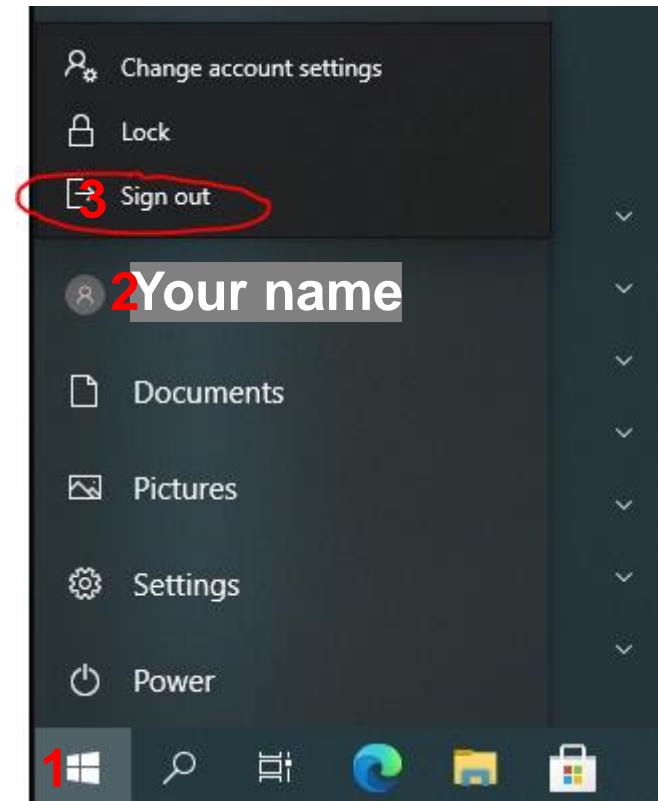
**IMPORTANT!** Please remember to do ‘Sign Out’ after the session (NOT Disconnect). Click your username in Start and click ‘Sign Out’.

**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.



**DREAM3D**[Home](#)[About](#)[Download](#)[Latest Release Notes](#)[License](#)[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
<a href="#">MacOS - DREAM3D-6.5.160-OSX.dmg</a>	MacOS 10.14 and greater required, including macOS 11.0. Download is a Disk Image
<a href="#">MacOS - DREAM3D-6.5.160-OSX.zip</a>	MacOS 10.14 and greater required, including macOS 11.0. Download is a Zip file
<a href="#">Windows - DREAM3D-6.5.160-Win64.zip</a>	Windows version 8 or 10
<a href="#">Linux - DREAM3D-6.5.160-Linux-x86_64.tar.gz</a>	Ubuntu 18.04 or Equivelant. Self contained tar archive.

[Table of contents](#)[Prebuilt Binaries](#)

[About](#) [Flavors](#) [Domains](#) [Resources](#) [Developer Tools](#) [Careers](#) [Download](#)

## Get the Software

You can either download binaries or source code archives for the latest stable or previous release or access the current development (aka nightly) distribution through Git. Specific license information can be found [here](#). This software may not be exported in violation of any U.S. export laws or regulations. For more information regarding Export Control matters please go to [https://kitware.com/export\\_control/index.html](https://kitware.com/export_control/index.html).

Version

v5.10



### Release Candidates

[Sources](#) **Windows** [Linux](#) [macOS](#)

Previews of ParaView's next release.

- [ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.zip](#)
- [ParaView-5.10.0-RC1-MPI-Windows-Python3.9-msvc2017-AMD64.zip](#)
- [ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.exe](#)
- [ParaView-5.10.0-RC1-MPI-Windows-Python3.9-msvc2017-AMD64.exe](#)

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

### Documentation

Quick start, tutorial, and user guides for ParaView and Catalyst.

- [ParaViewGettingStarted-5.10.0.pdf](#)
- [ParaViewCatalystGuide-5.10.0.pdf](#)
- [ParaViewTutorial-5.10.0.pdf](#)

Sep 27 20:11	1.3M
Sep 27 20:10	4.5M
Sep 22 10:40	44.7M

### Documentation files

# DREAM.3D & ParaView Extraction

Name	Status	Date modified	Type	Size
ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.exe	🕒 R		Application	247,593 KB
DREAM3D-6.5.160-Win64.zip	🕒 R		Compressed (zipp...)	207,048 KB
ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.zip	🕒 R		Compressed (zipp...)	572,396 KB

Extract the DREAM.3D/ParaView .zip file



Name	Status	Date modified	Type	Size
DREAM3D-6.5.160-Win64	🕒 R		File folder	
ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64	🕒 R		File folder	
ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.exe	🕒 R		Application	247,593 KB
DREAM3D-6.5.160-Win64.zip	🕒 R		Compressed (zipp...)	207,048 KB
ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64.zip	🕒 R		Compressed (zipp...)	572,396 KB

# DREAM.3D & ParaView running

02 Exercises > DREAM3D-6.5.160-Win64 > DREAM3D-6.5.160-Win64

	Status	Date modified	Type	Size
Data	⟳ R		File folder	
lib	⟳ R		File folder	
Plugins	⟳ R		File folder	
PrebuiltPipelines			File folder	
Anisotropy.plugin	⟳ H		PLUGIN File	1,160 KB
concr140.dll	⟳ R		Application exten...	325 KB
DDDAnalysisToolbox.plugin	⟳ R		PLUGIN File	619 KB
<b>DREAM3D.exe</b>	⟳ R		Application	1,729 KB
DREAM3DLicense.txt	⟳ R		TXT File	4 KB

Run DREAM3D.exe

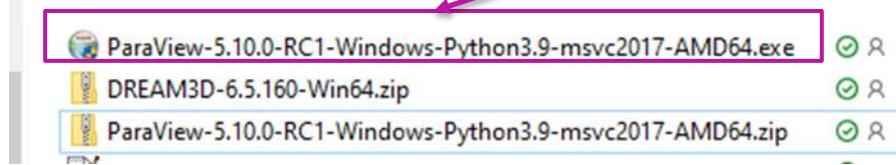
02 Exercises > ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64 > ParaView-5.10.0-RC1-Windows-Python3.9-msvc2017-AMD64

Name	Status	Date modified	Type	Size
optix.6.0.0.dll	⟳ R		Application exten...	189 KB
ospray.dll	⟳ R			186 KB
ospray_module_denoiser.dll	⟳ R			25 KB
ospray_module_ispc.dll	⟳ R			5,832 KB
paraview.conf	⟳ R		CONF File	1 KB
<b>paraview.exe</b>	⟳ R		Application	911 KB

Run ParaView.exe in folder 'bin'  
if you use the uninstalled version.

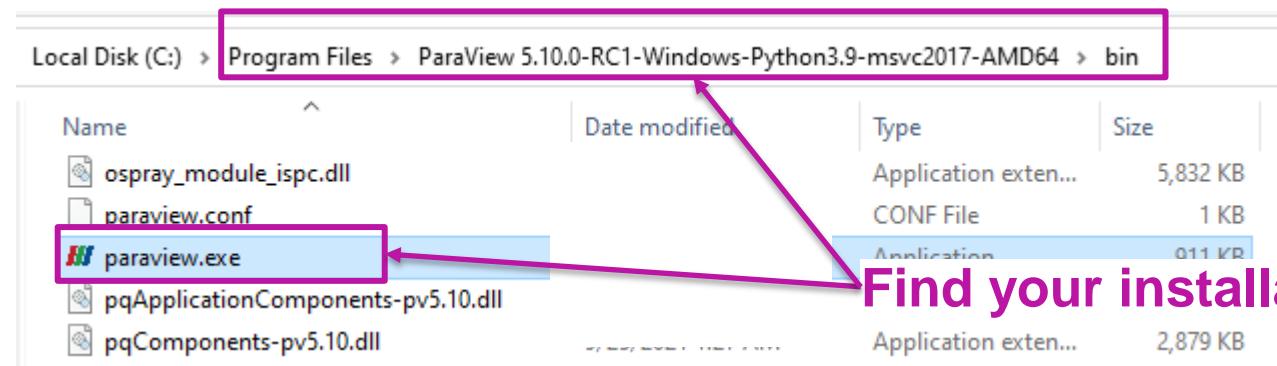
# ParaView installation

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

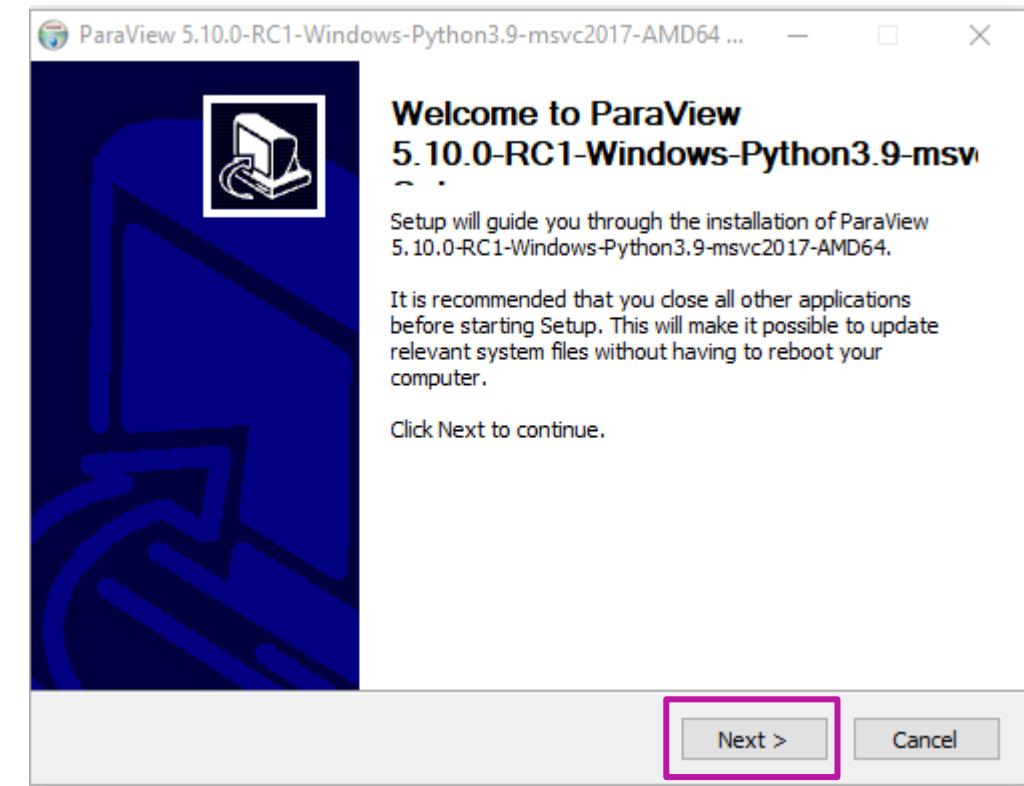


You are probably asked for the confirmation to run an .exe application in windows system.

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

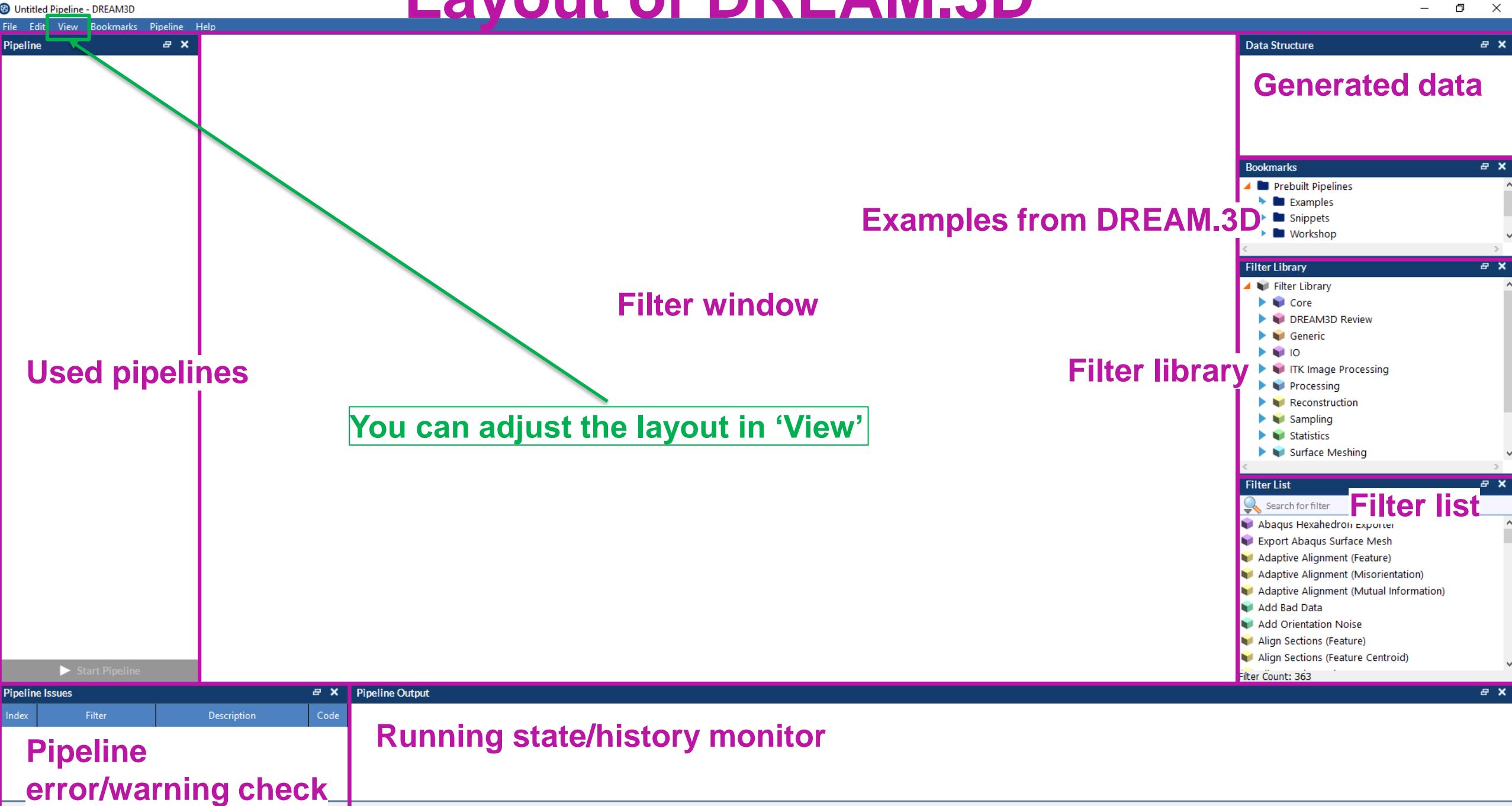


Find your installation folder and run **Paraview.exe**



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

# Layout of DREAM.3D



# Build up a pipeline

## Bookmarks

- Prebuilt Pipelines
  - Examples
  - Snippets
- Workshop
  - EBSD Reconstruction
  - EBSD Statistics
  - EBSD SurfaceMeshing
  - Image Reconstruction
- 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

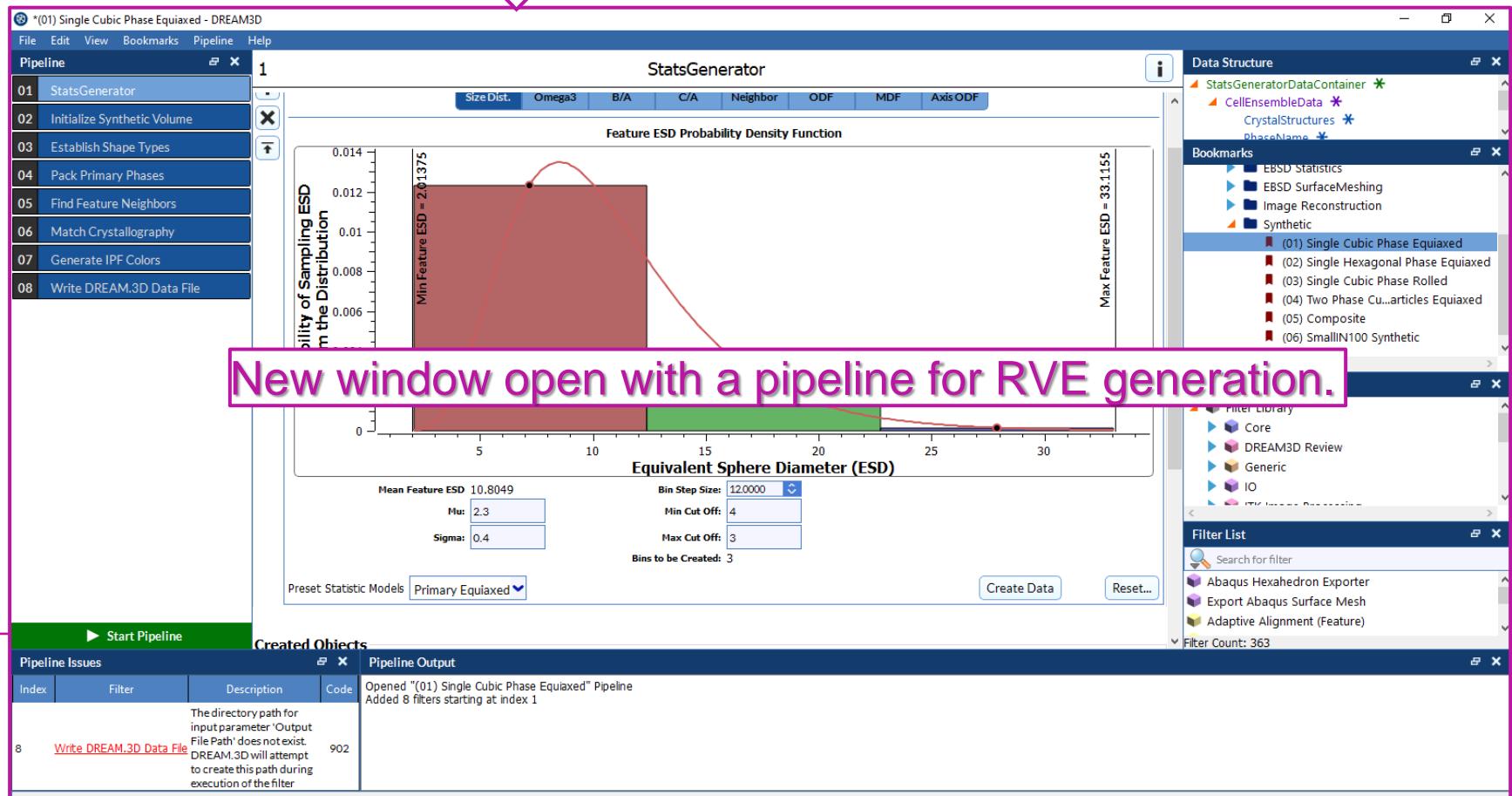
## Filter List

- Search for filter
- Abaqus Hexahedron Exporter
- Export Abaqus Surface Mesh
- Adaptive Alignment (Feature)

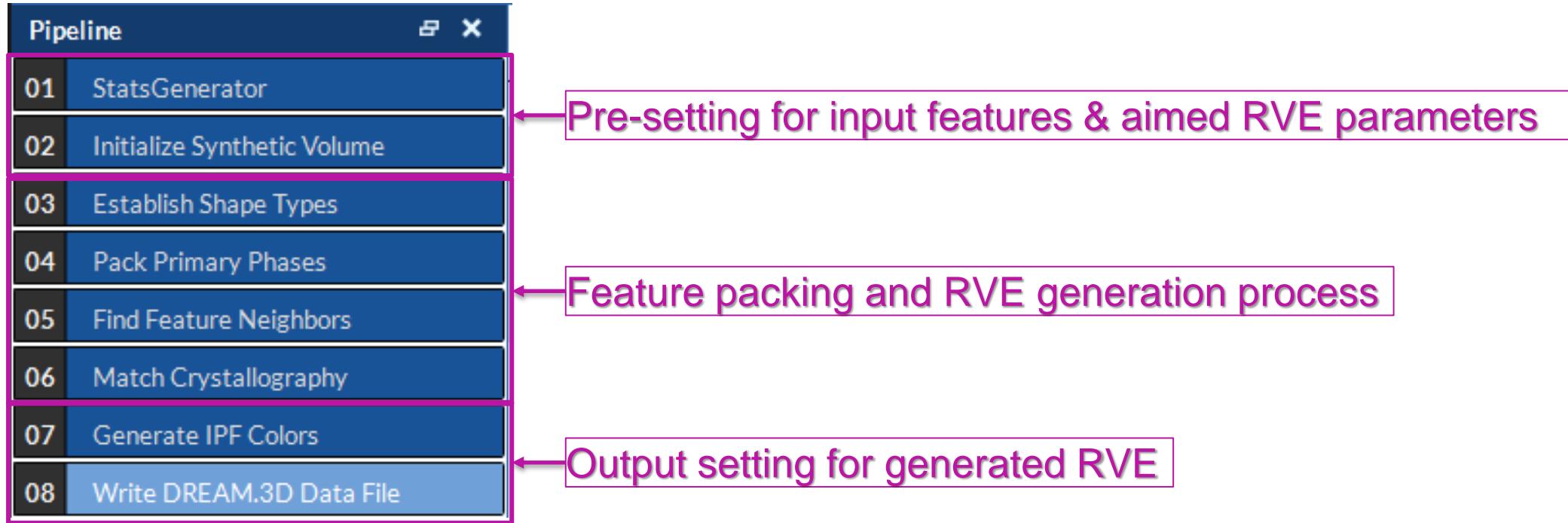
Filter Count: 363

## Bookmarks-Prebuilt pipelines: Examples from DREAM.3D

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



# 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

i

1

single phase tab

Parameters



Primary



grain shape

StatsGenerator

website documentation

Size Dist.

Omega3

B/A

C/A

Neighbor

ODF

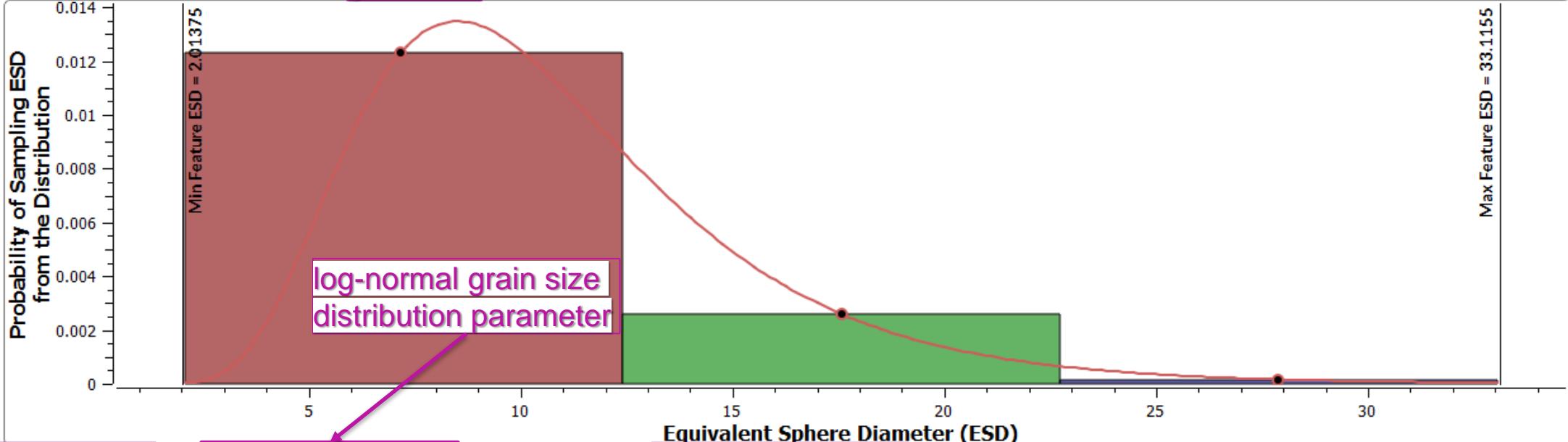
MDF

Axis ODF

grain orientation  
and misorientation

grain size

Feature ESD Probability Density Function



general/pre control for grain shape

Mean Feature ESD 10.8049

Mu: 2.3

Sigma: 0.4

Bin Step Size: 12.0000  
Min Cut Off: 4  
Max Cut Off: 3  
Bins to be Created: 3

grain size range control and generate data group for other features, e.g. grain shape

Preset Statistic Models Primary Equiaxed

Create Data

Reset...

Created Objects

Created Data Container

Statistics Data Container Name StatsGeneratorDataContainer

Created Ensemble AttributeMatrix

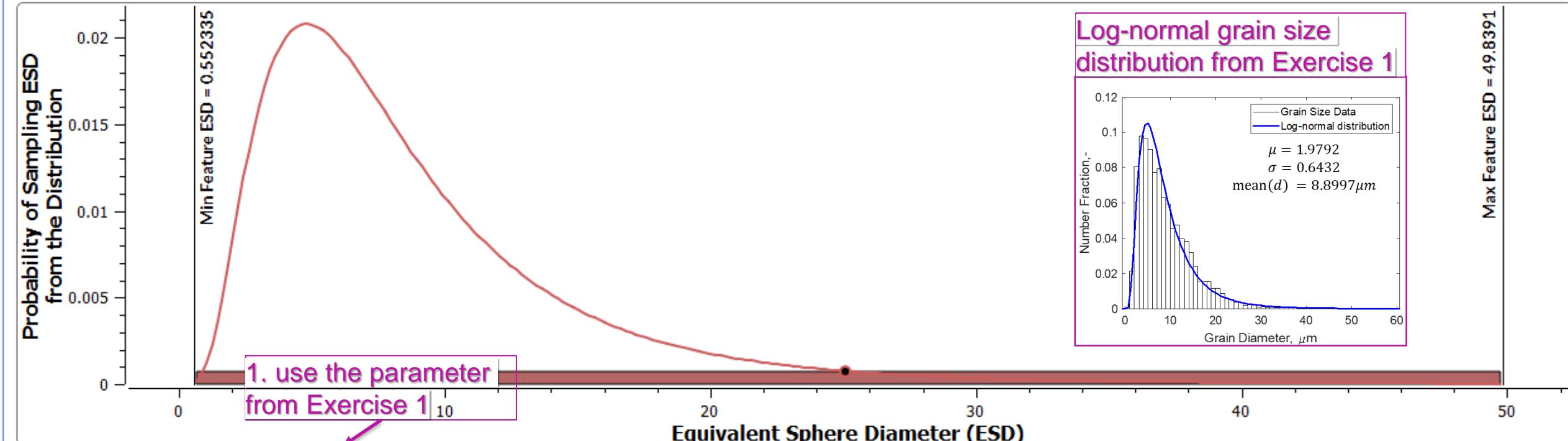
Cell Ensemble Attribute Matrix Name CellEnsembleData

the data structure generated in this filter

create grain data with the input parameters

22

## Feature ESD Probability Density Function



2. grain size range control and generate data group for other features, e.g. grain shape change the 'Bin Step Size' to create only one bin

Bin Step Size: 50.0000

Min Cut Off: 4

Max Cut Off: 3

Bins to be Created: 1

Create Data

Reset...

3. general/pre control for grain shape

choose 'Equiaxed' for the first shape type: 1:1:1

4. create grain data with the input parameters

23

# Step2 Initialize Synthetic Volume

2

Initialize Synthetic Volume

i

## Parameters

 Estimate Number of Features

Estimated Primary Features 811

1. Estimated grain number

Dimensions

100 100 100

2. Number of elements on each dimension

Resolution

1 1 1

3. Size of elements on each dimension, the unit is consistent with the grain size distribution, e.g.  $\mu\text{m}$ .

Origin

0 0 0

4. Origin point of RVE, as default

X Range: 0 to 100 (Delta: 100)

Box Size in Length Units Y Range: 0 to 100 (Delta: 100)

Z Range: 0 to 100 (Delta: 100)

## Required Objects

Cell Ensemble Data

Statistics StatsGeneratorDataContainer / CellEnsembleData / Statistics

Phase Types StatsGeneratorDataContainer / CellEnsembleData / PhaseTypes

## Created Objects

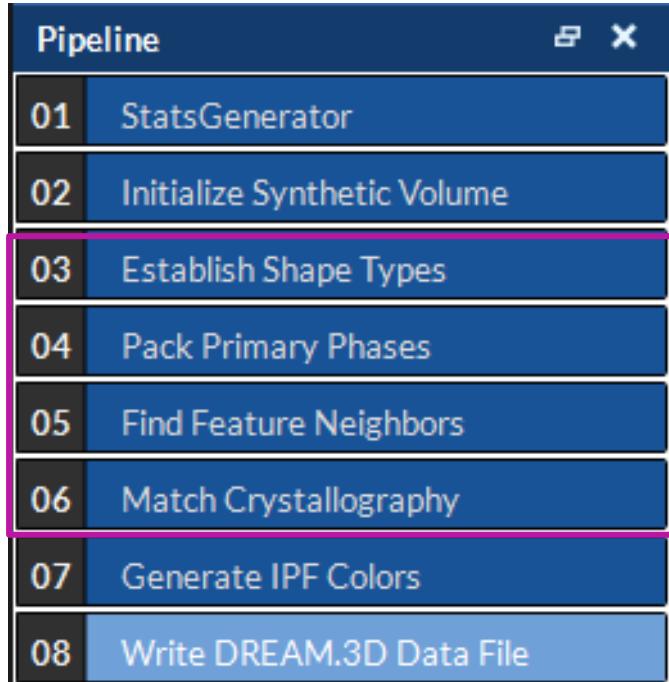
Synthetic Volume Data Container SyntheticVolumeDataContainer

Cell Data

Cell Attribute Matrix CellData

Ensemble Attribute Matrix CellEnsembleData

# DREAM.3D - Generation process



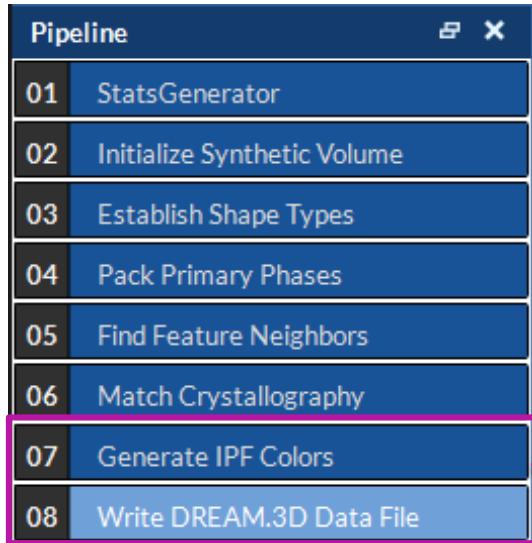
## Feature packing and RVE generation process:

- 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/](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’.

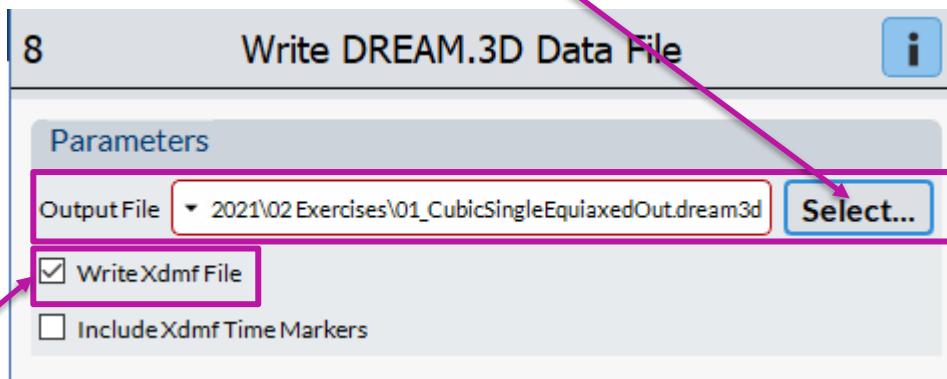
# DREAM.3D - RVE output



## Step4 Output setting for generated RVE

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

4.1. ‘Write DREAM.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.

► Start Pipeline

Step5: Click to run the generator

\*(01) Single Cubic Phase Equiaxed - DREAM3D

**DREAM.3D - Running**

Estimated running time for every step

Cancel Pipeline

**Pipeline Issues**

Index	Filter	Description	Code
No issues found.			

**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

**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

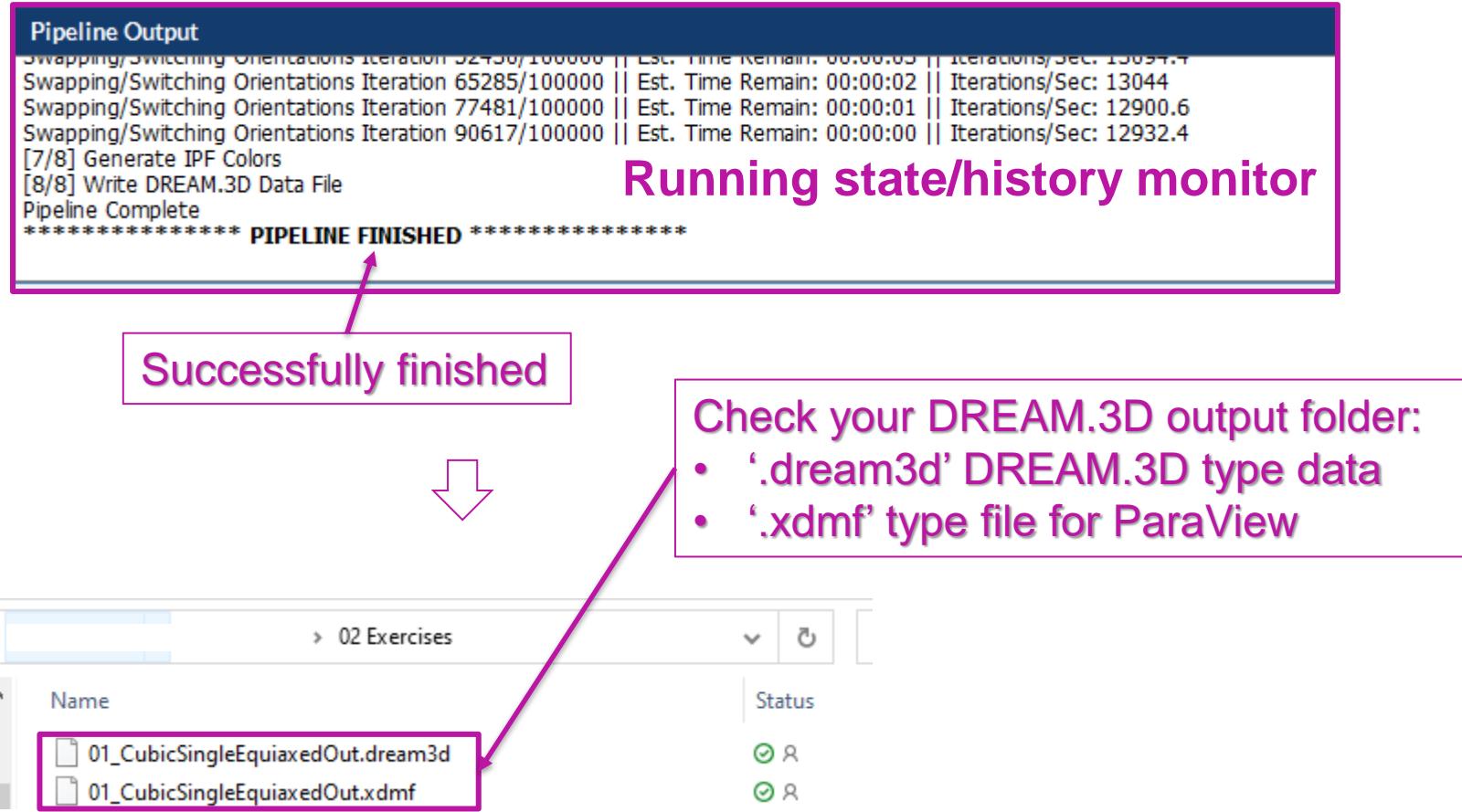
**Filter List**

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)

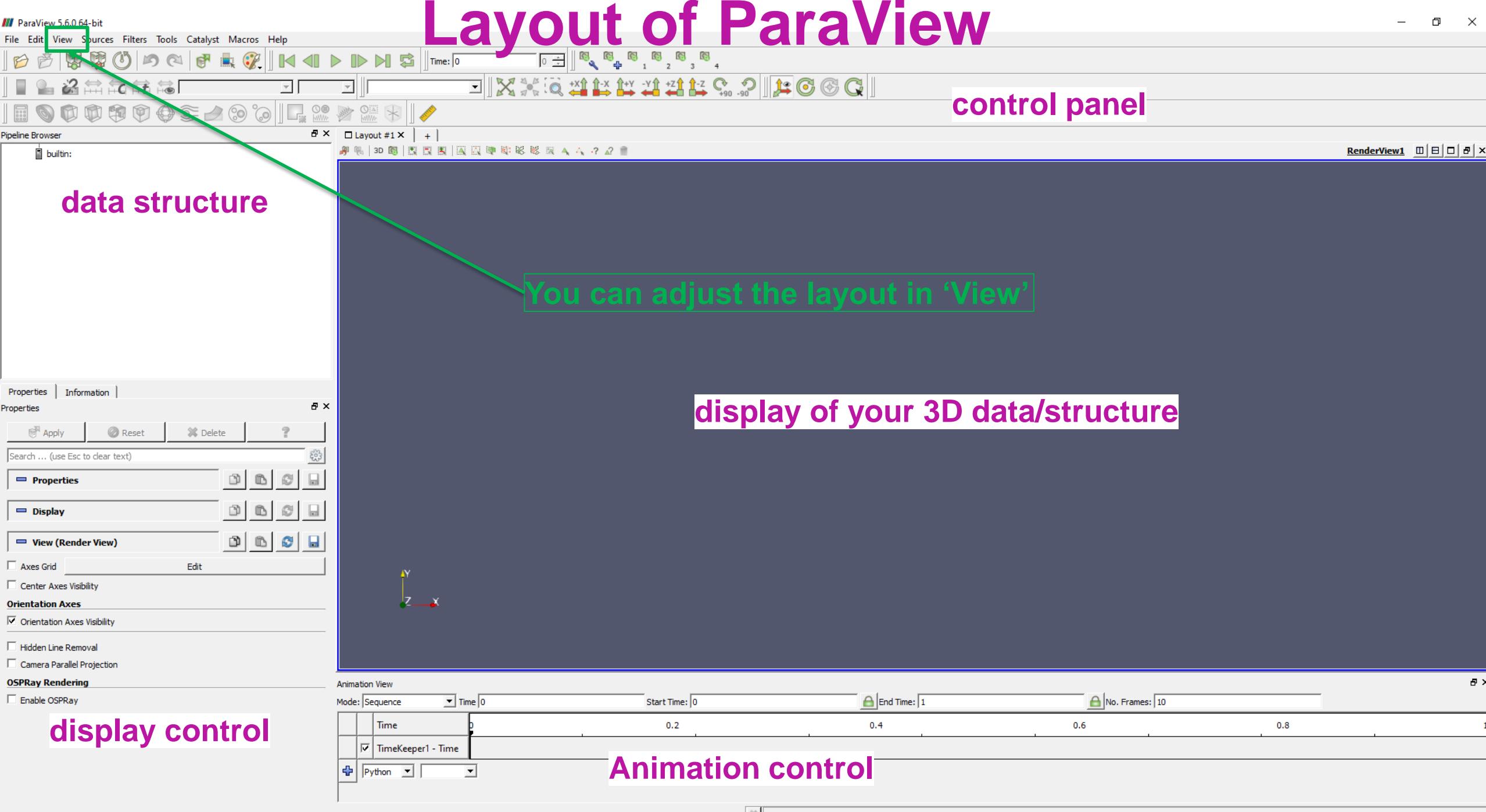
Filter Count: 363

# DREAM.3D - Data files

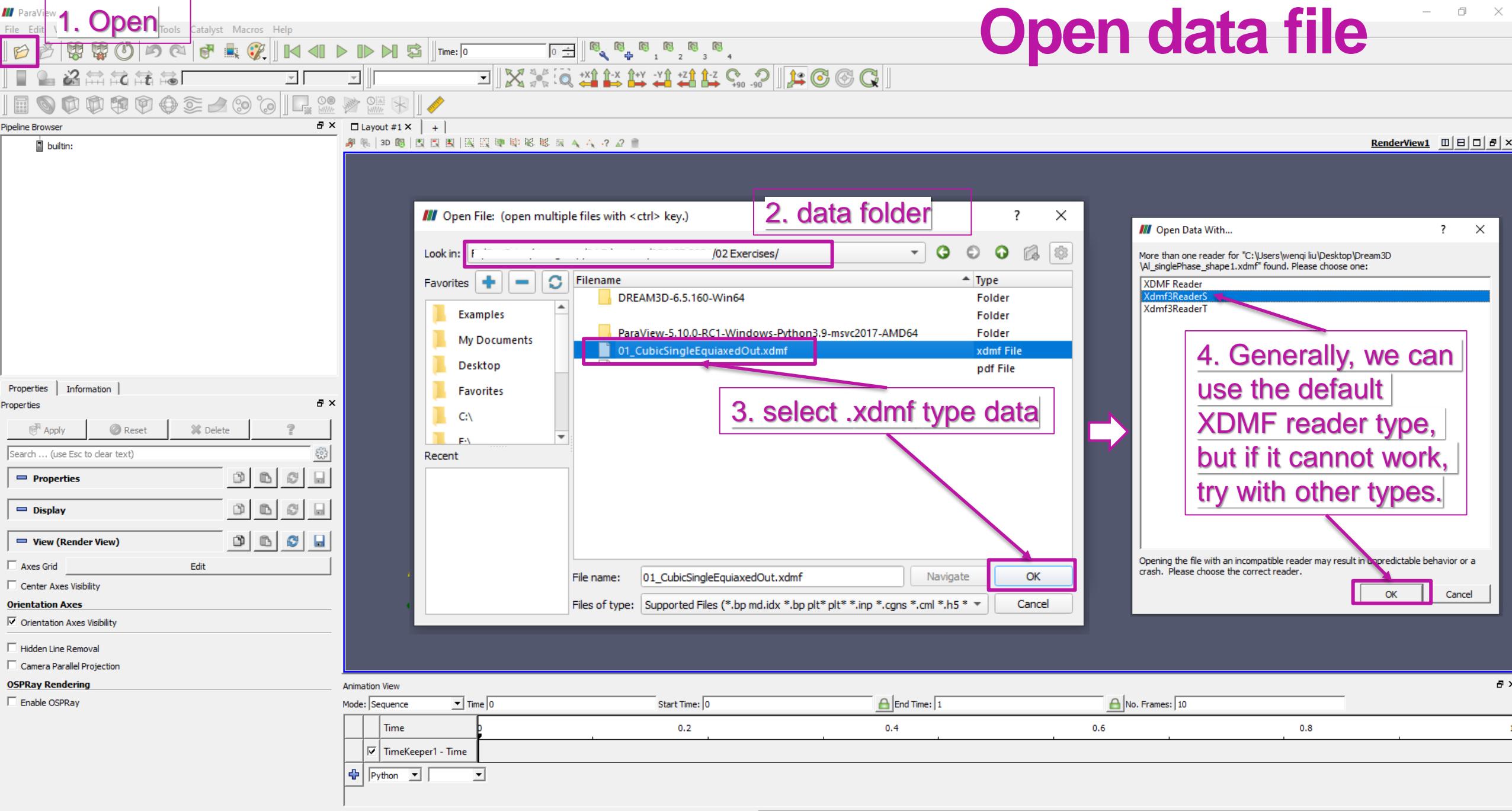


# ParaView operation

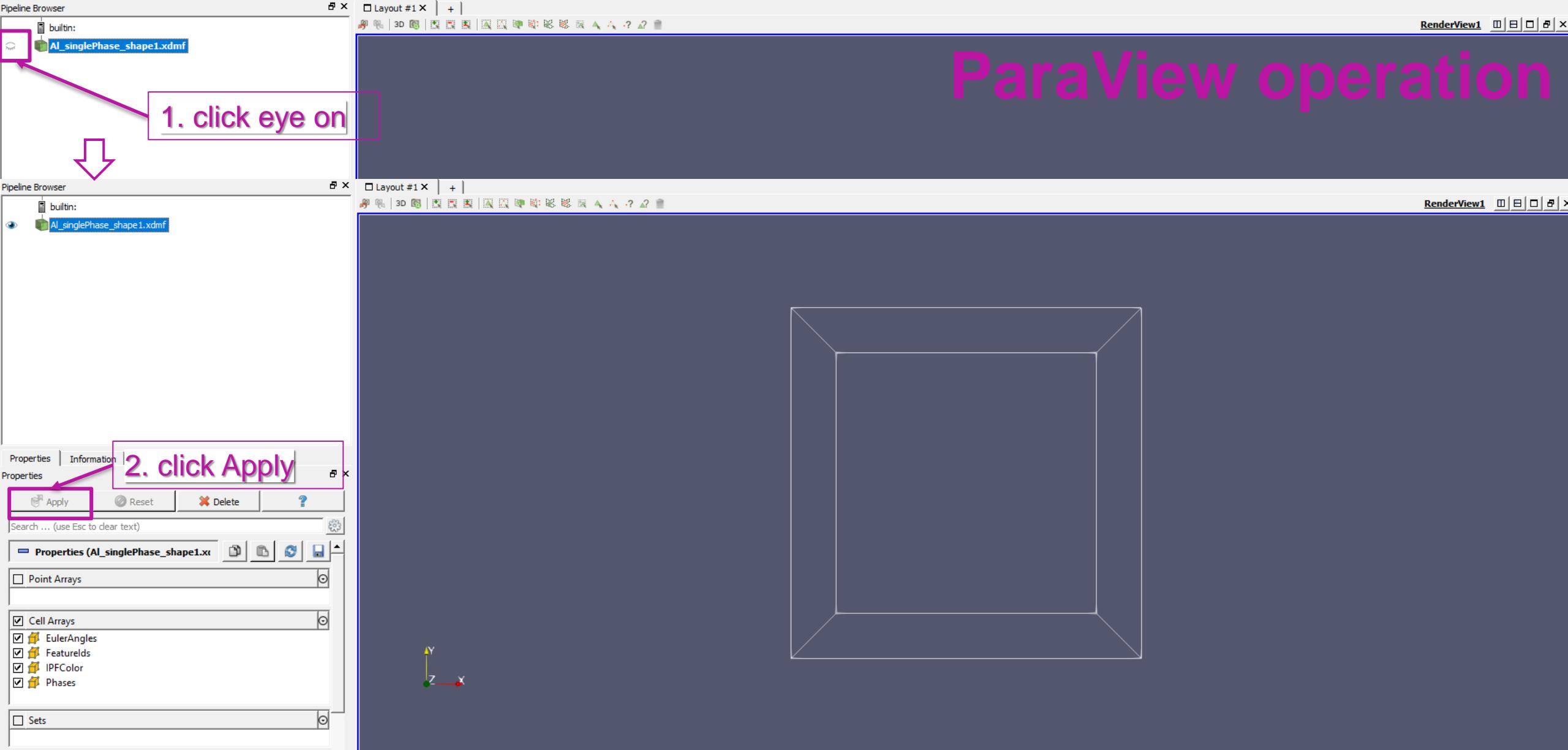
# Layout of ParaView



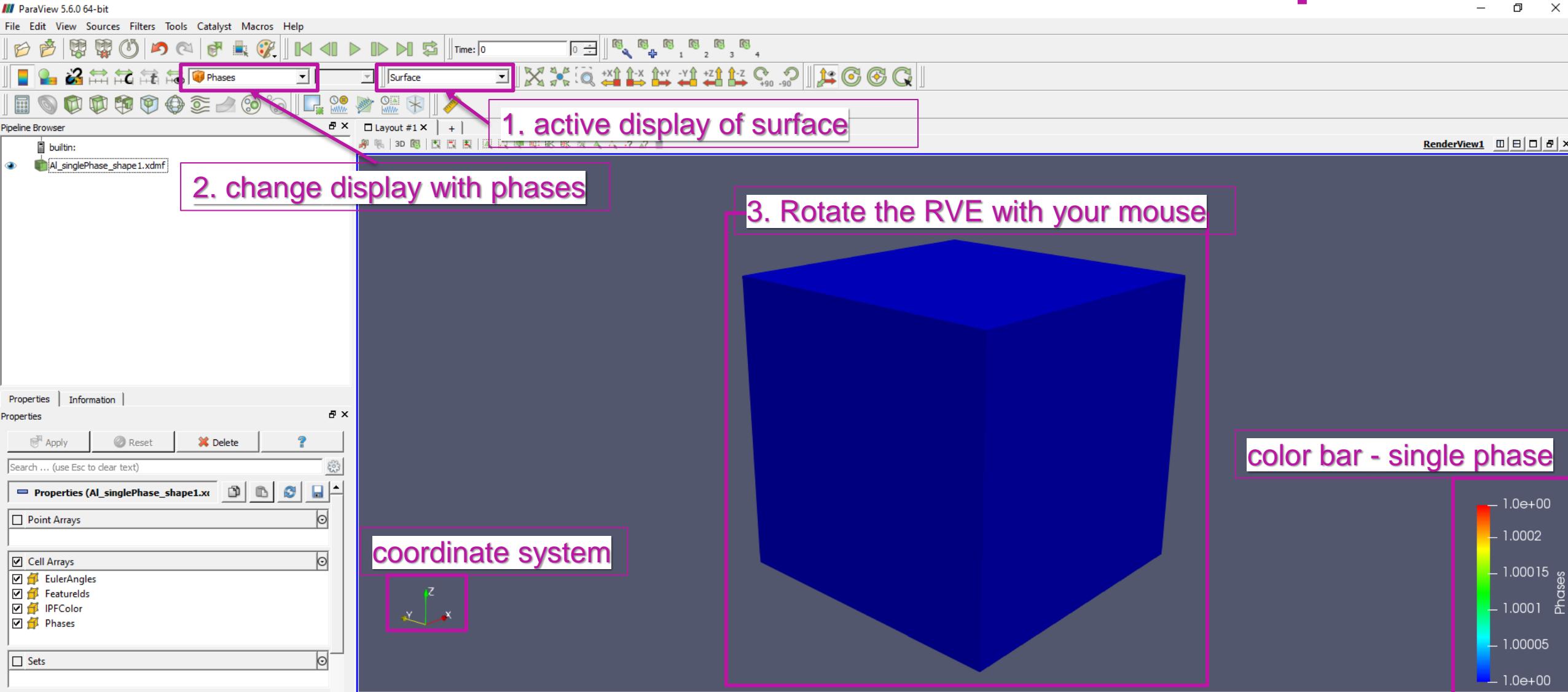
# Open data file



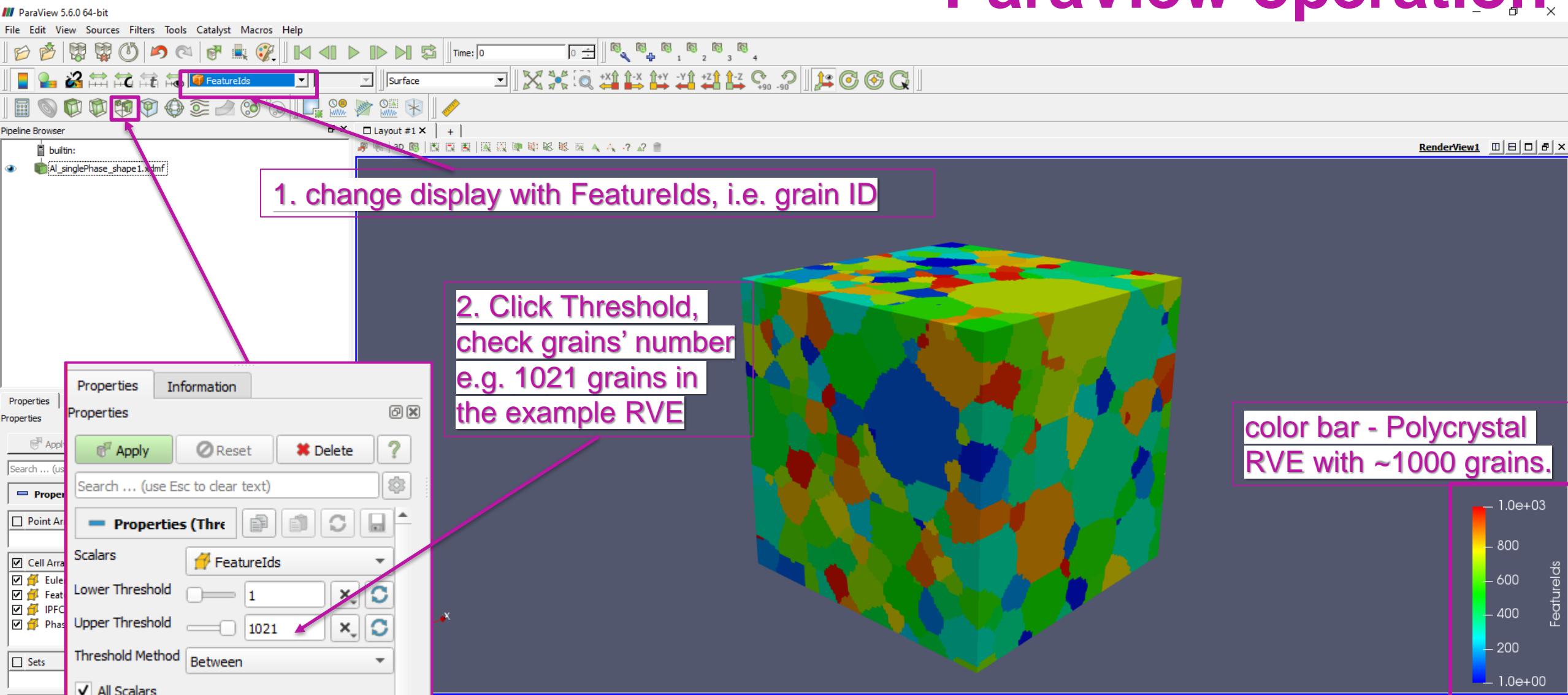
# ParaView operation



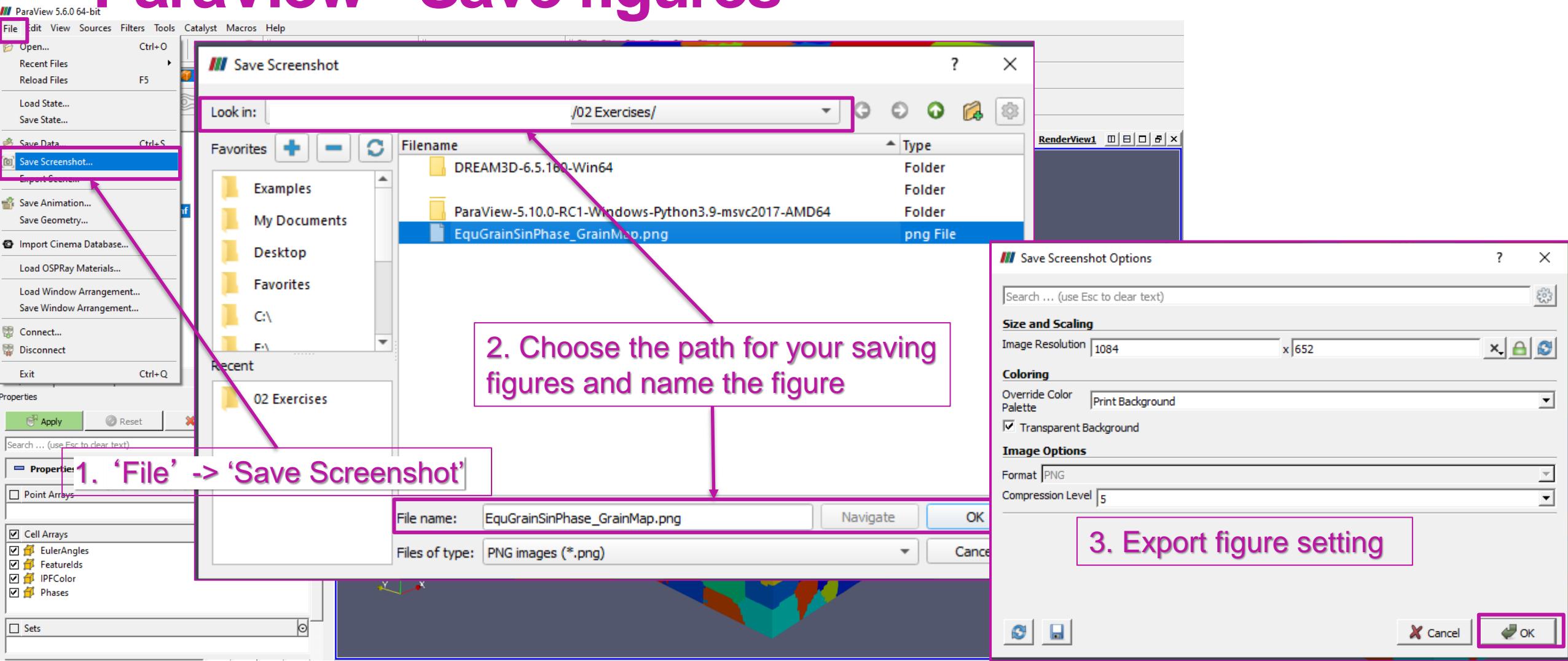
# ParaView operation



# ParaView operation



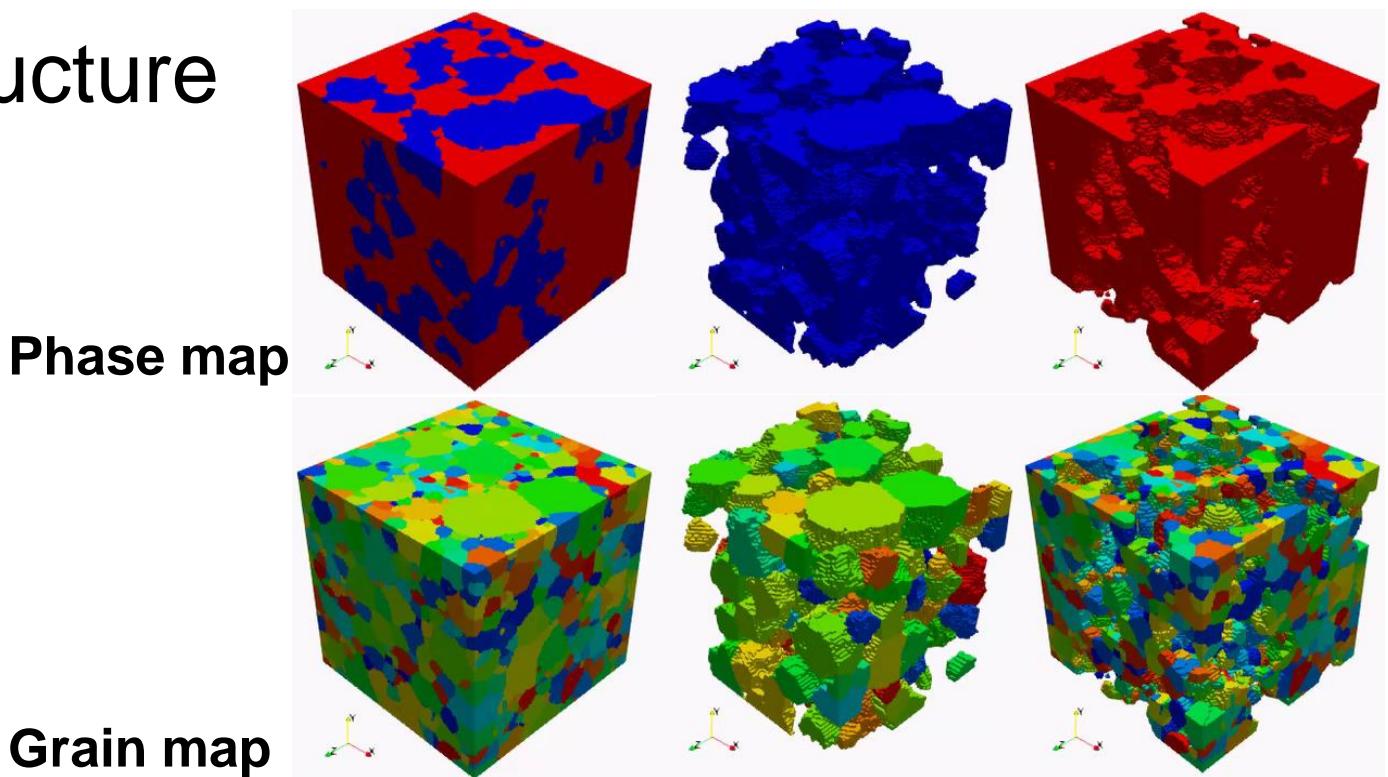
# ParaView - Save figures



# Advanced DREAM.3D operation

# DREAM.3D For more features

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



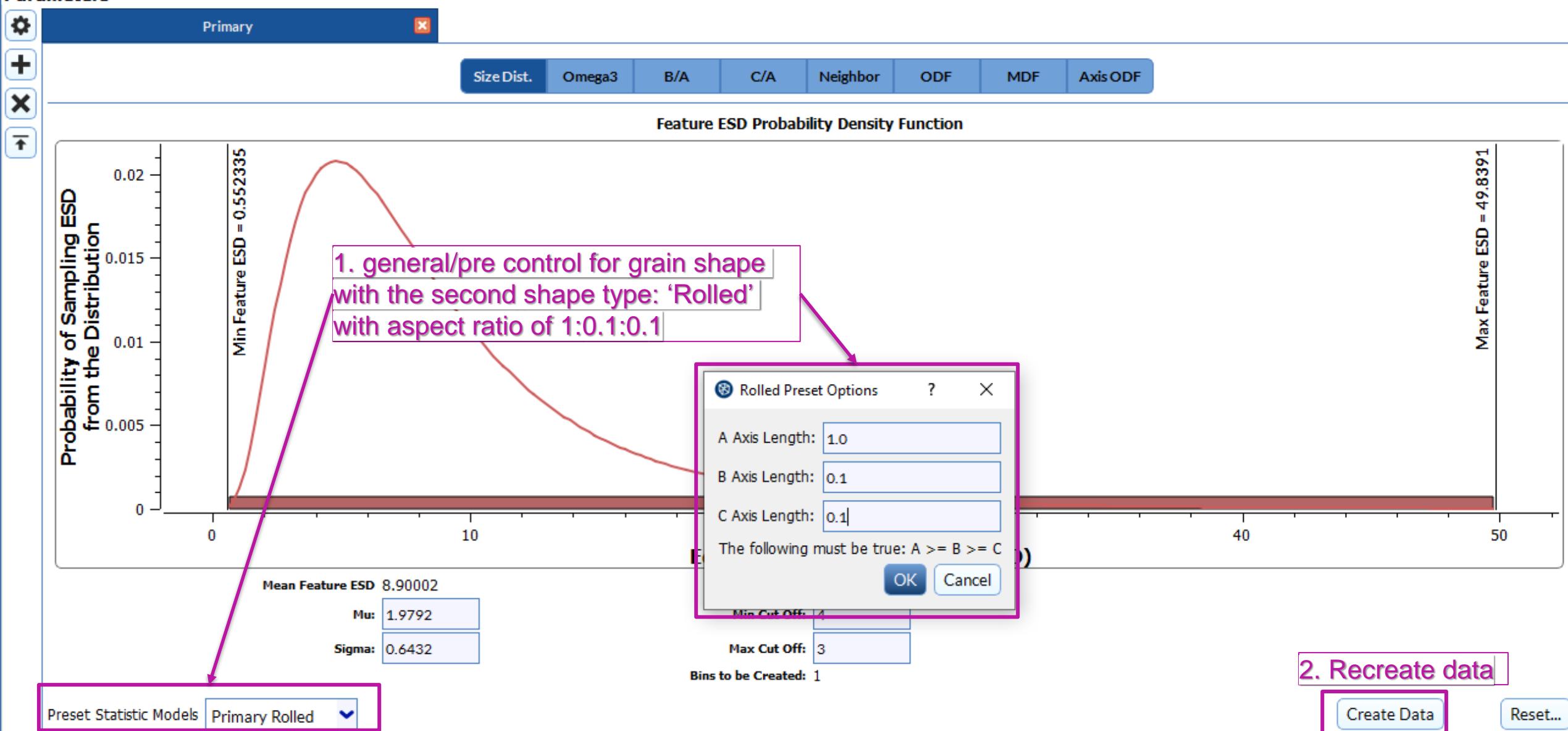
## 2. DREAM.3D - Rolled grain structure

1

StatsGenerator

i

Parameters



# 2. DREAM.3D - Rolled grain structure

\*(01) Single Cubic Phase Equiaxed - DREAM3D

File Edit View Bookmarks Pipeline Help

Pipeline 8 Write DREAM.3D Data File

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

Parameters

Output File C:\Users\wenqi.liu\Desktop\Dream3D\AI\_singlePhase\_shape2.dream3d Select...

Write Xdmf File

Include Xdmf Time Markers

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.

A"

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

Look in: Dream3D/

Filename Type

DREAM3D-6.5.141-Win64 Folder

Dream3D\_RVE Folder

AI\_singlePhase\_shape..xdmf Group

AI\_singlePhase\_shape1.xdmf xdmf File

AI\_singlePhase\_shape2.xdmf xdmf File

File name: AI\_singlePhase\_shape2.xdmf

OK Cancel

Files of type: Supported Files (plt\*.inp\*.cgns\*.cml\*.csv\*.txt\*.CSV\*.TSV\*.TXT\*.dem\*.dcm\*.do\*)

1.1e+03

800

600

400

200

1.0e+00

Features

Y

Z

X

### 3. DREAM.3D - Grain shape distribution

1 StatsGenerator

Parameters Primary

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

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

3. Use the parameter from E1, see the distribution curve change, then close this small data window.

4. Do the same for C/A.

5. Recreate data

B/A Shape Distribution

Frequency

Number Fraction, -

Grain Shape Aspect Ratio, -

Bin Alpha Beta

0.552335 6.2604 2.6321

Grain Shape Data Beta distribution

$\alpha = 6.2604$

$\beta = 2.6321$

$\text{mean}(\text{asp}) = 0.7041$

Preset Statistic Models Primary Rolled Create Data Reset... 40

The screenshot shows the StatsGenerator software interface. At the top, there's a toolbar with icons for settings, plus, minus, and other functions. Below it is a menu bar with 'Parameters' and 'Primary'. A sub-menu bar has tabs for 'Size Dist.', 'Omega3', 'B/A', 'C/A', 'Neighbor', 'ODF', 'MDF', and 'Axis ODF'. The 'B/A' tab is highlighted. A callout box labeled '1.' points to the 'B/A' tab. Another callout box labeled '2.' points to a button labeled 'Edit Data' on a small window titled 'Edit B/A Distribution Values Data'. This window contains a table with columns 'Bin', 'Alpha', and 'Beta', and a row with values 0.552335, 6.2604, and 2.6321 respectively. A callout box labeled '3.' points to a histogram titled 'Beta grain shape distribution from Exercise 1'. The histogram plots 'Number Fraction, -' against 'Grain Shape Aspect Ratio, -' (ranging from 0 to 1). It shows a red beta distribution curve overlaid on a grey bar chart. Text in the histogram area specifies parameters:  $\alpha = 6.2604$ ,  $\beta = 2.6321$ , and  $\text{mean}(\text{asp}) = 0.7041$ . A callout box labeled '4.' points to a text box stating 'Do the same for C/A.'. A final callout box labeled '5.' points to a 'Create Data' button at the bottom right. The overall background is light blue with some dark blue header sections.

# 3. DREAM.3D - Grain shape distribution

1

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

Parameters

Primary

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

C/A Shape Distribution

Step4 in last page, the same setting for 'C/A'

Frequency

0.01

0.008

0.006

0.004

0.002

0

0 0.2 0.4 0.6 0.8

Bin Alpha Beta

0.552335 6.2604 2.6321

Preset Statistic Models Primary Rolled

Create Data Reset...

8

Write DREAM.3D Data File

Parameters

Output File \Dream3D\AI\_singlePhase\_shape3.dream3d Select...

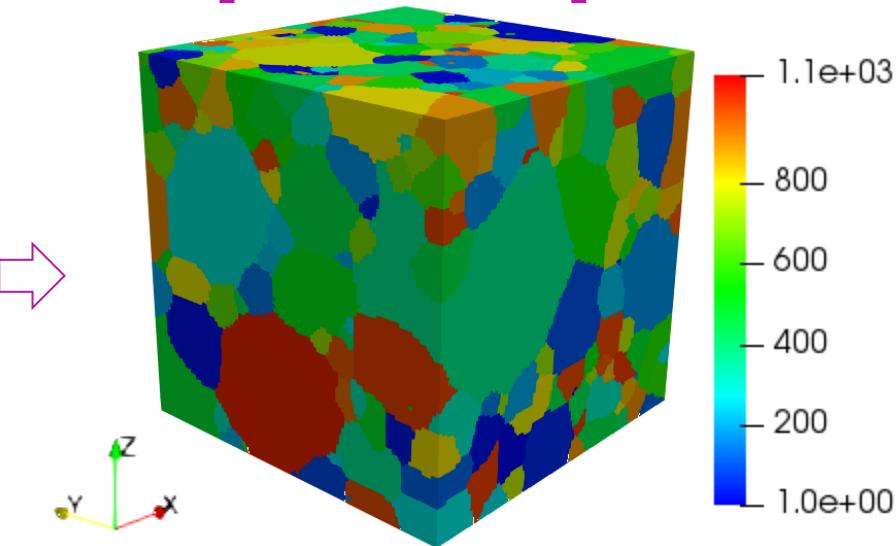
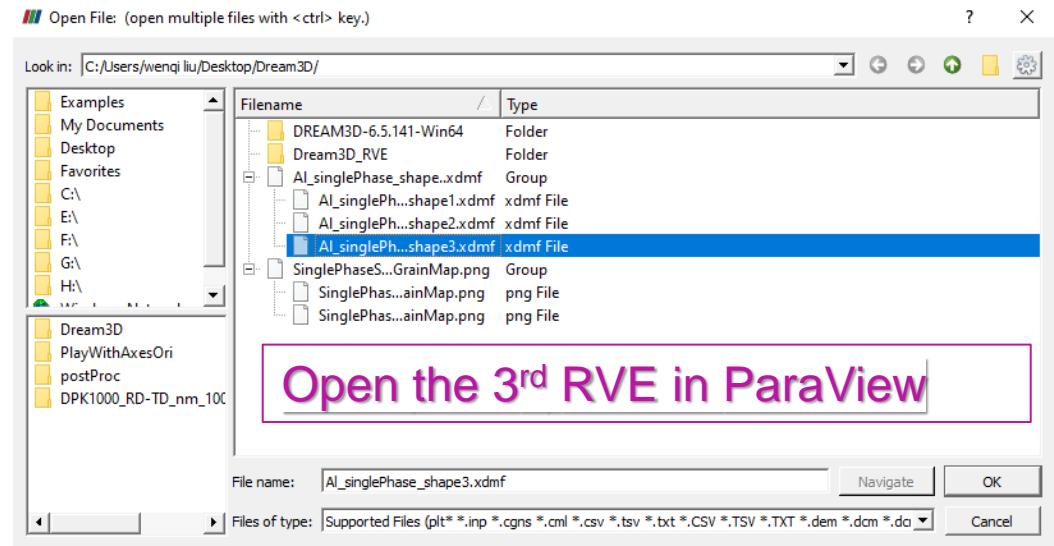
Write Xdmf File

Include Xdmf Time Markers

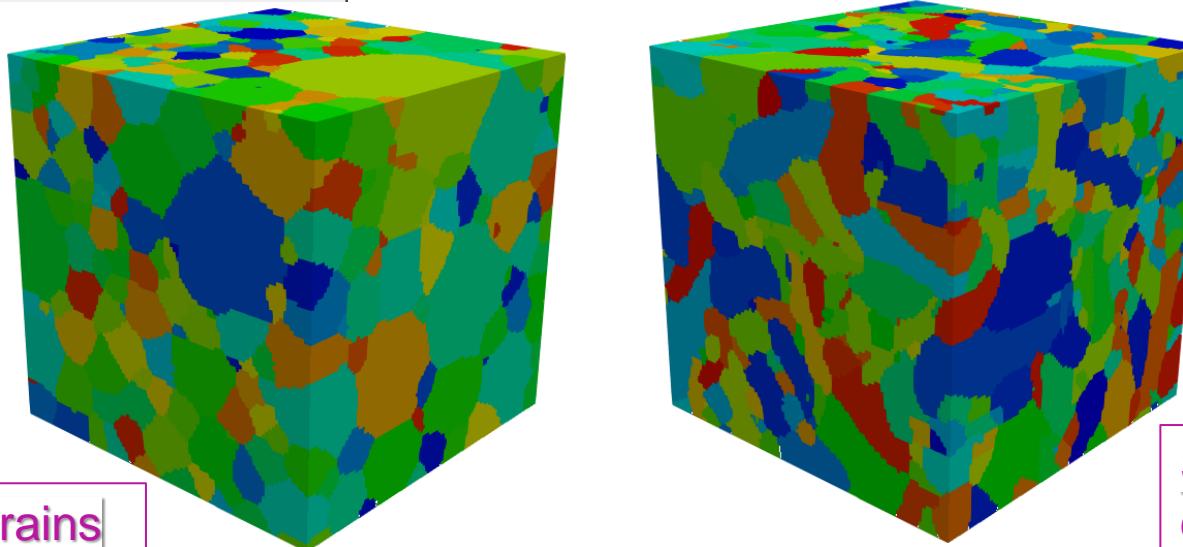
2. Change output filename to avoid overwrite in Filter 08

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

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



Open the 3<sup>rd</sup> RVE in ParaView



Shape 1: Equiaxed grains

Shape 2: Extremely elongated/rolled grains

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

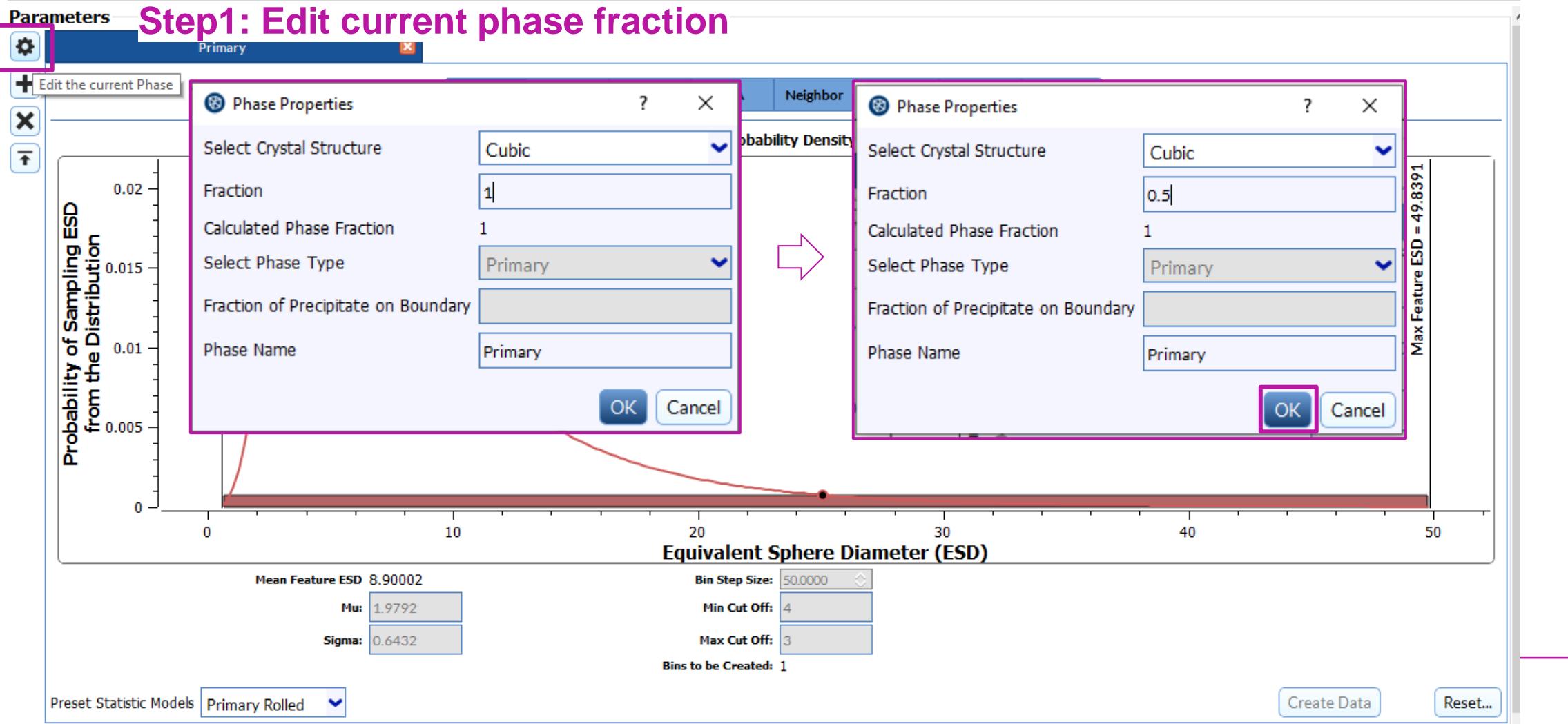
# 4. DREAM.3D - Dual-phase structure

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

1

StatsGenerator

i



# 4. DREAM.3D - Dual-phase structure

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

1

StatsGenerator



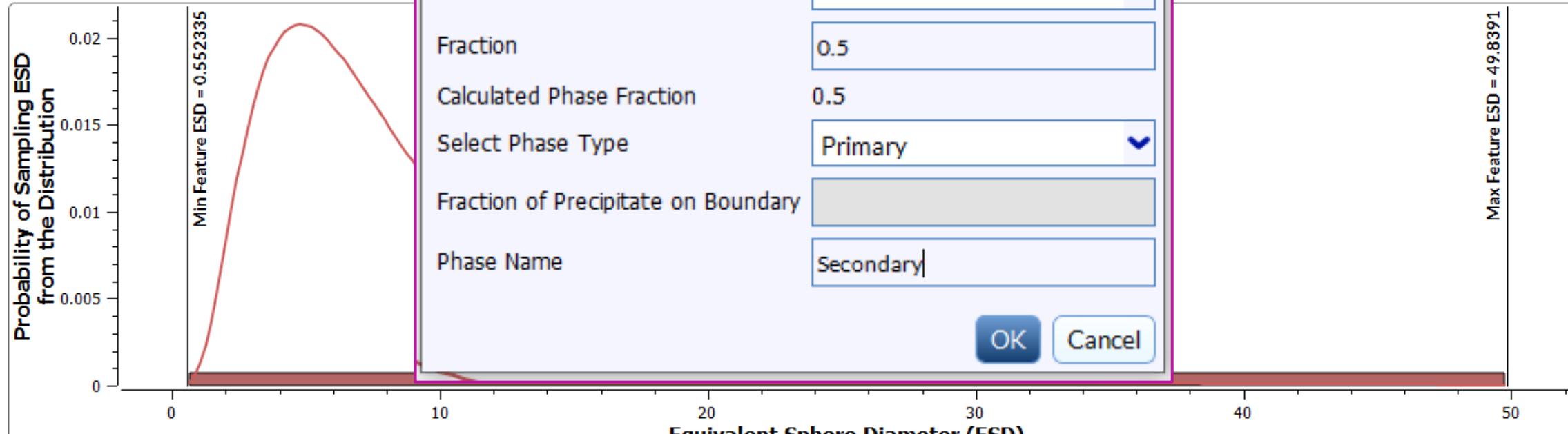
Parameters



X Add a new Phase

Primary

Step2: Add the second primary phase with 50% fraction



Preset Statistic Models Primary Rolled

Create Data

Reset...

# 4. DREAM.3D - Dual-phase structure

1

StatsGenerator

i

Parameters

Primary

Secondary

Size Dist.

Omega3

B/A

C/A

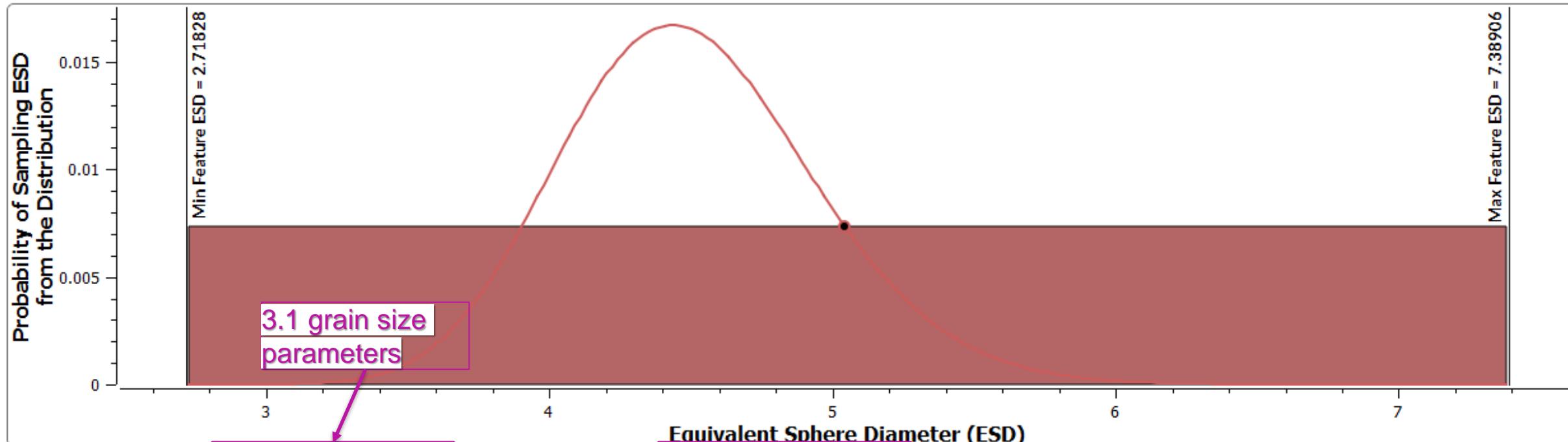
Neighbor

ODF

MDF

Axis ODF

Feature ESD Probability Density Function



3.1 grain size parameters

Mean Feature ESD 4.50415  
Mu: 1.5  
Sigma: 0.1

Equivalent Sphere Diameter (ESD)

Bin Step Size: 16532.0000  
Min Cut Off: 5  
Max Cut Off: 5  
Bins to be Created: 1

3.2 change the 'Bin Step Size' to create only one bin

3.4 create grain data for phase 2

3.3 Equiaxed shape

Preset Statistic Models Primary Equiaxed

Create Data

45

Reset...

# 4. DREAM.3D - Dual-phase structure

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\_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

Cancel Pipeline

Pipeline Issues

Index	Filter	Description	Code
1			

Pipeline Output

```
Swapping/Moving/Adding Features Iteration 25215/100000 || Est. Time Remain: 00:00:00 || Iterations/Sec: 12097.4
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

Data Structure

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

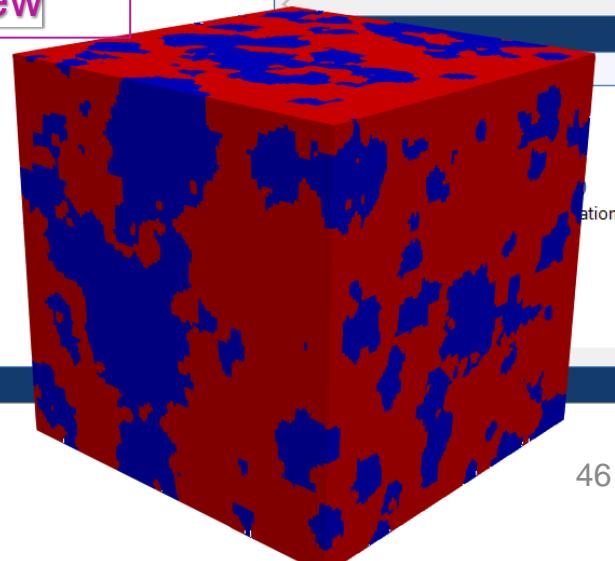
Bookmarks

- 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

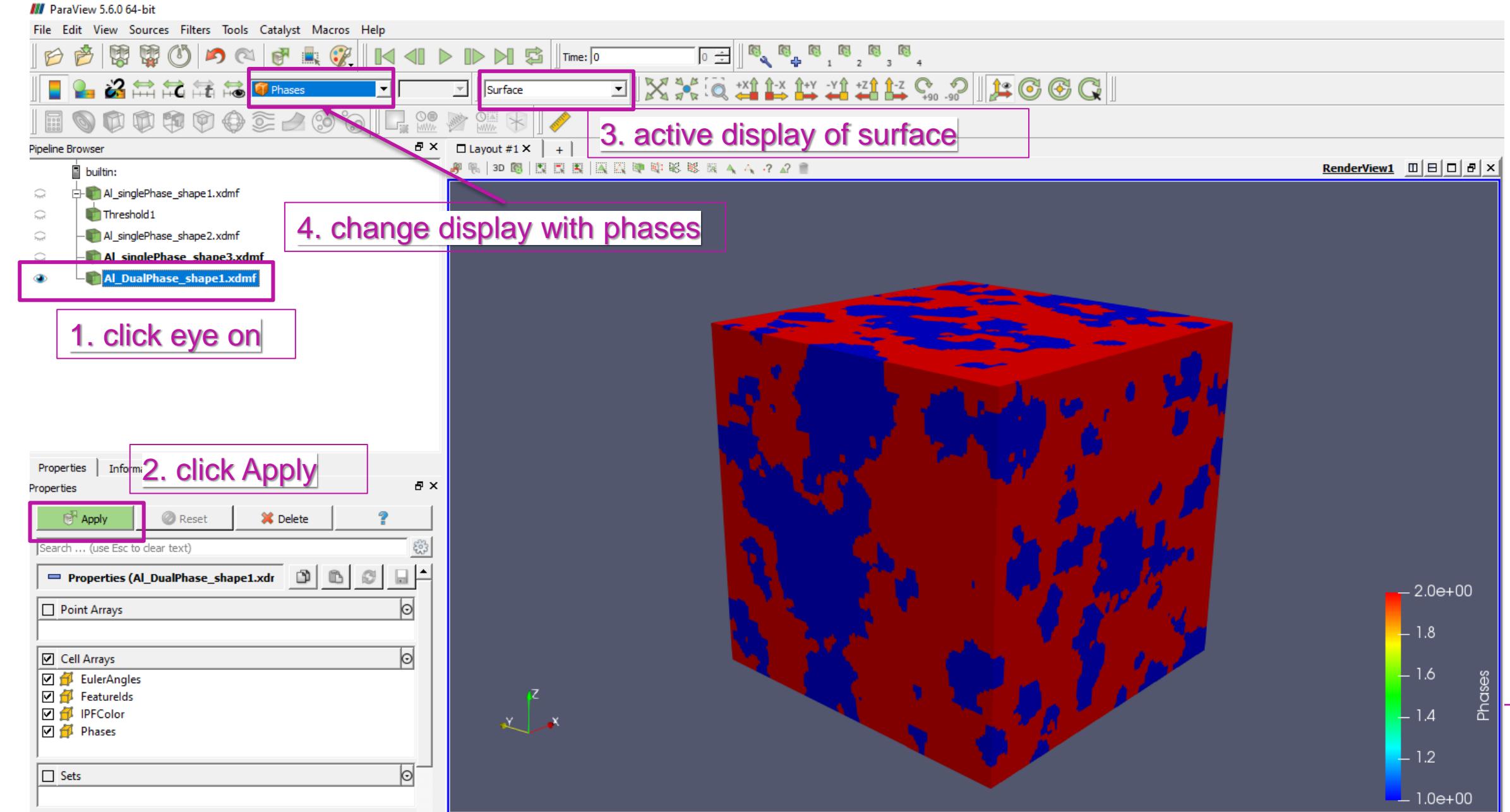
- Filter Library
  - Core
  - DREAM3D Review
  - Generic
  - IO
  - ITK Image Processing
  - Processing

Step8: Open new RVE in ParaView

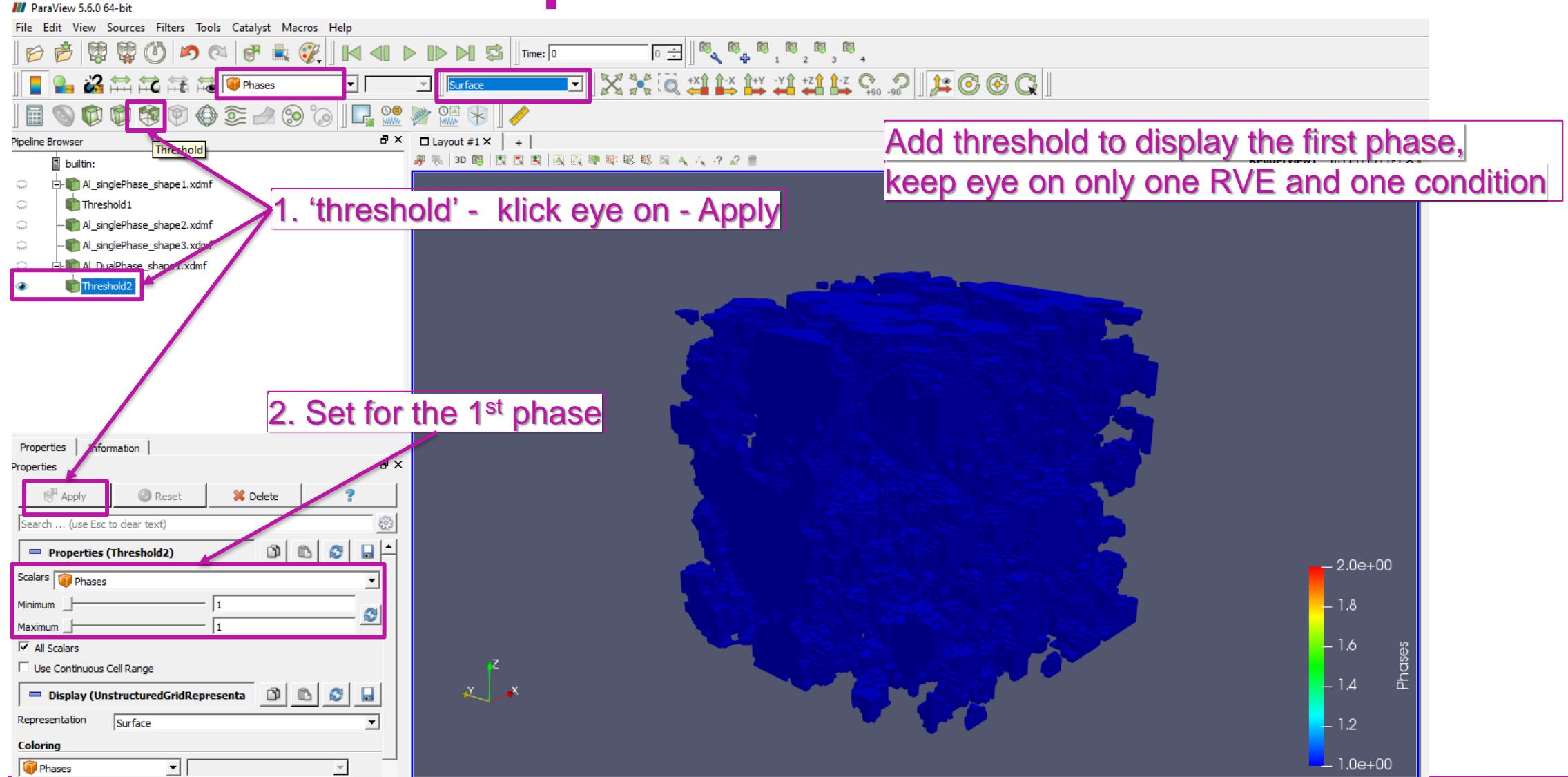


46

# 4. ParaView - Dual-phase structure

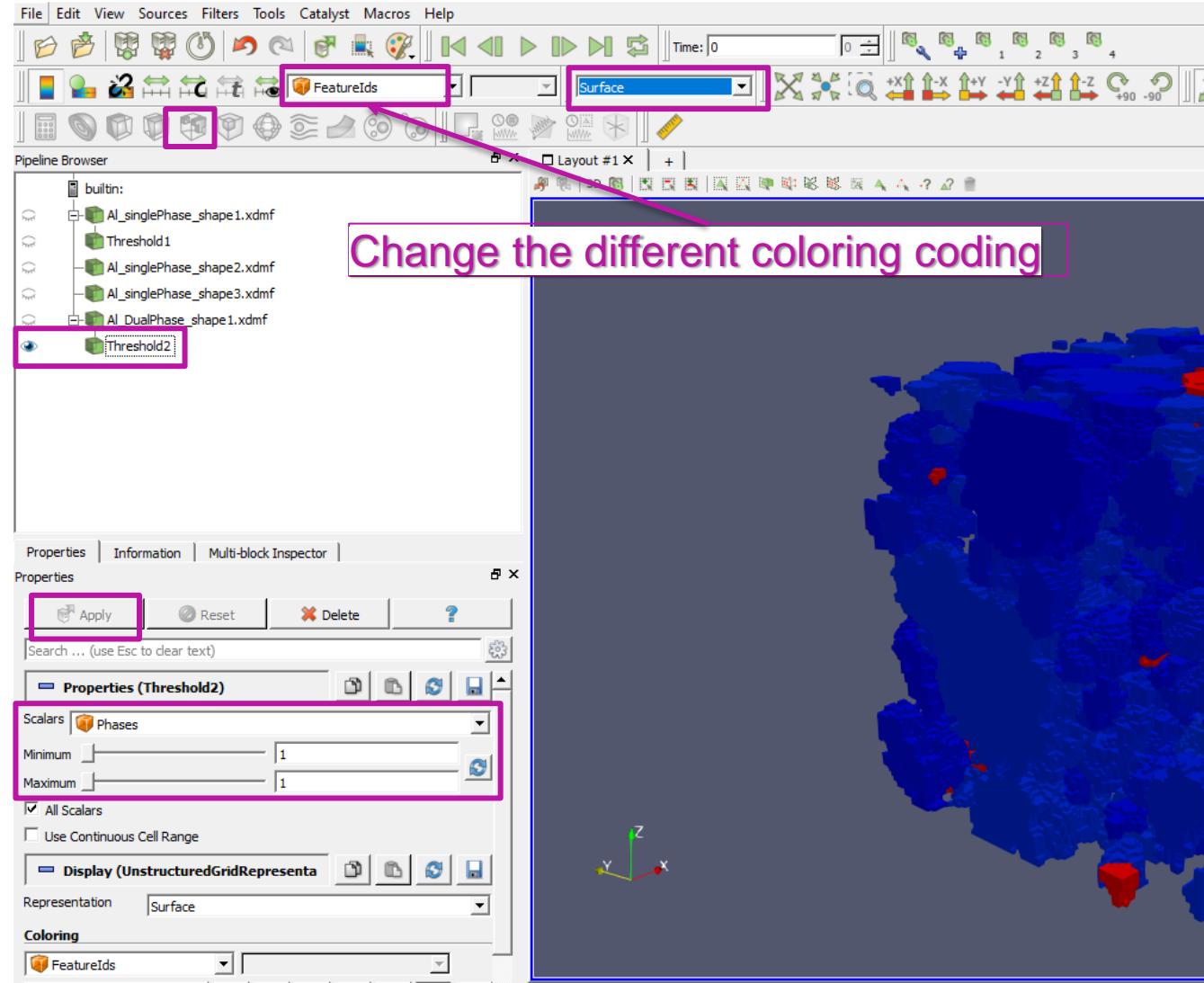


# 4. ParaView - Dual-phase structure



# 4. ParaView - Dual-phase structure

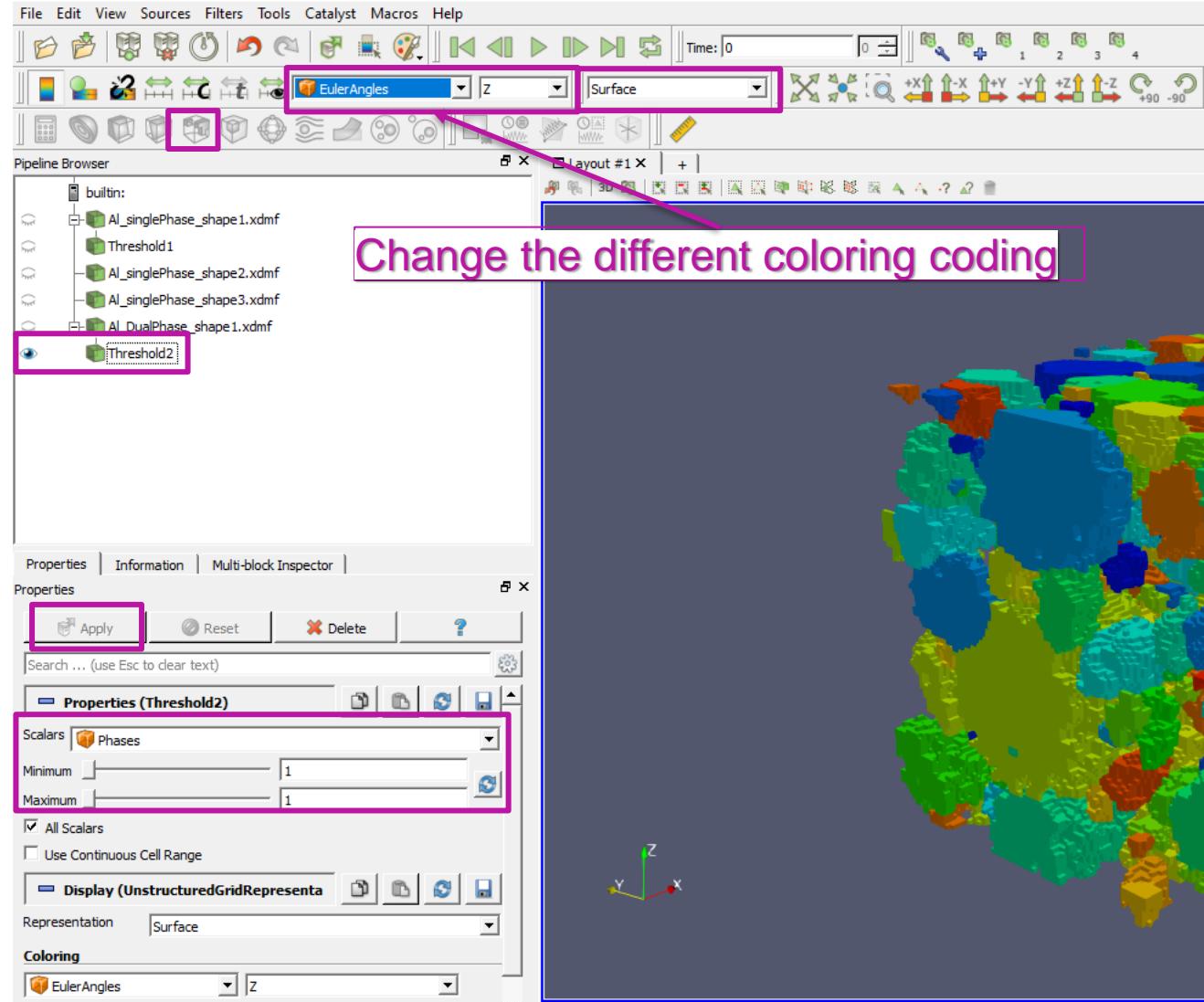
ParaView 5.6.0 64-bit



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

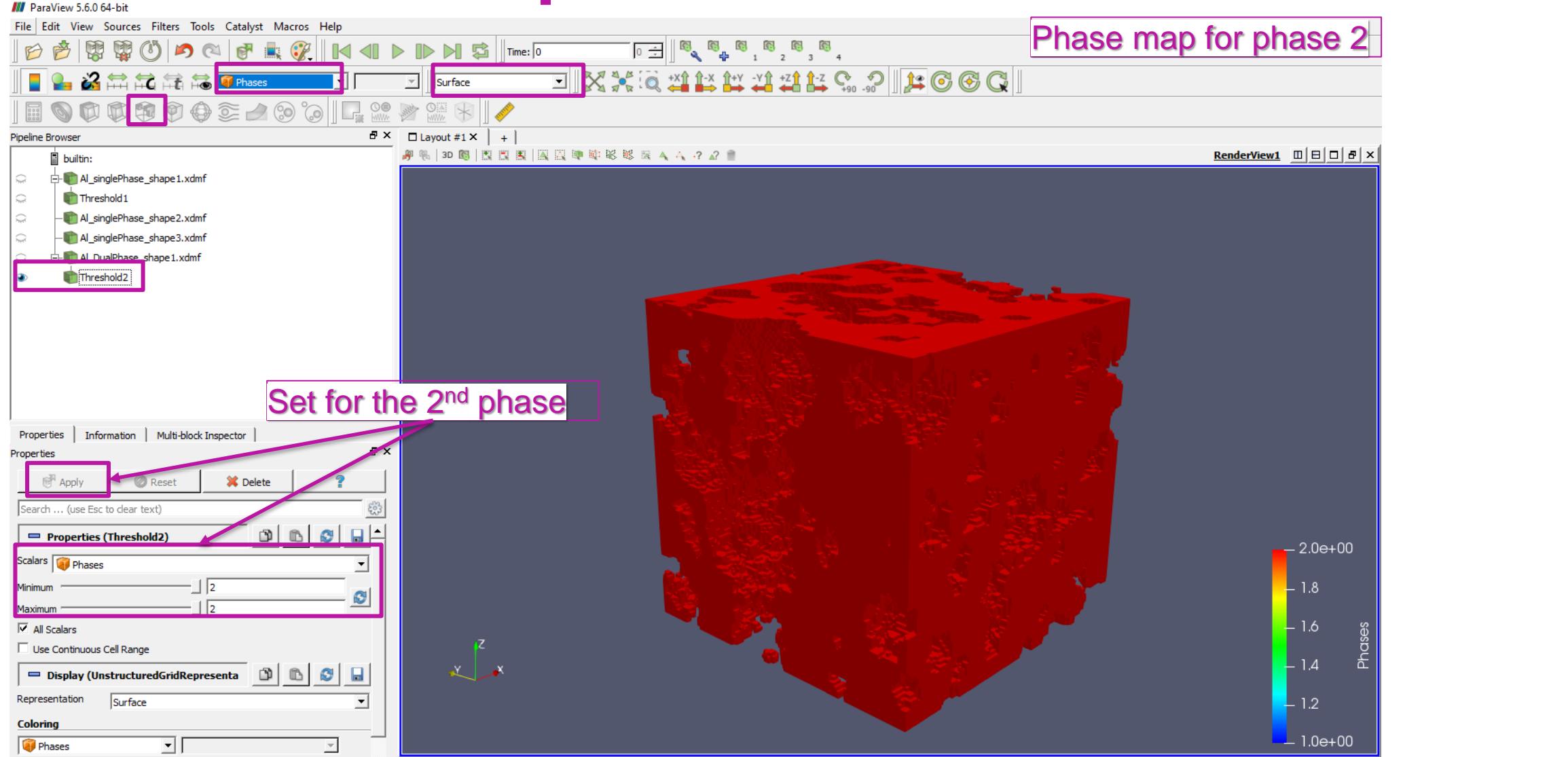
ParaView 5.6.0 64-bit



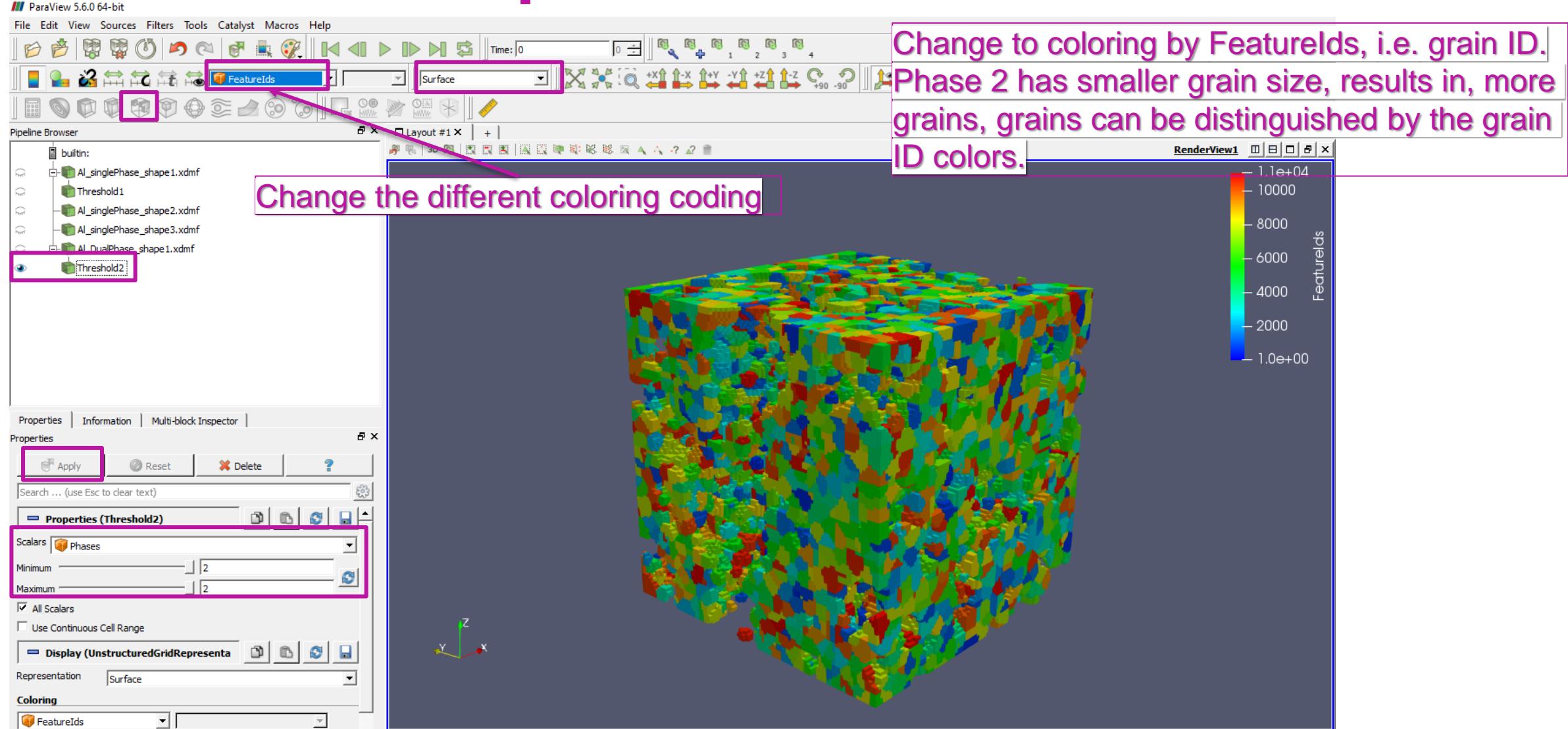
Change to coloring by FeatureIds, i.e. grain ID  
but the grain ID is ordered according to phase,  
the color code is too closed for grains in one  
phase. -> Try to coloring by EulerAngles-Z

Change the different coloring coding

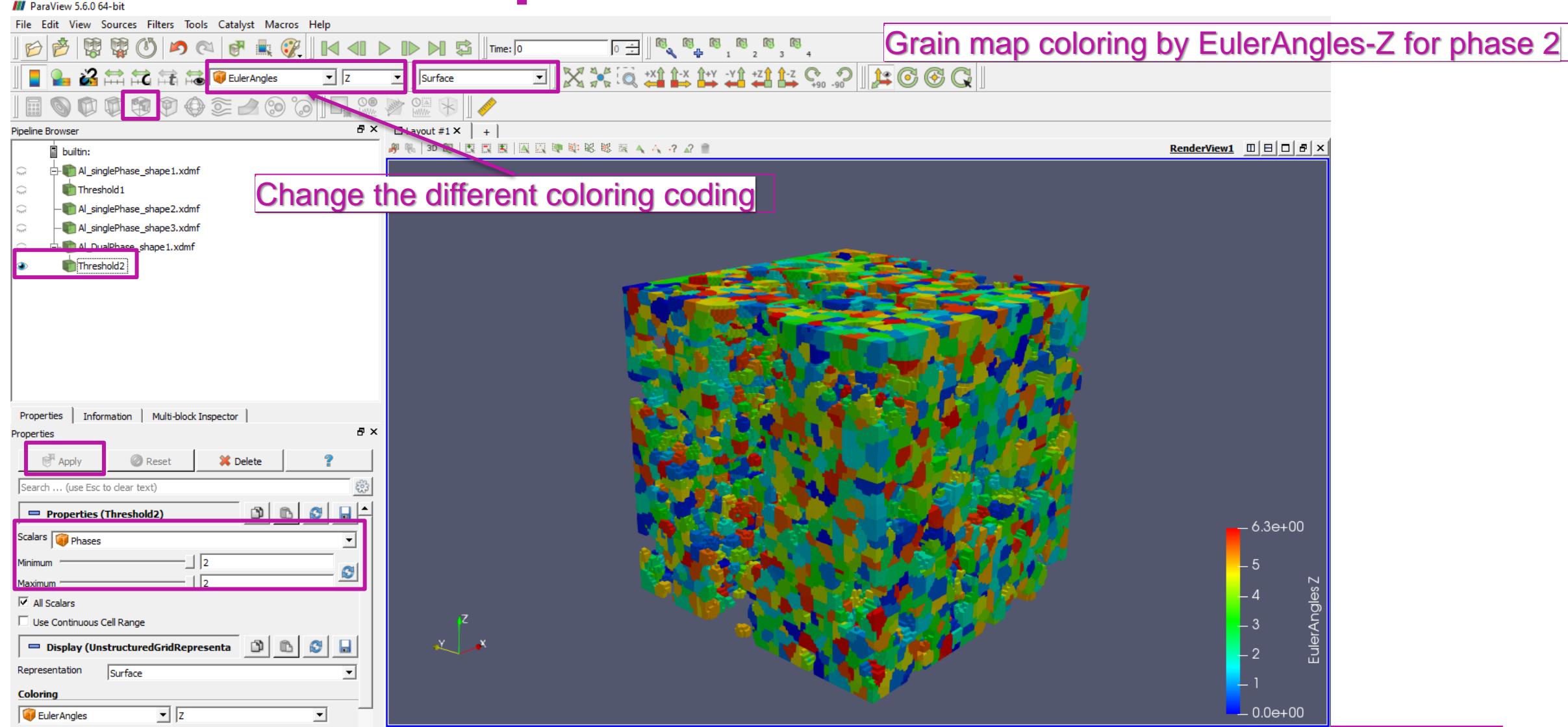
# 4. ParaView - Dual-phase structure



# 4. ParaView - Dual-phase structure



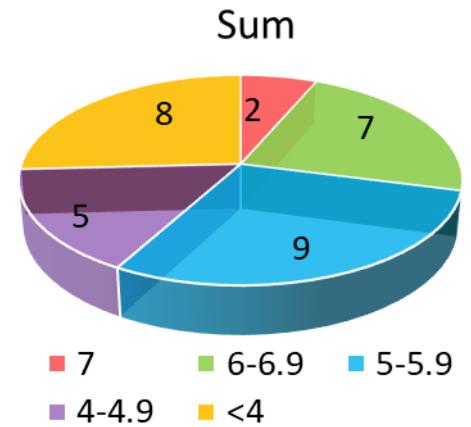
# 4. ParaView - Dual-phase structure



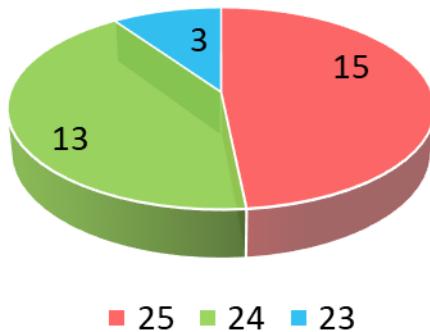
# Feedback - Assignment

# Assignment 01 - Summary

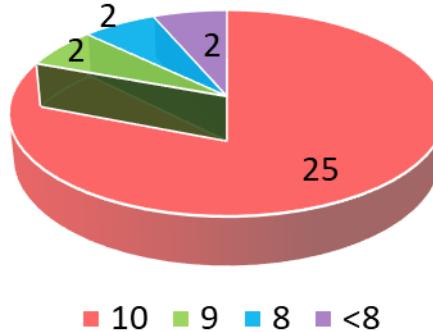
- Submission: 31
- Full points: 100, is calculated as 7 points in the final grade system.
- Due date: 18:00, 07.11.2021 (3 delayed submission)
- Grading criteria are listed in the assignment solution.
- Tolerant grading, **high points ≠ exactly accurate answers!**
- **Check the assignment solution carefully!**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



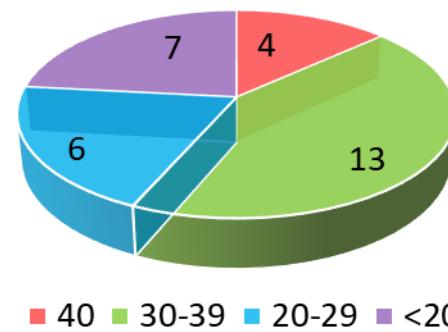
Task 1: 31, 25 points



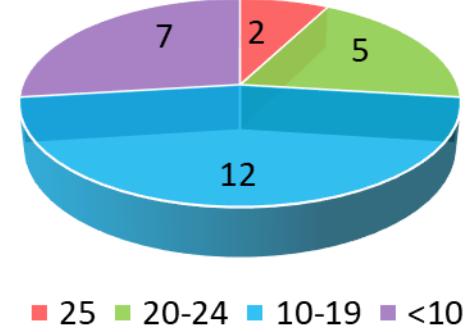
Task 2: 31, 10 points



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,  $r = 5.3 \text{ nm} = 5.3 \times 10^{-9} \text{ m}$ , 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  $\epsilon_0$  is the vacuum permittivity constant ( $8.85 \times 10^{-12} \text{ F/m}$ ),  $e$  is the elementary charge ( $1.602 \times 10^{-19} \text{ C}$ ),  $Z$  is the chemical valence of ion. Combining Eq. 1 and Eq. 2:

$$E_A = -\frac{1}{4\pi \left(8.85 \times 10^{-12} \frac{C^2}{N \cdot m^2}\right) (5.3 \times 10^{-9} \text{ m})} [|+2|(1.602 \times 10^{-19} \text{ C})][|-1|(1.602 \times 10^{-19} \text{ C})] = -8.7082 \times 10^{-20} \text{ J} \quad \text{(2 points)}$$

Mathematically, energy (E) and force (F) are related as:  $E = \int F \, dr$  (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:

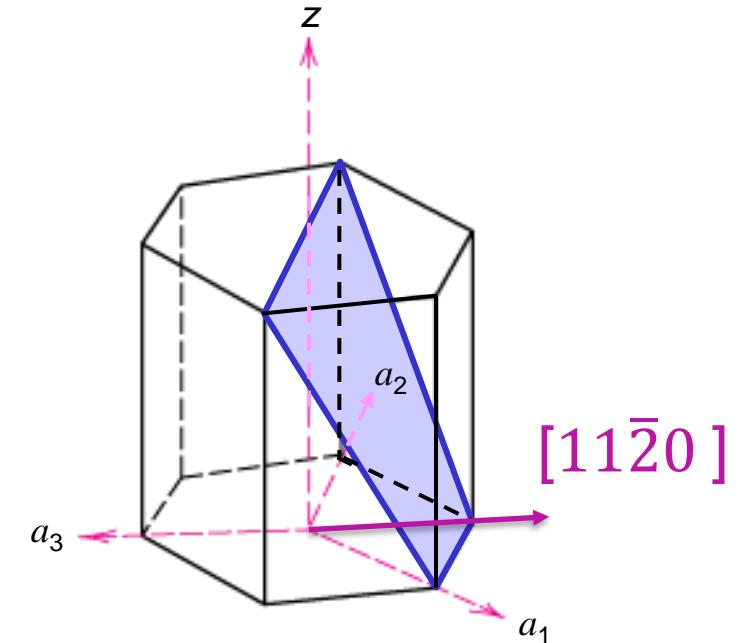
$$F_A = \frac{A}{r^2} = \frac{1}{4\pi \left(8.85 \times 10^{-12} \frac{C^2}{N \cdot m^2}\right) (5.3 \times 10^{-9} \text{ m})^2} [|+2|(1.602 \times 10^{-19} \text{ C})][|-1|(1.602 \times 10^{-19} \text{ C})] = 1.6430 \times 10^{-11} \text{ N} \quad \text{(2 points)}$$

# 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	$a$	$\infty a$	$c$
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	$i = -(h + k)$	$i = -(1 + 0) = -1$	$a_1 + a_2 + a_3 = 0$
7. Miller-Bravais Indices	( $10\bar{1}1$ )		$h + k + i = 0$



# Crystal structure

Miller indices - Cube

Miller-Bravais indices - HCP

Crystal plane:  $(hkl)$   $(hkil)$

Crystal plane family:  $\{hkl\}$   $\{hkil\}$

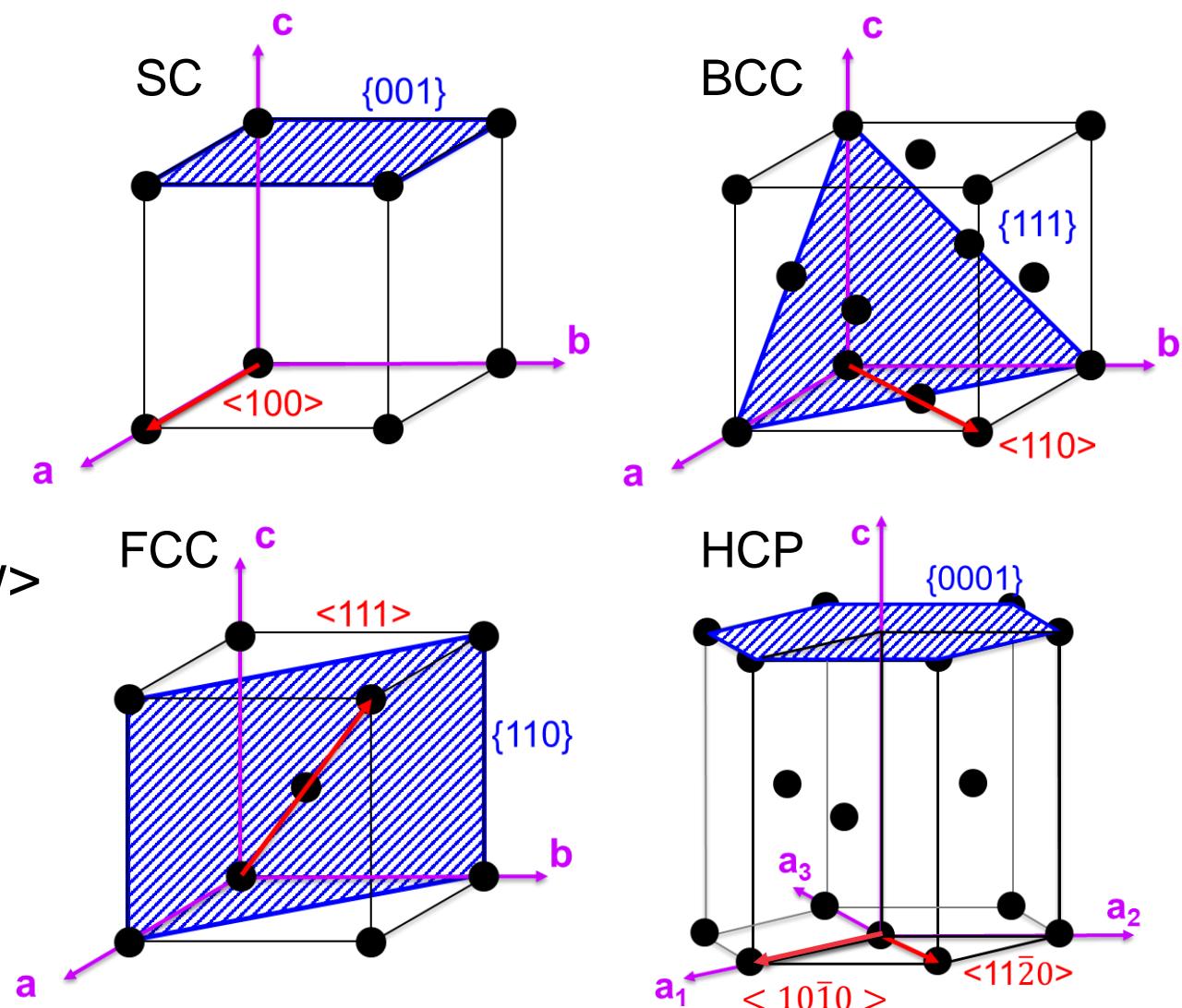
Crystal direction:  $[uvw]$   $[uvtw]$

Crystal direction family:  $\langle uvw \rangle$   $\langle uvtw \rangle$

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

e.g. for HCP most closed packet planes:

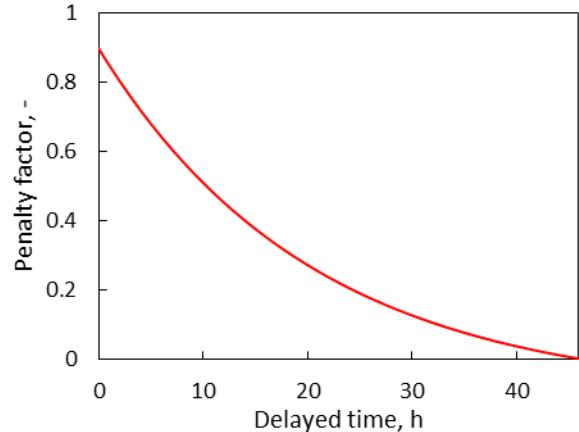
$\langle 11\bar{2}0 \rangle$  ✓  
 $\langle 11-20 \rangle$  ✗  
 $\langle 110 \rangle$  ✗



# 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.**