

A”

Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

Exercise 2

Prof. Junhe Lian

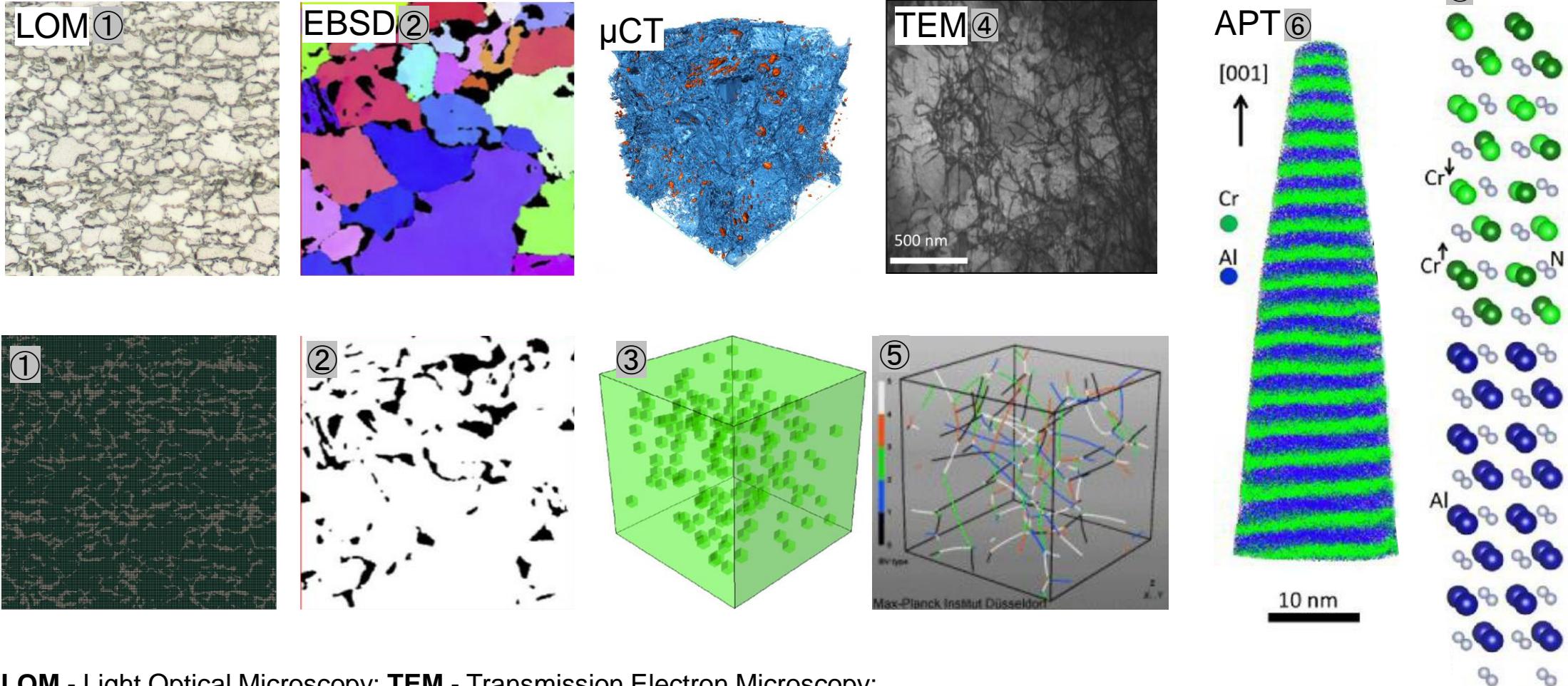
Wenqi Liu (Teaching assistant)

Outline

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

Microstructure modeling

Microstructure modeling



LOM - Light Optical Microscopy; **TEM** - Transmission Electron Microscopy;

EBSD - Electron Backscatter Diffraction; **μCT** - micro Computed Tomography; **APT** - atom probe tomography

Microstructure modeling

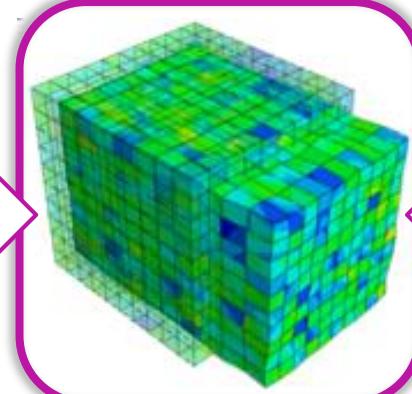
Microstructure - property relation & microstructure -based material design



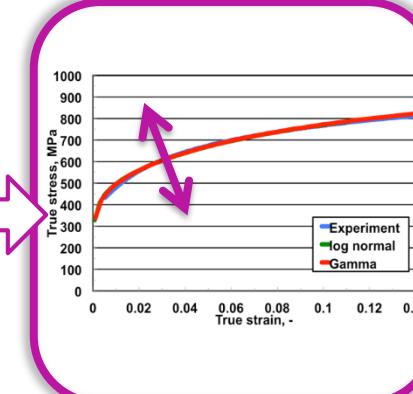
Microstructure measurement



Microstructure modeling

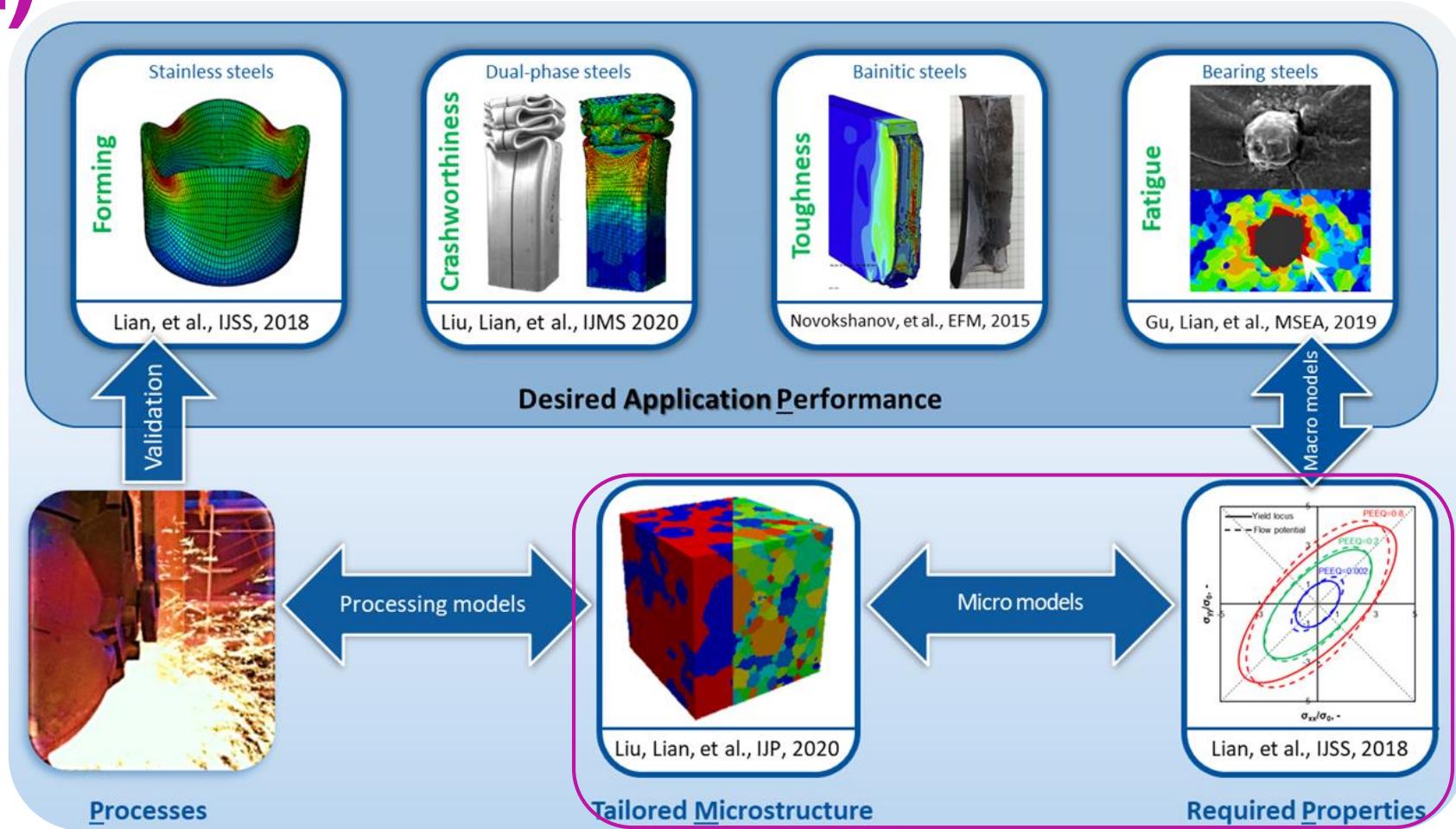


Virtual laboratory



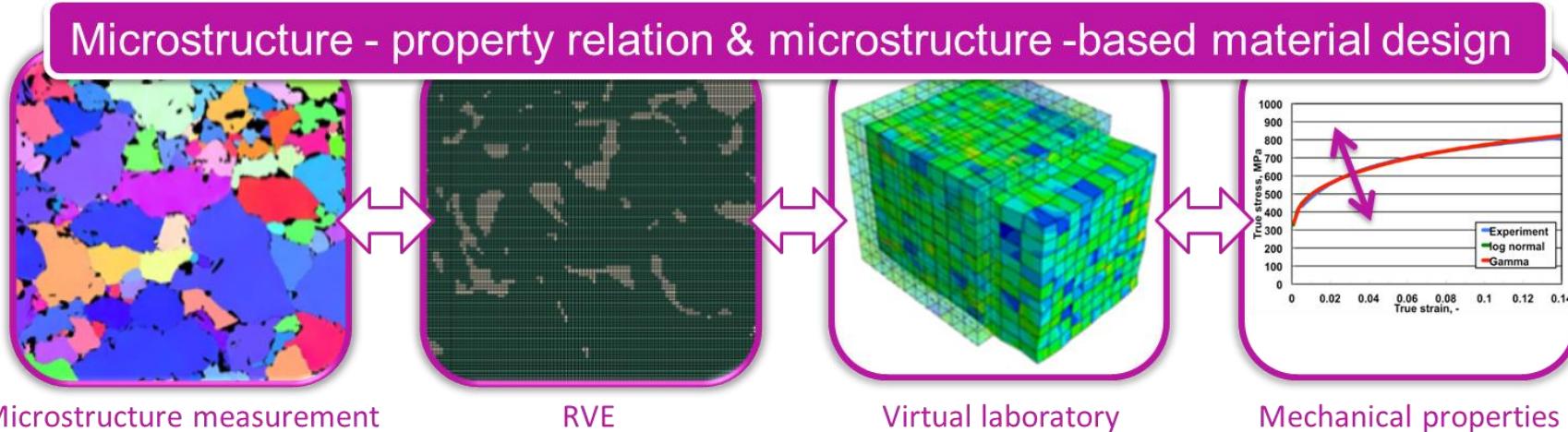
Mechanical properties

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

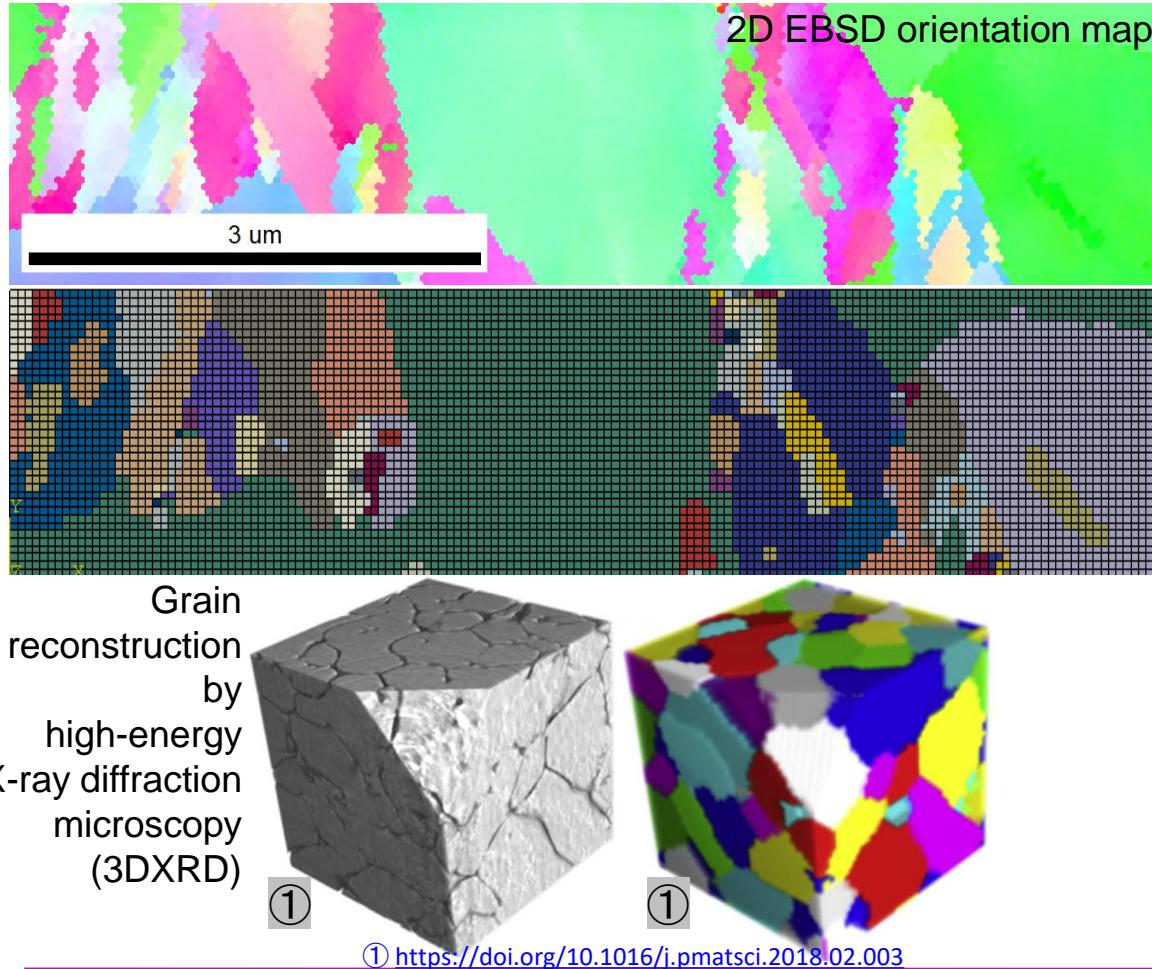
$L^M \gg L^{RVE} \gg L^\mu$

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.)

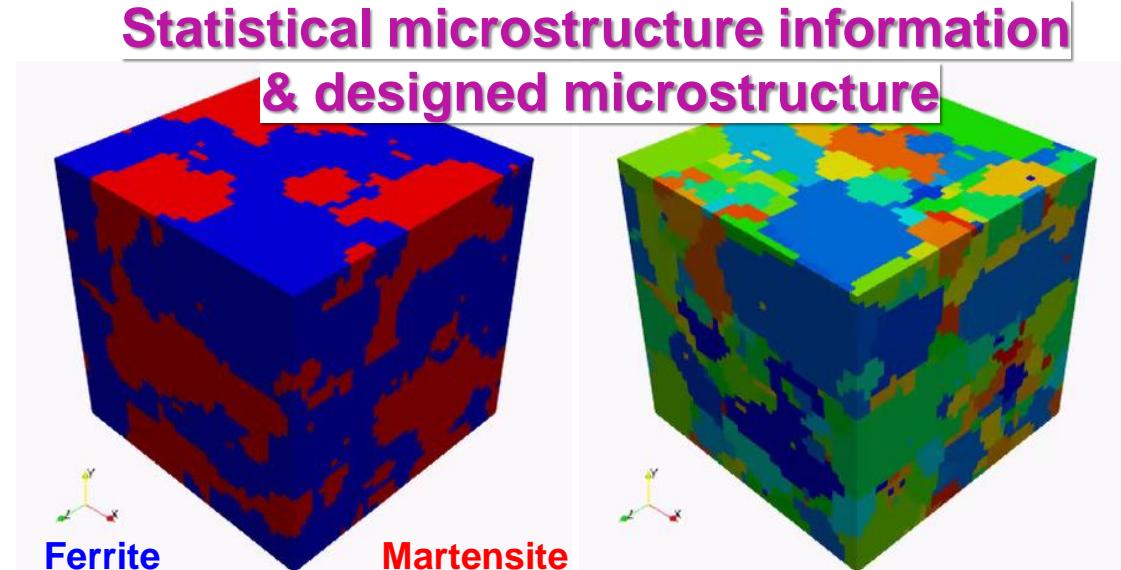
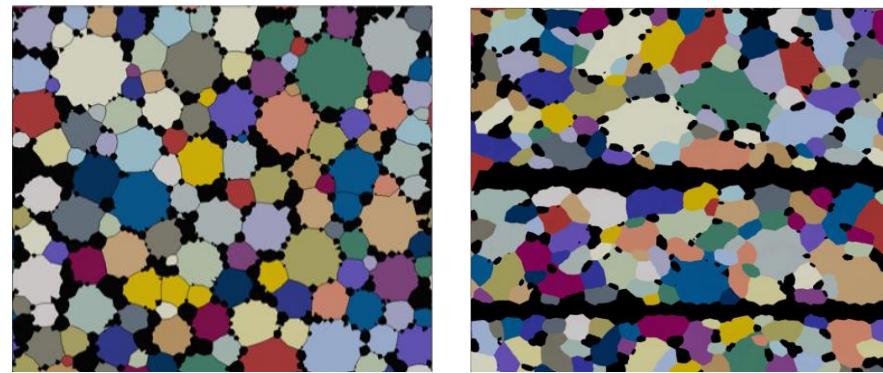
[1] <https://doi.org/10.1016/j.jpmatsci.2018.02.003>

Microstructure modeling - RVE

- Real microstructure RVE

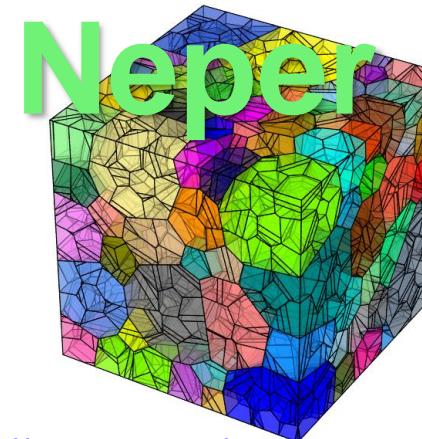


- Artificial/synthetic microstructure RVE



Microstructure modeling - RVE

- Generation



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



simpleware

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

- Visualization



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

DREAM.3D & ParaView preparation

Software preparation

DREAM.3D: open-source/freeware software <http://dream3d.bluequartz.net>

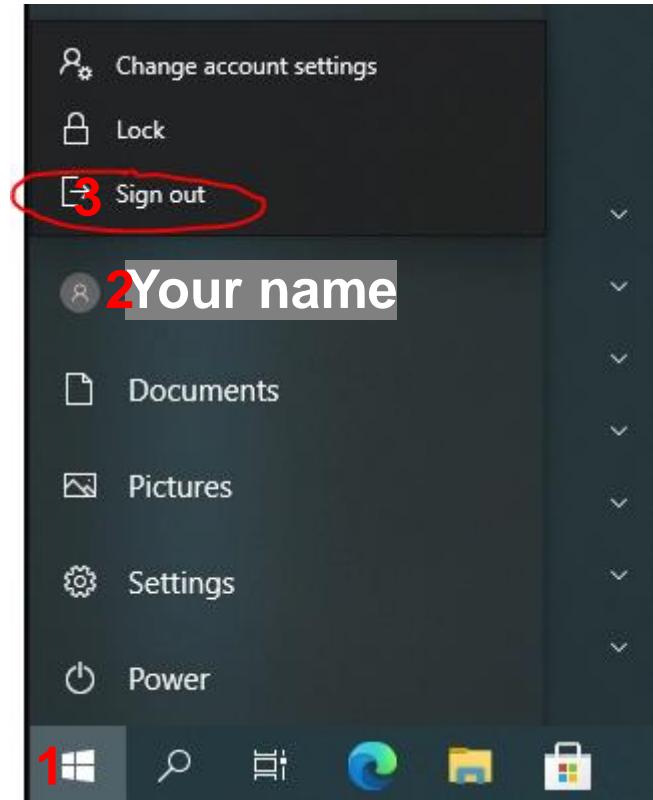
ParaView: freeware software <https://www.paraview.org/download/>

Aalto VDI system: mfavdi.aalto.fi, 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.



Interactive presentation software | Course: COE-C2004 - Materials S | DREAM.3D | Download | ParaView | +

Not secure | dream3d.bluequartz.net | Apps

DREAM.3D Download

<http://dream3d.bluequartz.net>



DREAM.3D

Home About Download Help Posts Search

DREAM.3D Version 6.5 (OS X)
DREAM.3D Version 6.5 (Linux x64)
DREAM.3D Version 6.5 (Windows x64)

DREAM.3D 6.5 New Features

There are some terrific new features in DREAM.3D version 6.5 and we are here to let you in on some of the major additions. A Fresh New Look We stripped DREAM.3D down and gave it a fresh ...

Choose the version according to your operating system.

© 2018/06/29 Demo, New Feature, Official Release, Training Mike Jackson

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.

dream3d.bluequartz.net/?page_id=536

<http://dream3d.bluequartz.net>

DREAM.3D Download



DREAM.3D

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Search

[Return to Download](#)

DREAM.3D Version 6.5 (Windows x64)

Please answer the simple math question below to download this version of DREAM.3D.

This download is compatible with the following systems: **64 Bit versions of Windows 8.1/10**

Fields marked with an * are required

We would like to make sure you are a human. What
is $20 + 10$ *

30

[Download](#)

Download

Interactive presentation software Course: COE-C2004 - Materials S DREAM3D Version 6.5 (Windows) Download | ParaView

ParaView Download

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

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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.

Version v5.8

ParaView

Sources **Windows** Linux macOS

Full suite of ParaView tools, including the ParaView GUI client, pypython, pvserver, and pvbatch. Versions with MPI in the name require MS-MPI.

- [!\[\]\(d055e740a24011074151377df88bf8de_img.jpg\) ParaView-5.8.1-Windows-Python3.7-msvc2015-64bit.zip](#)
- [!\[\]\(bd41e4ded8bc9f7822dec4e6c39801ba_img.jpg\) ParaView-5.8.1-Windows-Python3.7-msvc2015-64bit.exe](#)
- [!\[\]\(9abadd8da856b8c30a90f8699372d5a7_img.jpg\) ParaView-5.8.1-MPI-Windows-Python3.7-msvc2015-64bit.zip](#)
- [!\[\]\(72248d629b65dfc3dab3a5d21ed3e2af_img.jpg\) ParaView-5.8.1-MPI-Windows-Python3.7-msvc2015-64bit.exe](#)
- [!\[\]\(8729def1b55d42f94c7d42be3e368c01_img.jpg\) ParaView-5.8.0-Windows-Python3.7-msvc2015-64bit.zip](#)
- [!\[\]\(c4ec5b3adf6b09dea4d40dc97a2df580_img.jpg\) ParaView-5.8.0-Windows-Python3.7-msvc2015-64bit.exe](#)
- [!\[\]\(d10777cdada3063c66813646fb4e1f42_img.jpg\) ParaView-5.8.0-MPI-Windows-Python3.7-msvc2015-64bit.zip](#)
- [!\[\]\(8e066b970ada6d2d030fbf119365235c_img.jpg\) ParaView-5.8.0-MPI-Windows-Python3.7-msvc2015-64bit.exe](#)

Aug 4 23:09 464.1M
Aug 4 23:09 464.1M
Aug 4 21:47 194.2M
Feb 18 2020 463.0M
Feb 18 2020 192.4M
Feb 18 2020 467.2M
Feb 18 2020 193.5M

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

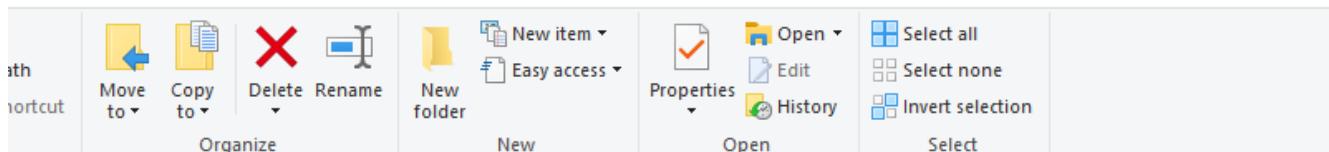
Documentation

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

- [!\[\]\(0e1ff9e7d838def2bf6dbccc7af86e56_img.jpg\) ParaViewTutorial-5.8.1.pdf](#)
- [!\[\]\(bf87b9106a236f546265691e3de3d6d2_img.jpg\) ParaViewTutorial-5.8.0.pdf](#)
- [!\[\]\(8656d6a83af0f8e5d736c949169854e8_img.jpg\) ParaViewGuide-5.8.1.pdf](#)
- [!\[\]\(a161899ae011056c4839aeaa6166021a_img.jpg\) ParaViewGuide-5.8.0.pdf](#)
- [!\[\]\(a37753b72b9f6b34b712513e11a73bc3_img.jpg\) ParaViewGettingStarted-5.8.1.pdf](#)

Documentation files

- Jun 15 17:01 46.1M
- Jan 14 2020 46.1M
- Jun 15 16:58 49.3M
- Feb 18 2020 49.3M
- Jun 15 16:55 1.3M



03 MSE 2020 > 02 Exercises

The screenshot shows a Windows File Explorer window with the following details:

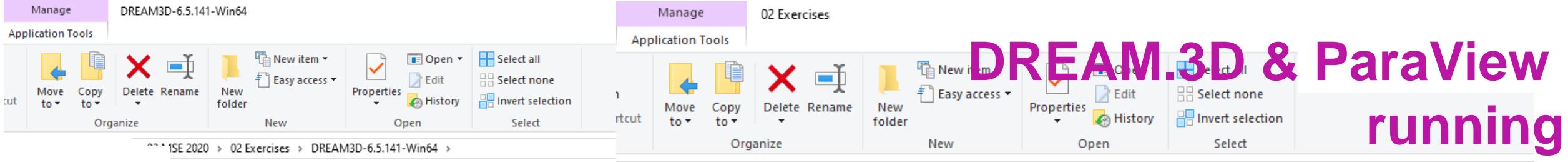
- Path:** 03 MSE 2020 > 02 Exercises
- Selected Item:** DREAM3D-6.5.141-Win64.zip (highlighted with a red box)
- Content List:**

Name	Status	Date modified	Type	Size
DREAM3D-6.5.141-Win64	Normal	09/03/2020 10:23	File folder	239,725 KB
DREAM3D-6.5.141-Win64.zip	Normal	09/03/2020 10:23	Compressed (zipp...)	28,997 KB
CTF File	Normal	09/03/2020 10:23	Microsoft PowerP...	28,536 KB
Microsoft PowerP...	Normal	09/03/2020 10:23	Foxit Reader PDF ...	6,723 KB
Foxit Reader PDF ...	Normal	09/03/2020 10:23	Microsoft PowerP...	28,749 KB
Microsoft PowerP...	Normal	09/03/2020 10:23	Microsoft PowerP...	28,540 KB
Microsoft PowerP...	Normal	09/03/2020 10:23	Compressed (zipp...)	160,895 KB
- Context Menu (Open):** A red box highlights the "Open" option in the context menu for the selected zip file.

Extract the Dream.3d .zip file

DREAM.3D & ParaView Extraction

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



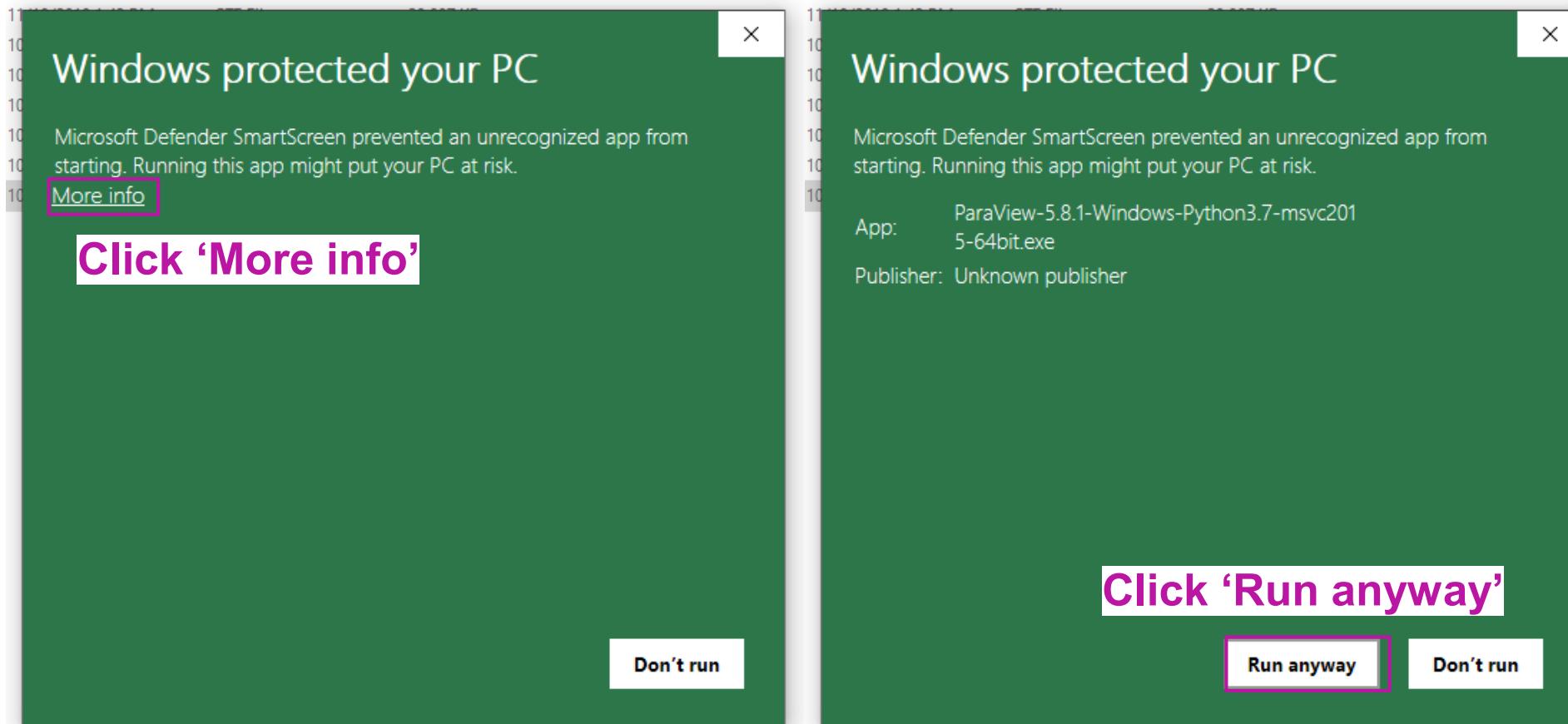
Name	Status	Date modified	Type	Size
Data	○ R	10/30/2020 8:32 PM	File folder	
Help	○ R	10/30/2020 8:32 PM	File folder	
lib	○ R	10/30/2020 8:32 PM	File folder	
Plugins	○ R	10/30/2020 8:32 PM	File folder	
PrebuiltPipelines	○ R	10/30/2020 8:32 PM	File folder	
Anisotropy.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
concr140.dll	○ R	10/30/2020 8:31 PM	Application exten...	
DDDAAnalysisToolbox.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
DREAM3D.exe	○ R	10/30/2020 8:31 PM	Application	
DREAM3DLicense.txt				
DREAM3DReview.plugin				
EbsdLib.dll				
EMMPM.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
EMMPMLib.dll	○ R	10/30/2020 8:31 PM	Application exten...	
Generic.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
H5Support.dll	○ R	10/30/2020 8:31 PM	Application exten...	
hdf5.dll	○ R	10/30/2020 8:31 PM	Application exten...	
hdf5_cpp.dll	○ R	10/30/2020 8:31 PM	Application exten...	
HEDMAssessment.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
ImportExport.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
ITKCommon-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKImageProcessing.plugin	○ R	10/30/2020 8:31 PM	PLUGIN File	
ITKIOBioRad-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOBMP-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOGE-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOIPL-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOImageBase-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOIPL-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOJPEG-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOMeta-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIMRC-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIONIFTI-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIONRRD-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOPNG-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOStimulate-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	
ITKIOVTK-4.13.dll	○ R	10/30/2020 8:31 PM	Application exten...	

Run DREAM3D.exe

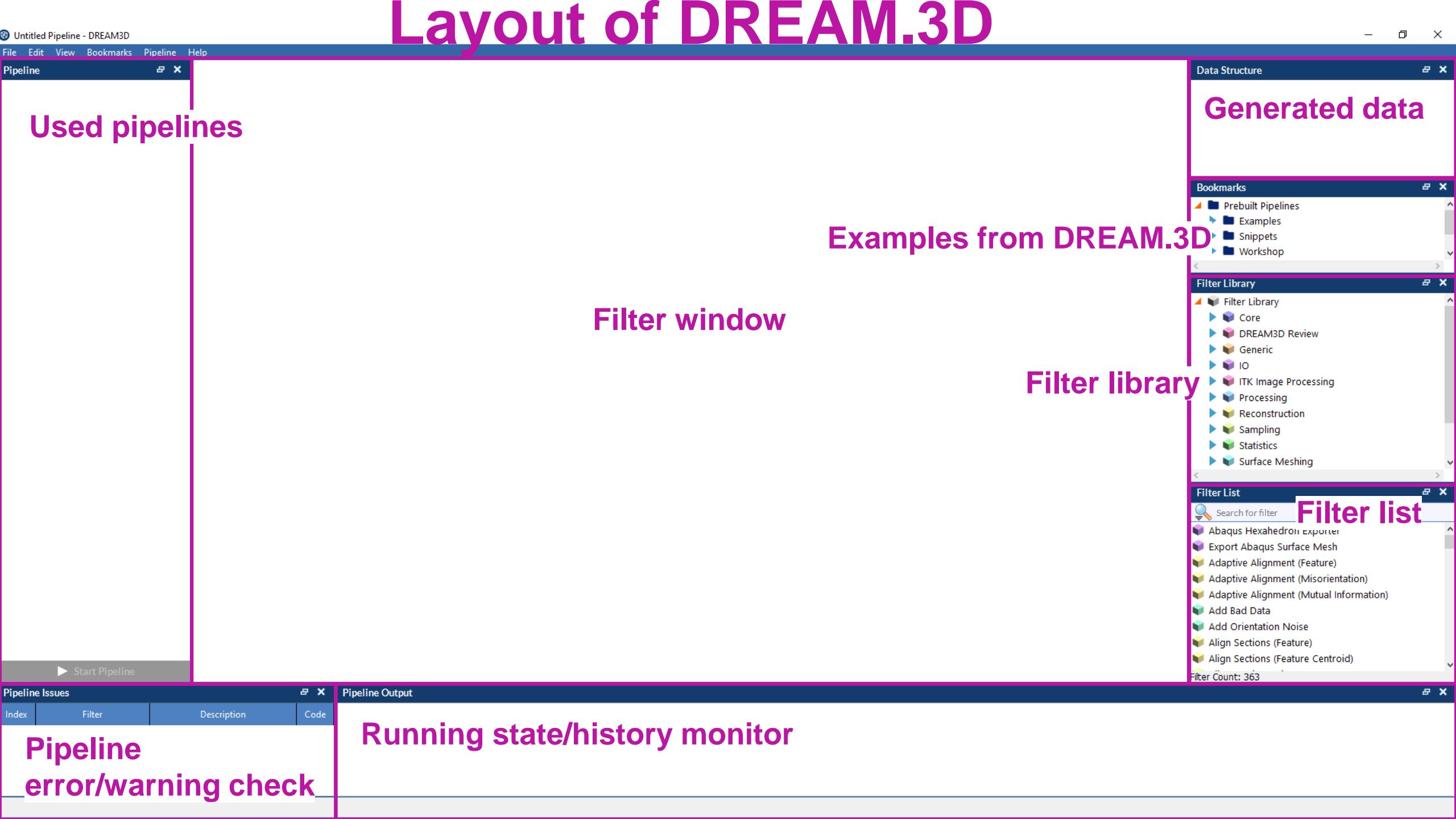
If you download the exe version, you need to install it first.
If you download the zip version, directly run the application.

DREAM.3D & ParaView installation

To run an .exe application in windows system



Basic DREAM.3D operation (Equiaxed single phase)



Used pipelines

Examples from DREAM.3D

Filter window

Filter library

Filter list

Pipeline
error/warning check

Running state/history monitor

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

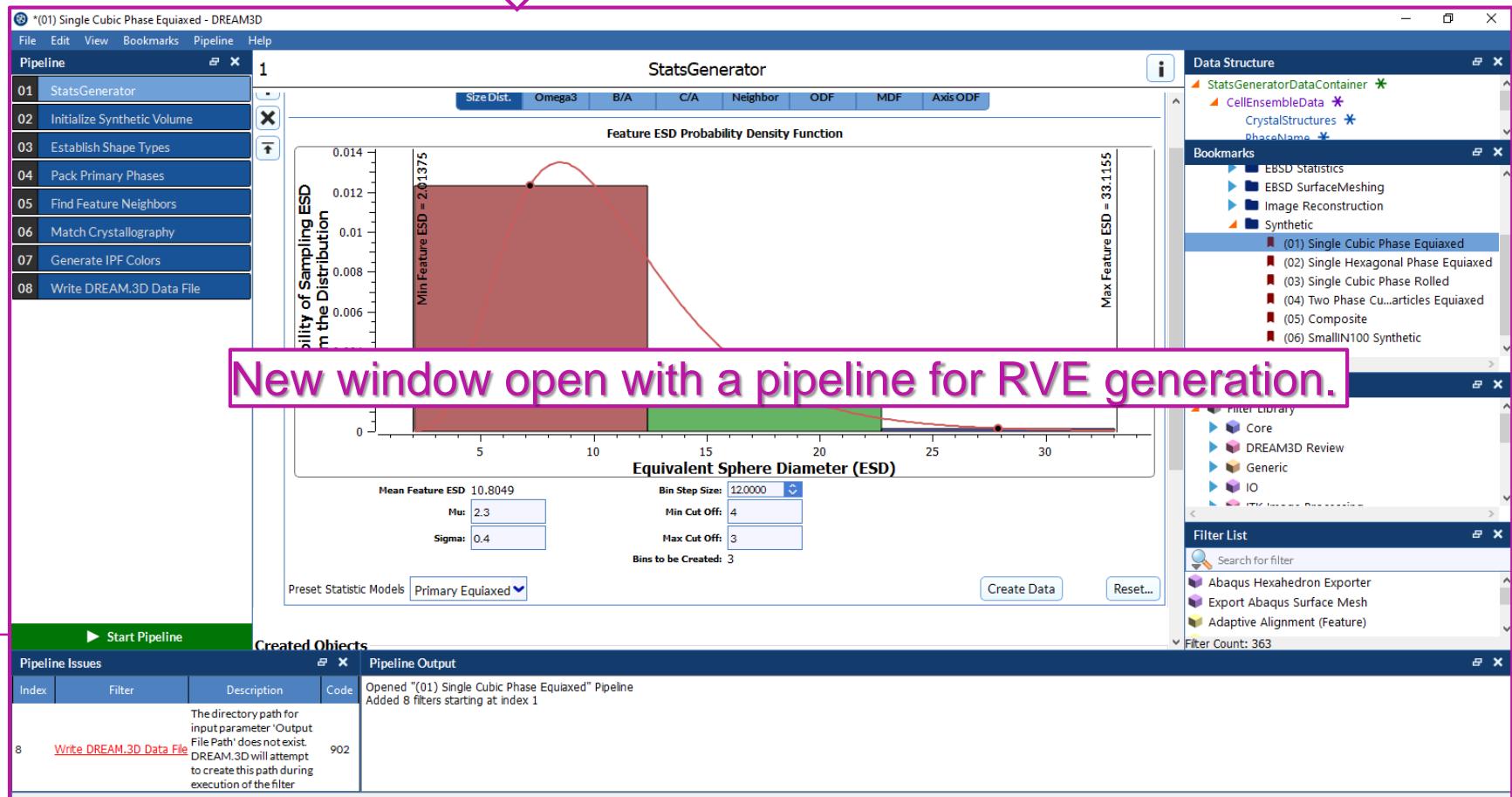
Filter List

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

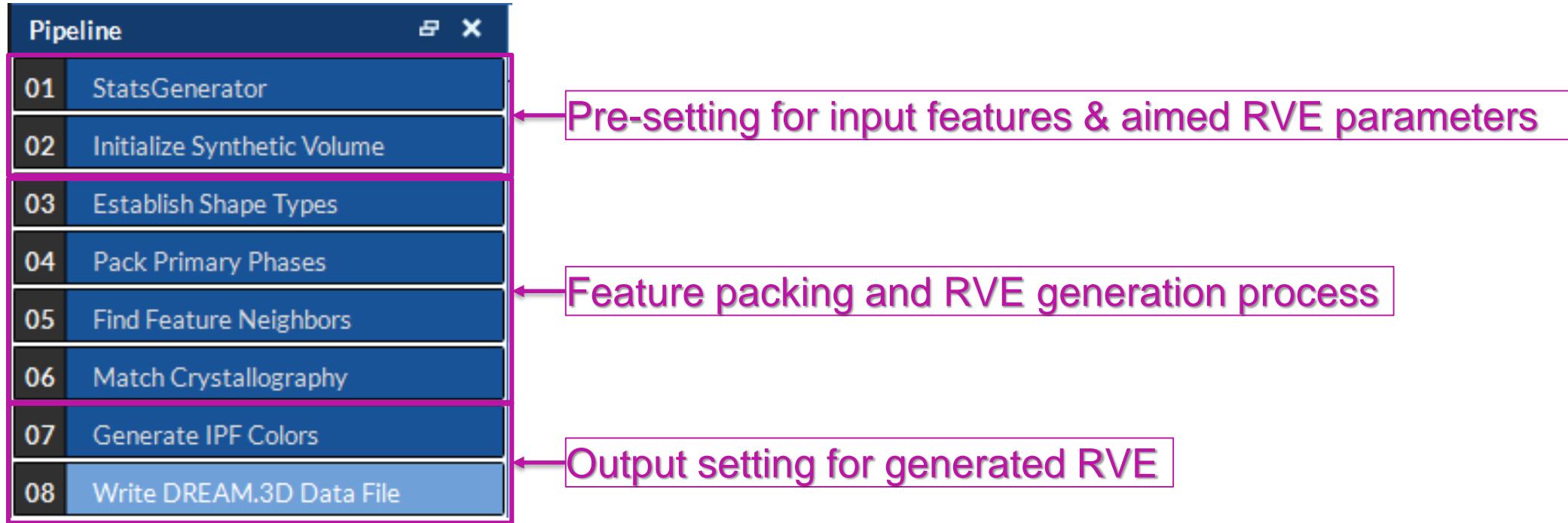
Filter Count: 363

Bookmarks-Prebuilt pipelines: Examples from DREAM.3D

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



DREAM.3D pipelines



StatsGenerator Layout



1

single phase tab

StatsGenerator

Parameters



Primary



grain shape



Size Dist.

Omega3

B/A

C/A

Neighbor

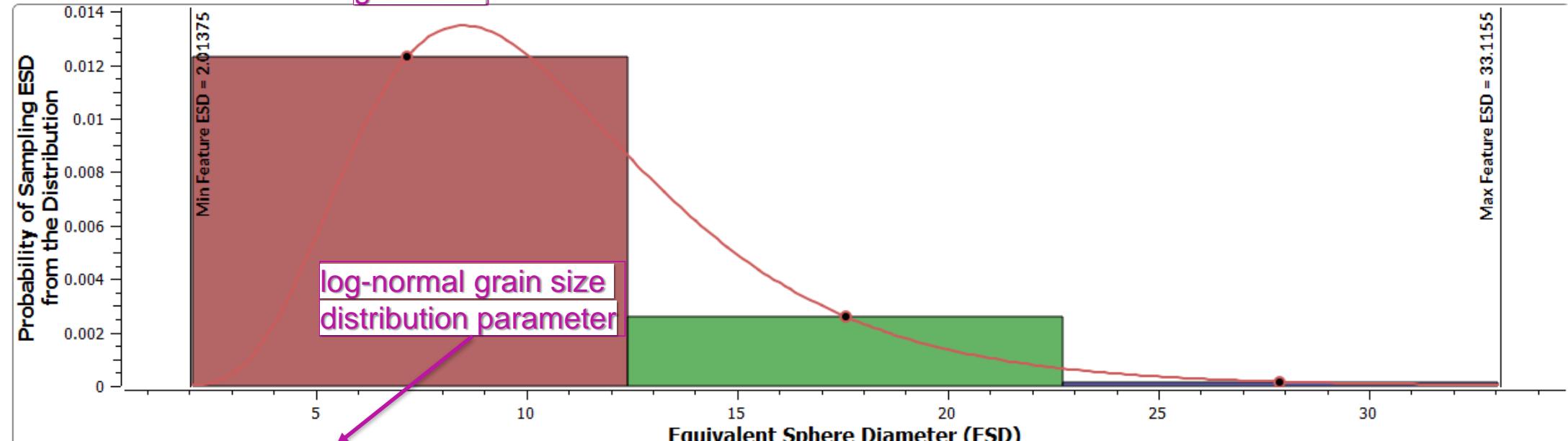
ODF

MDF

Axis ODF

grain orientation
and misorientationwebsite
documentation

Feature ESD Probability Density Function



general/pre control for grain shape

Mean Feature ESD 10.8049

Mu: 2.3
Sigma: 0.4Bin 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

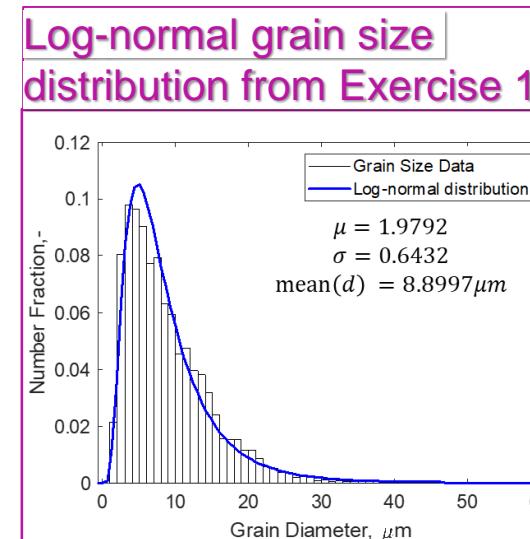
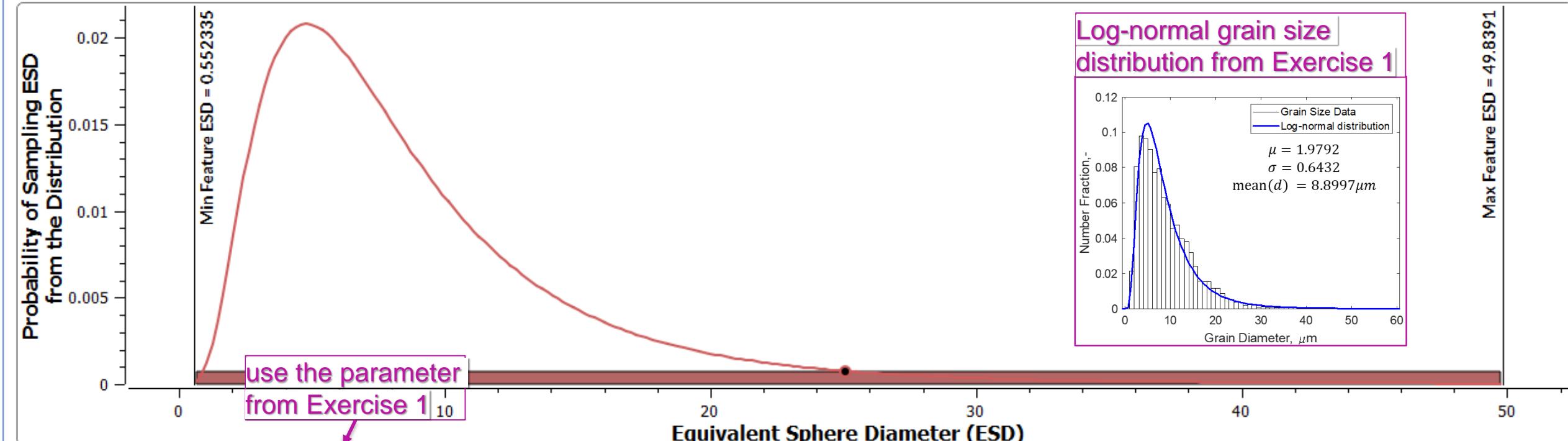
Cell Ensemble Attribute Matrix Name CellEnsembleData

the data structure generated in this filter

create grain data with the input parameters

22

Feature ESD Probability Density Function



Max Feature ESD = 49.8391

Mean Feature ESD 8.90002

Mu: 1.9792

Sigma: 0.6432

Bin Step Size: 50.0000

Min Cut Off: 4

Max Cut Off: 3

Bins to be Created: 1

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

Preset Statistic Models Primary Equiaxed

Create Data

Reset...

general/pre control for grain shape

1. first shape type: 1:1:1

create grain data with
the input parameters

Step2 Initialize Synthetic Volume

2

Initialize Synthetic Volume

i

Parameters

Estimate Number of Features
Estimated Primary Features 811

Dimensions 100 100 100

Resolution 1 1 1

Origin 0 0 0

X Range: 0 to 100 (Delta: 100)
Y Range: 0 to 100 (Delta: 100)
Z Range: 0 to 100 (Delta: 100)

Estimated grain number

Number of elements on each dimension

Size of elements on each dimension, the unit is consistent with the grain size distribution, e.g. μm .

Origin point of RVE

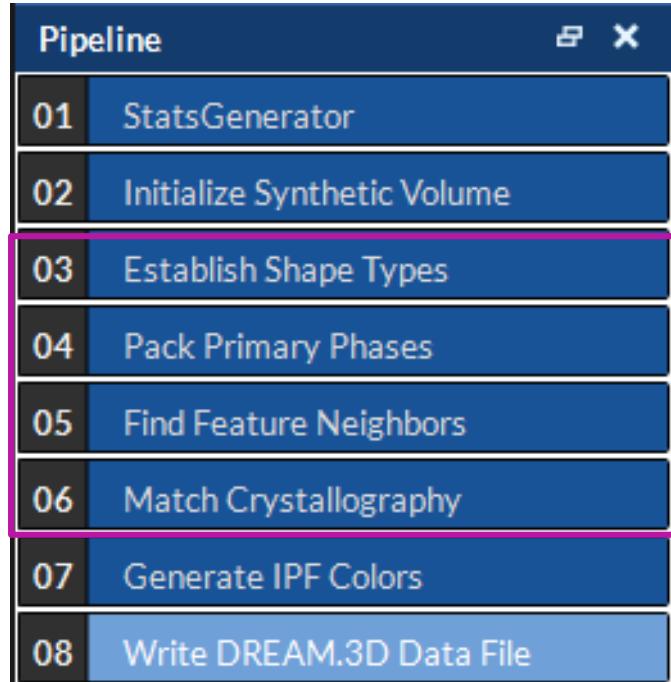
Required Objects

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



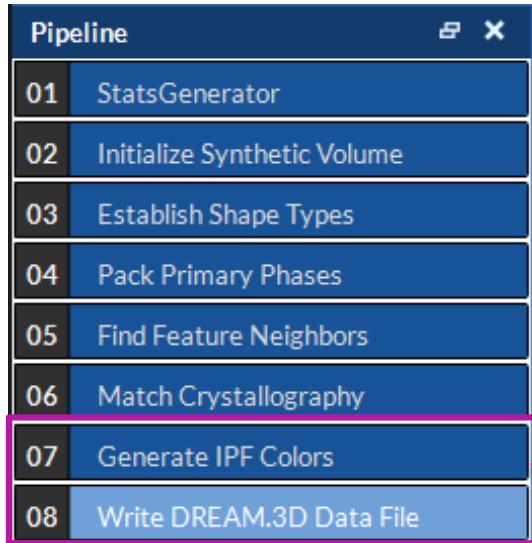
Feature packing and RVE generation process:

- 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://127.0.0.1:32456/2_Tutorials/SyntheticSinglePhase/

Step3 Generation process:

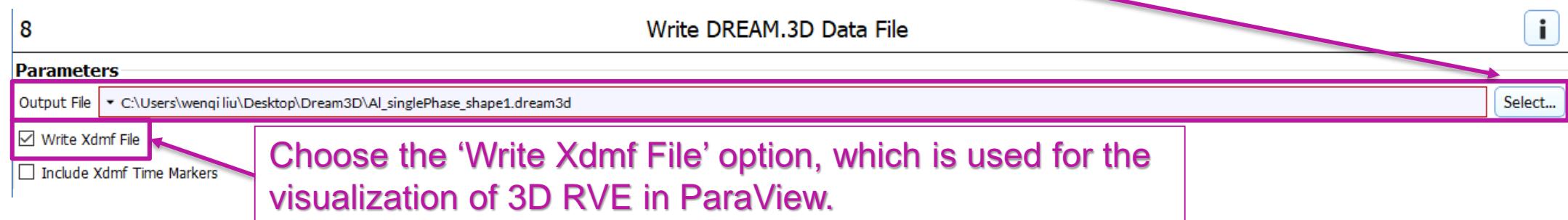
for these filters, directly use the default setting without any changes, but you need to click and review one by one and solve the probable error/missing data structure, which is shown in the 'Pipeline Issues'.

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



► Start Pipeline

Step5: Click to run the generator

*(01) Single Cubic Phase Equiaxed - DREAM3D

File Edit View Bookmarks Pipeline Help

Pipeline

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

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

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

27

DREAM.3D - Data files

```
Pipeline Output
Swapping/Switching Orientations Iteration 52450/100000 || Est. Time Remain: 00:00:05 || Iterations/Sec: 15094.7
Swapping/Switching Orientations Iteration 65285/100000 || Est. Time Remain: 00:00:02 || Iterations/Sec: 13044
Swapping/Switching Orientations Iteration 77481/100000 || Est. Time Remain: 00:00:01 || Iterations/Sec: 12900.6
Swapping/Switching Orientations Iteration 90617/100000 || Est. Time Remain: 00:00:00 || Iterations/Sec: 12932.4
[7/8] Generate IPF Colors
[8/8] Write DREAM.3D Data File
Pipeline Complete
***** PIPELINE FINISHED *****
```

Running state/history monitor

Successfully finished

- Check your DREAM.3D output folder:
- '.dream3d' DREAM.3D type data
 - '.xdmf' type file for ParaView

Name	Date modified	Type	Size
Dream3D_RVE		File folder	
DREAM3D-6.5.141-Win64		File folder	
AI_singlePhase_shape1.dream3d		DREAM3D File	22,855 KB
AI_singlePhase_shape1.xdmf		XDMF File	2 KB
RVE_Dream3d.pptx		Microsoft PowerP...	7,690 KB

ParaView operation

ParaView 5.6.0 64-bit

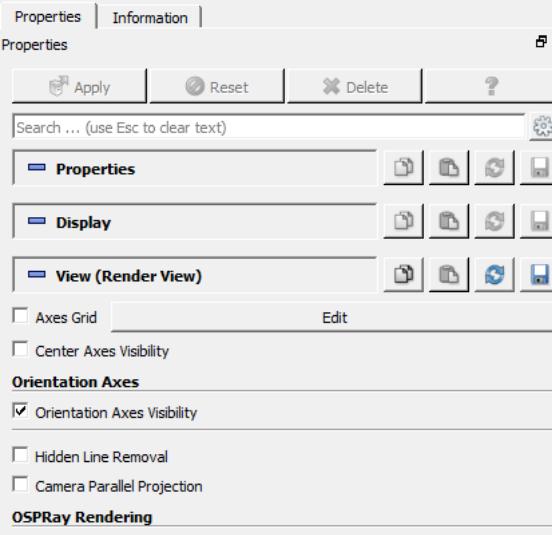
File Edit View Sources Filters Tools Catalyst Macros Help



Pipeline Browser

builtin:

data structure

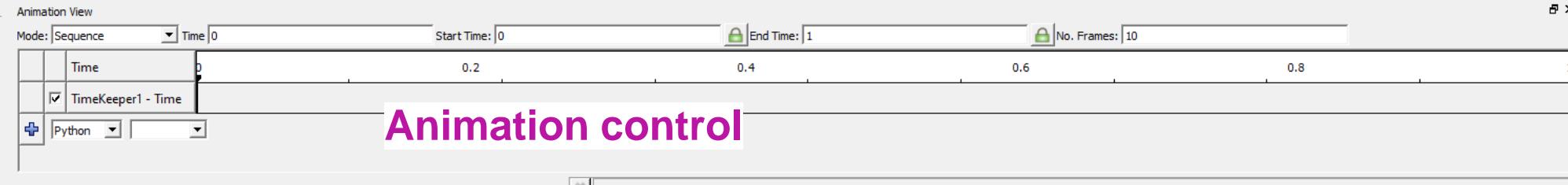


display control

Layout of ParaView

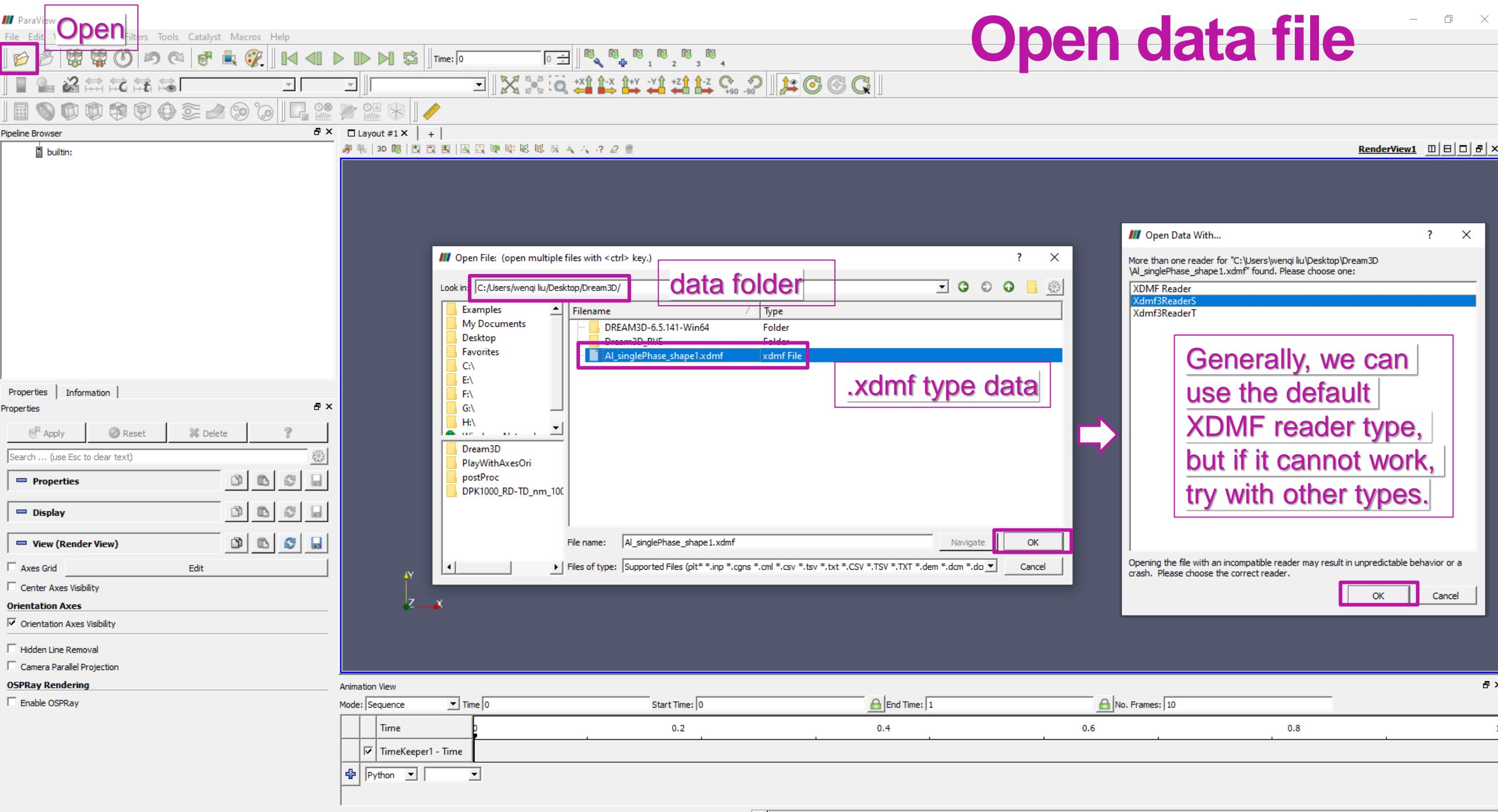
control panel

display of your 3D data/structure

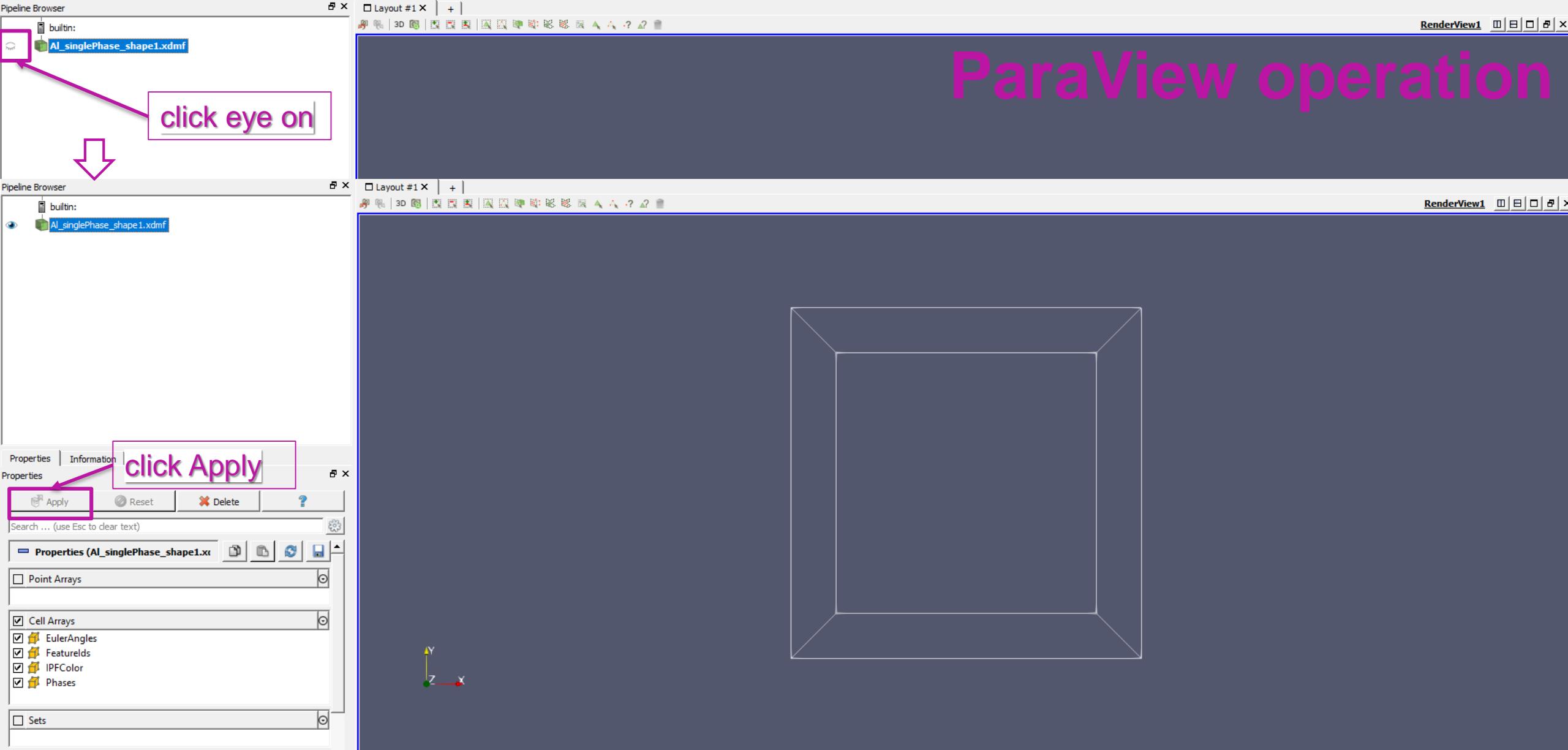


Animation control

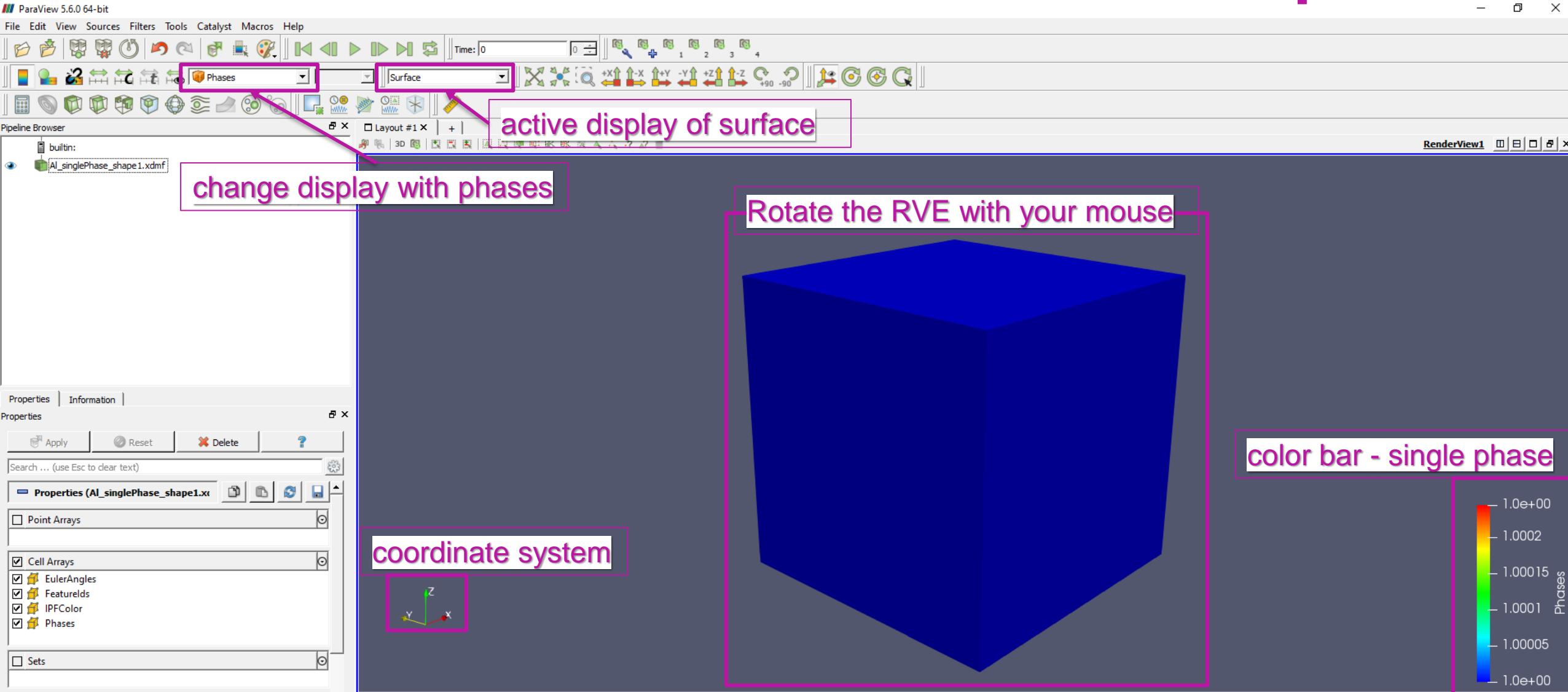
Open data file



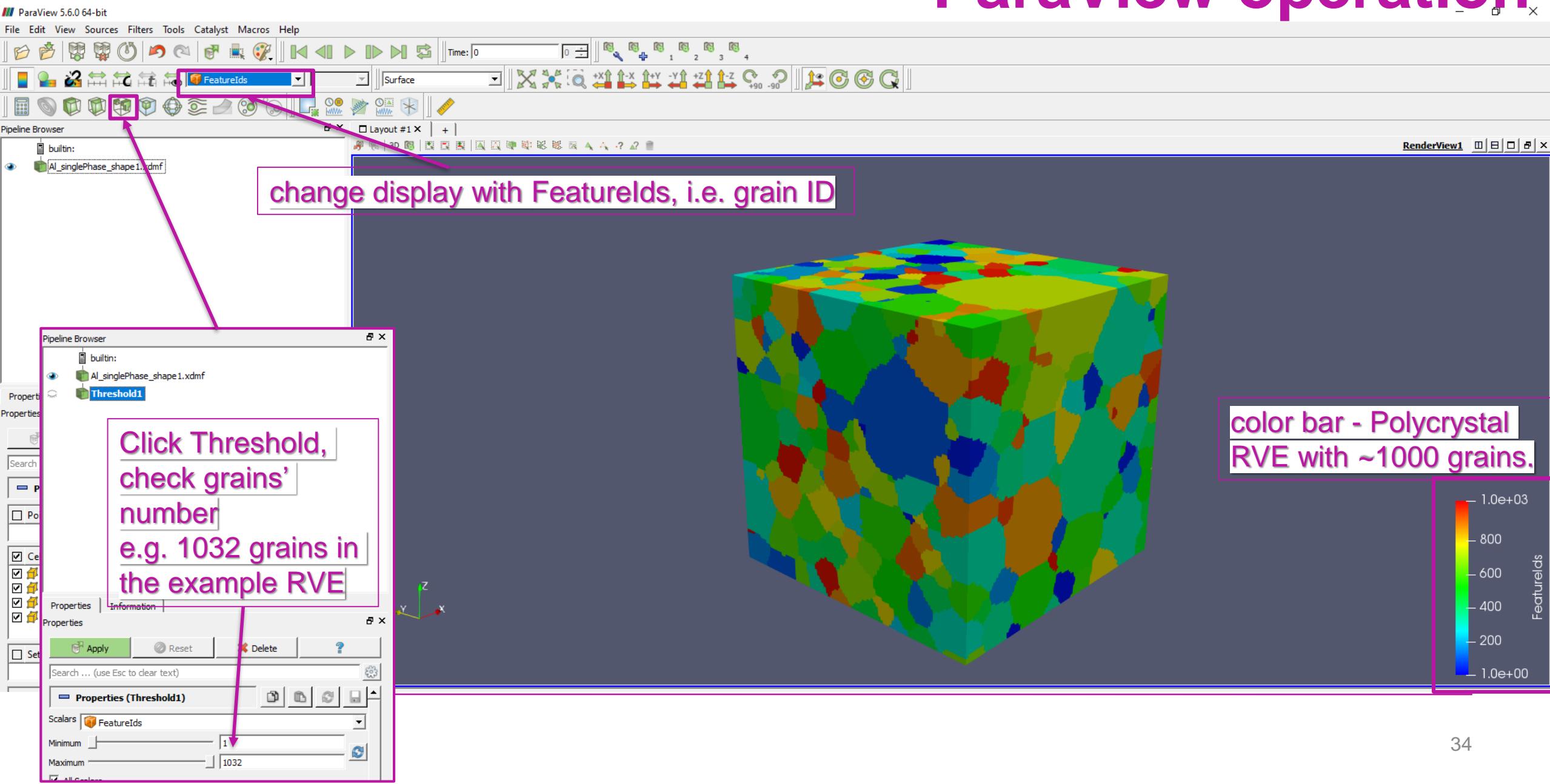
ParaView operation



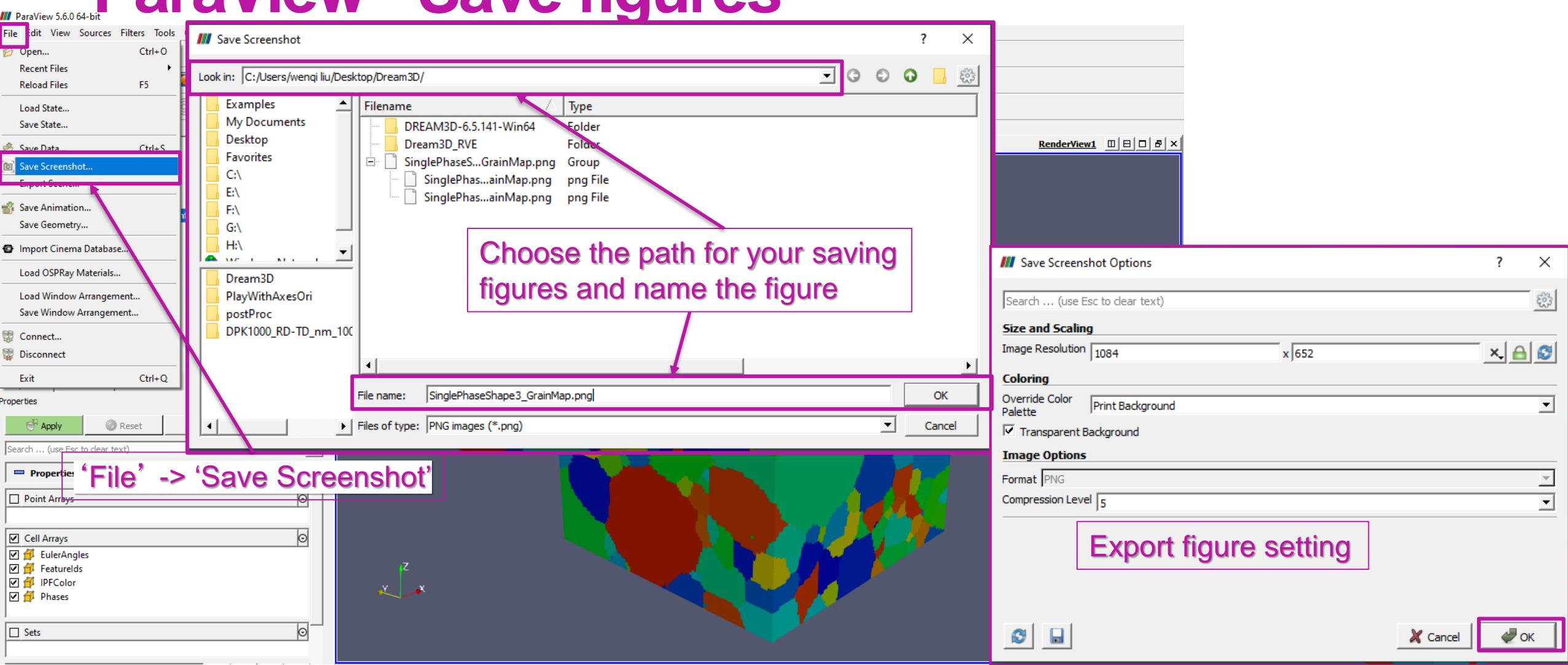
ParaView operation



ParaView operation



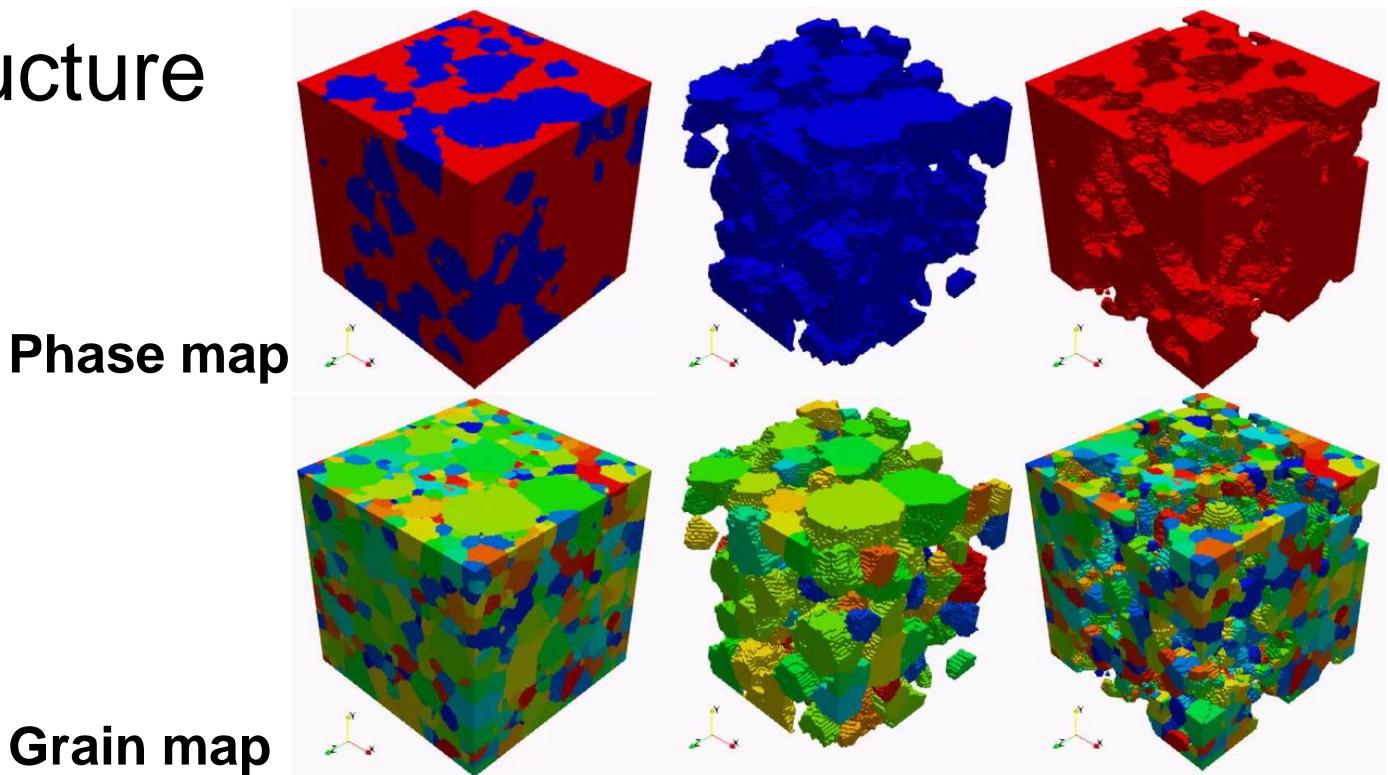
ParaView - Save figures



Advanced DREAM.3D operation

DREAM.3D For more features

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



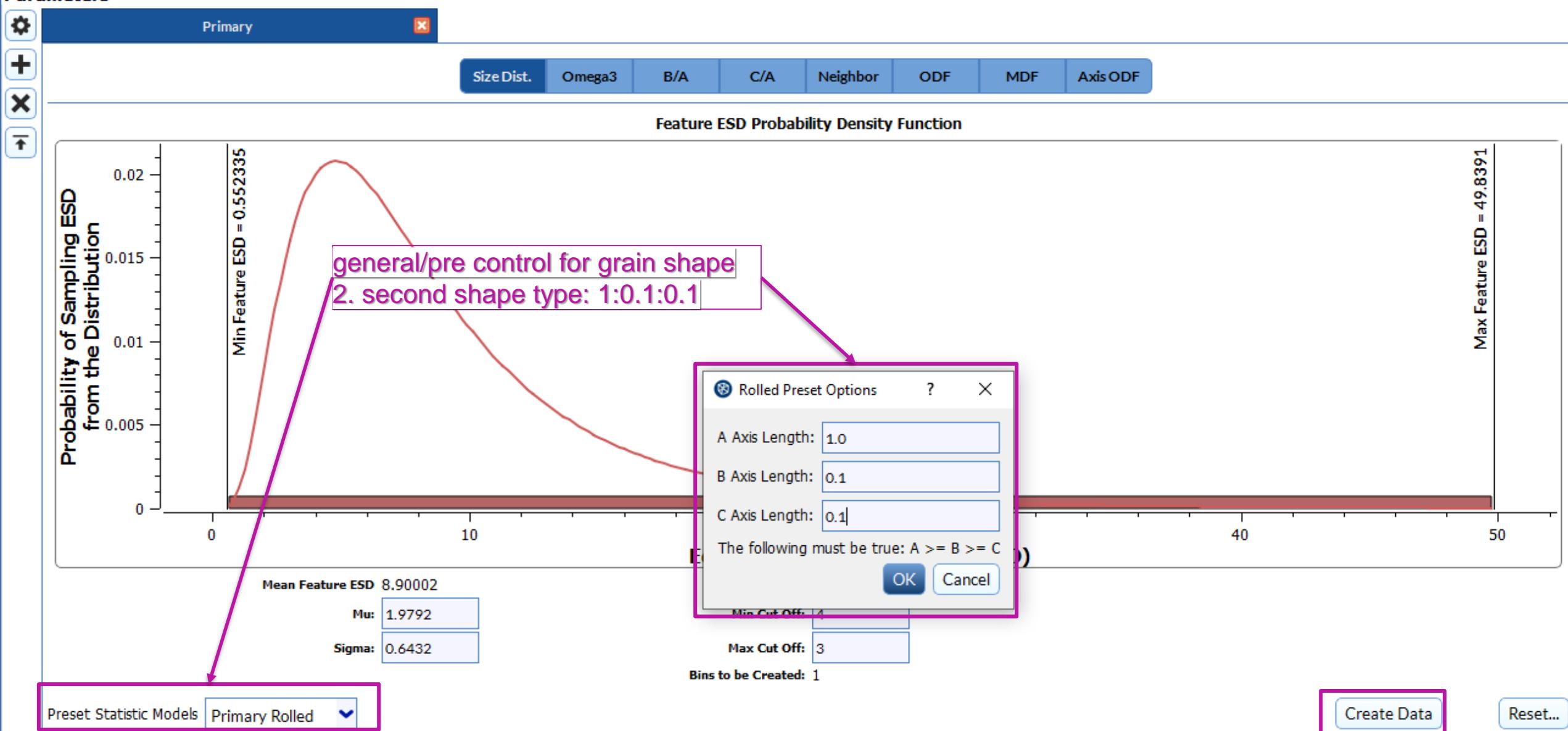
DREAM.3D - Rolled grain structure

1

StatsGenerator

i

Parameters



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

Write Xdmf File

Include Xdmf Time Markers

Parameters

Output File C:\Users\wenqi.liu\Desktop\Dream3D\AI_singlePhase_shape2.dream3d Select...

Change output filename to avoid overwrite

Start running

► Start Pipeline

Open new RVE in ParaView

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

File name: AI_singlePhase_shape2.xdmf

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

OK Cancel

A

extremely elongated/rolled grains

1.1e+03
800
600
400
200
1.0e+00

Features

39

DREAM.3D - Grain shape distribution

1

StatsGenerator

i

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

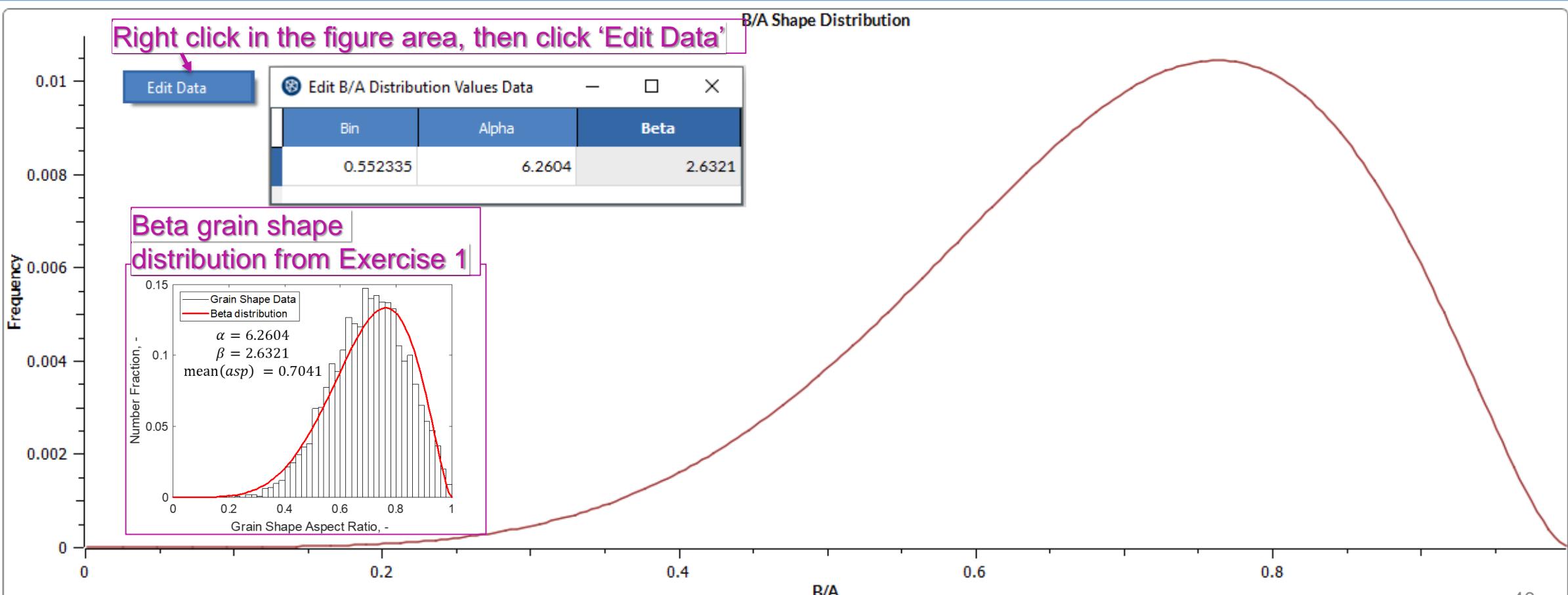
MDF

Axis ODF

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

Edit Data

Bin	Alpha	Beta
0.552335	6.2604	2.6321



Preset Statistic Models

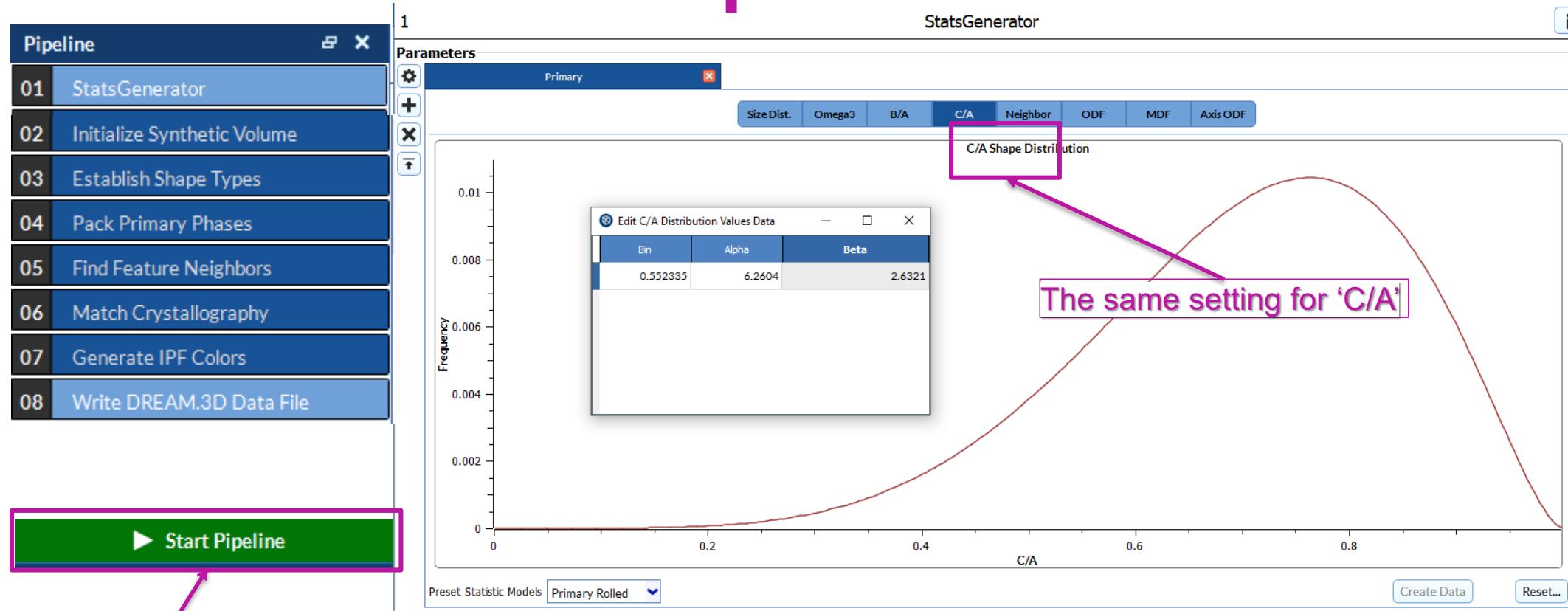
Primary Rolled

Create Data

Reset...

40

DREAM.3D - Grain shape distribution



8

Write DREAM.3D Data File

Parameters

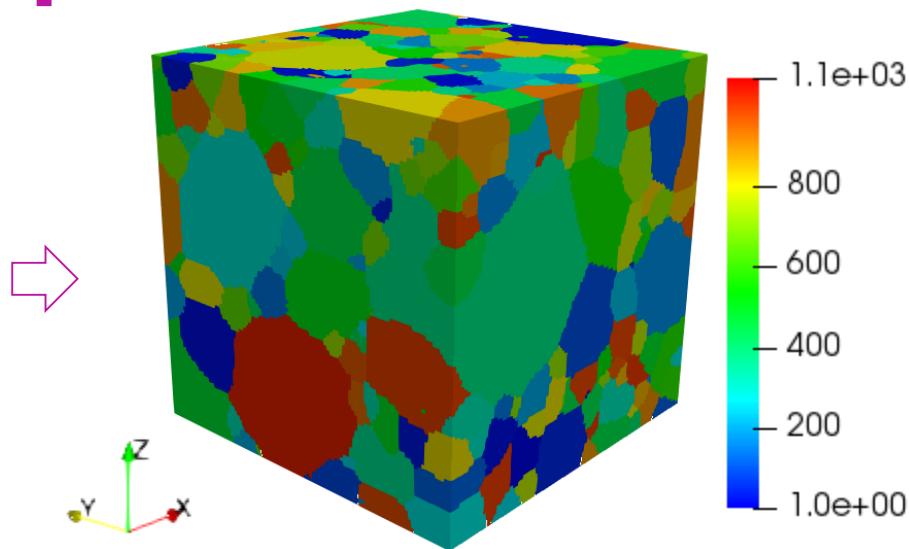
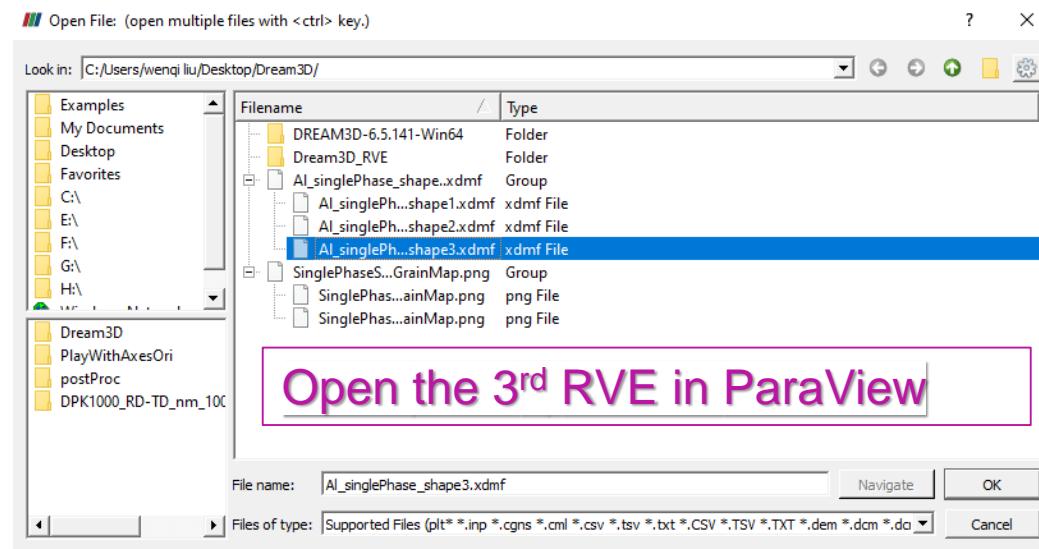
Output File C:\Users\wenqi liu\Desktop\Dream3D\AI_singlePhase_shape3.dream3d Select...

Write Xdmf File

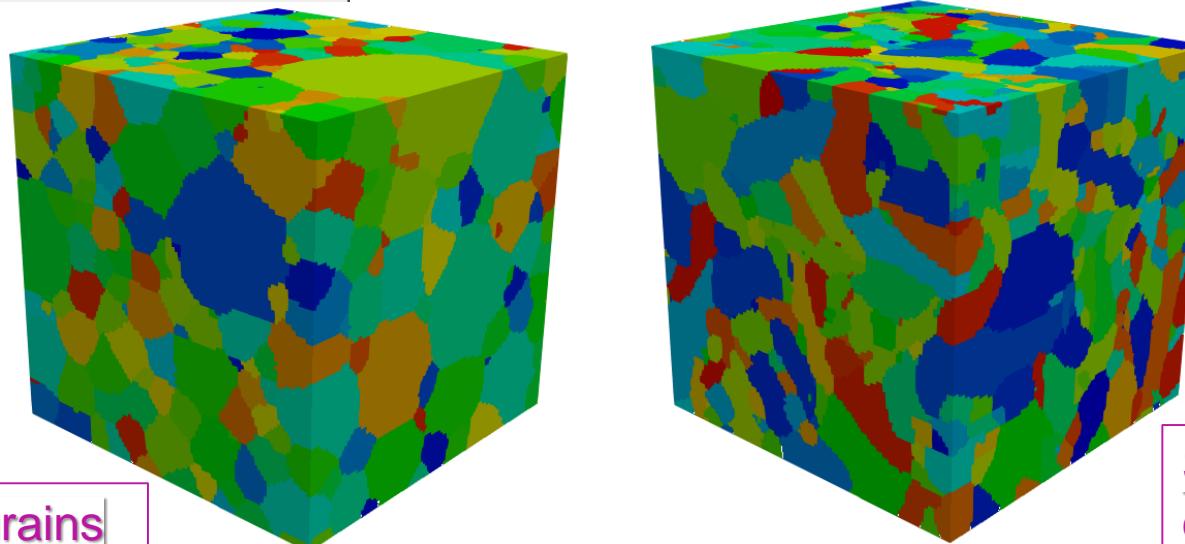
Include Xdmf Time Markers

Change output filename to avoid overwrite

DREAM.3D - Grain shape distribution



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



Shape 1: Equiaxed grains

**Shape 2: Extremely
elongated/rolled grains**

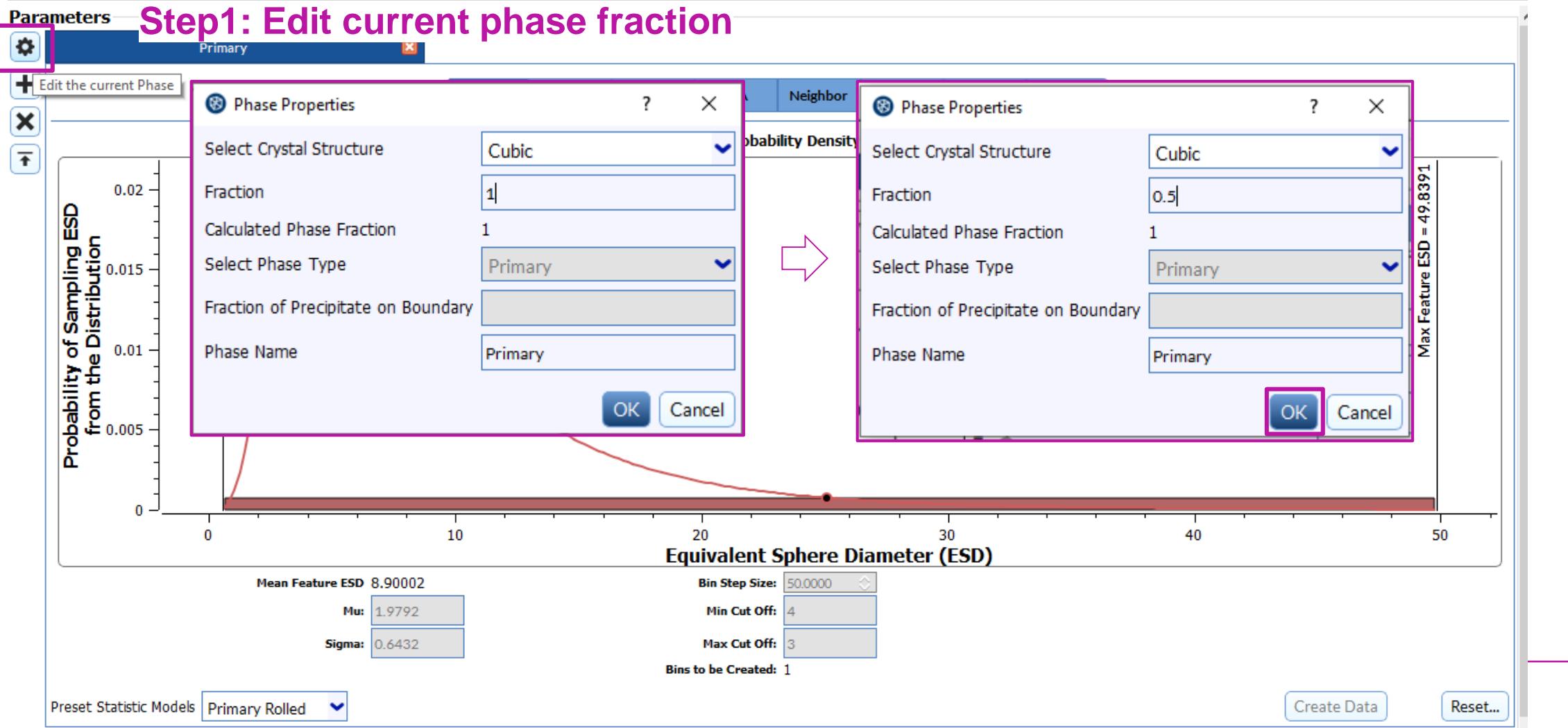
DREAM.3D - Dual-phase structure

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

1

StatsGenerator

i



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

Step2: Add the second primary phase with 50% fraction

Primary

Phase Properties



Cubic

0.5

0.5

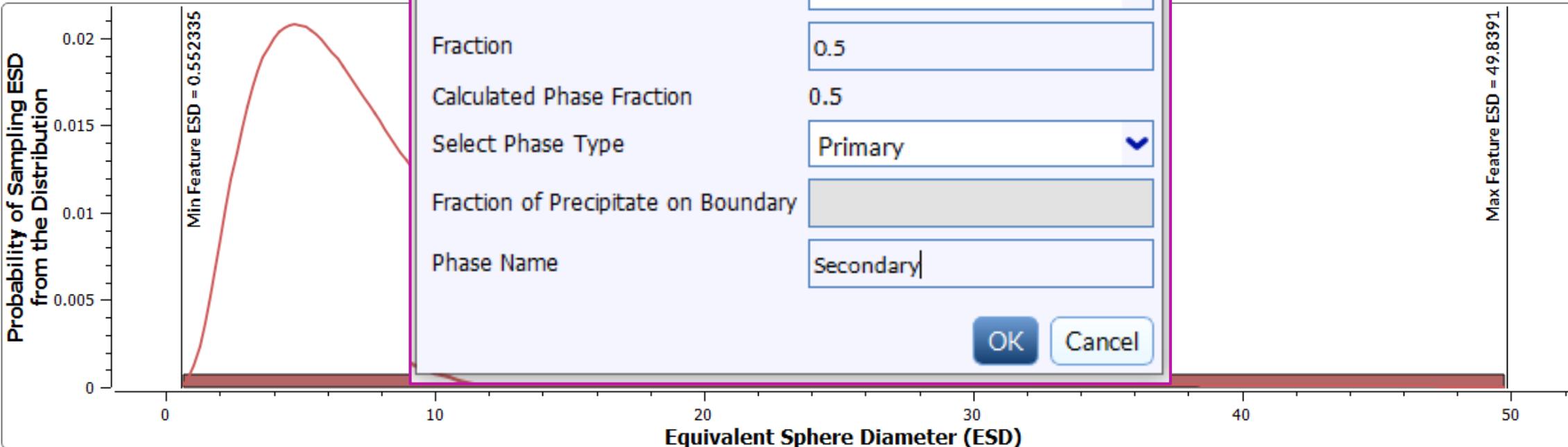
Primary



Secondary

OK

Cancel



Mean Feature ESD 8.90002

Mu: 1.9792

Sigma: 0.6432

Bin Step Size: 50.0000

Min Cut Off: 4

Max Cut Off: 3

Bins to be Created: 1

Preset Statistic Models

Primary Rolled

Create Data

Reset...

DREAM.3D - Dual-phase structure

1

StatsGenerator

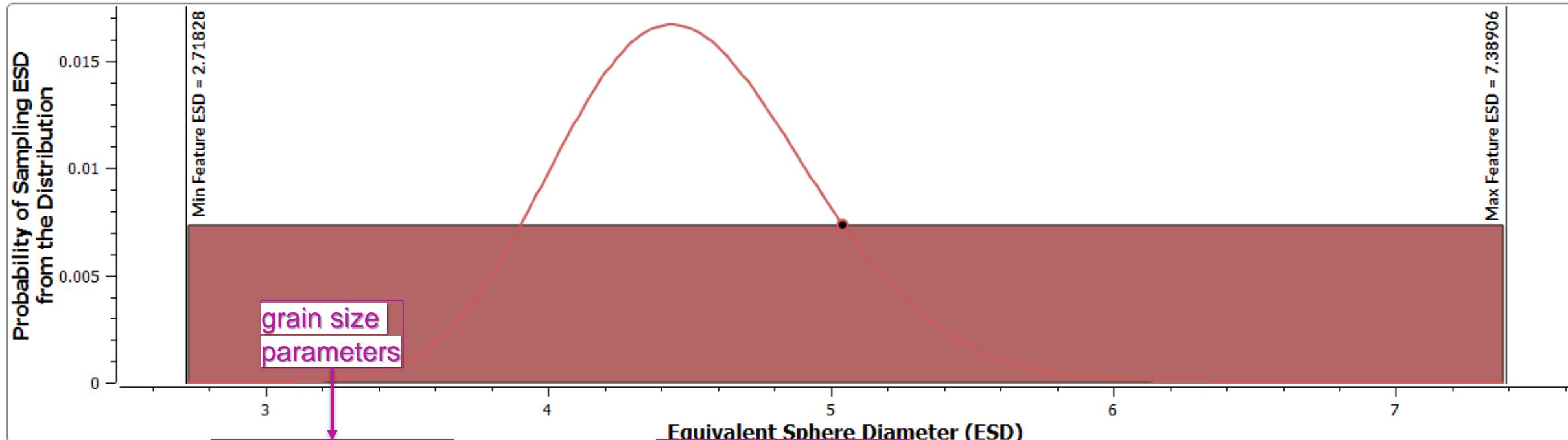
i

Parameters

Primary Secondary

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

Feature ESD Probability Density Function



Equiaxed shape

Preset Statistic Models

Primary Equiaxed

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

create grain data for phase 2

Create Data

45

Reset...

DREAM.3D - Dual-phase structure

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

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

Step4: Check every filter to solve errors/warnings.

Step6: Start running

Cancel Pipeline

Pipeline Issues

Index	Filter	Description	Code

Pipeline Output

```
Swapping/Moving 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

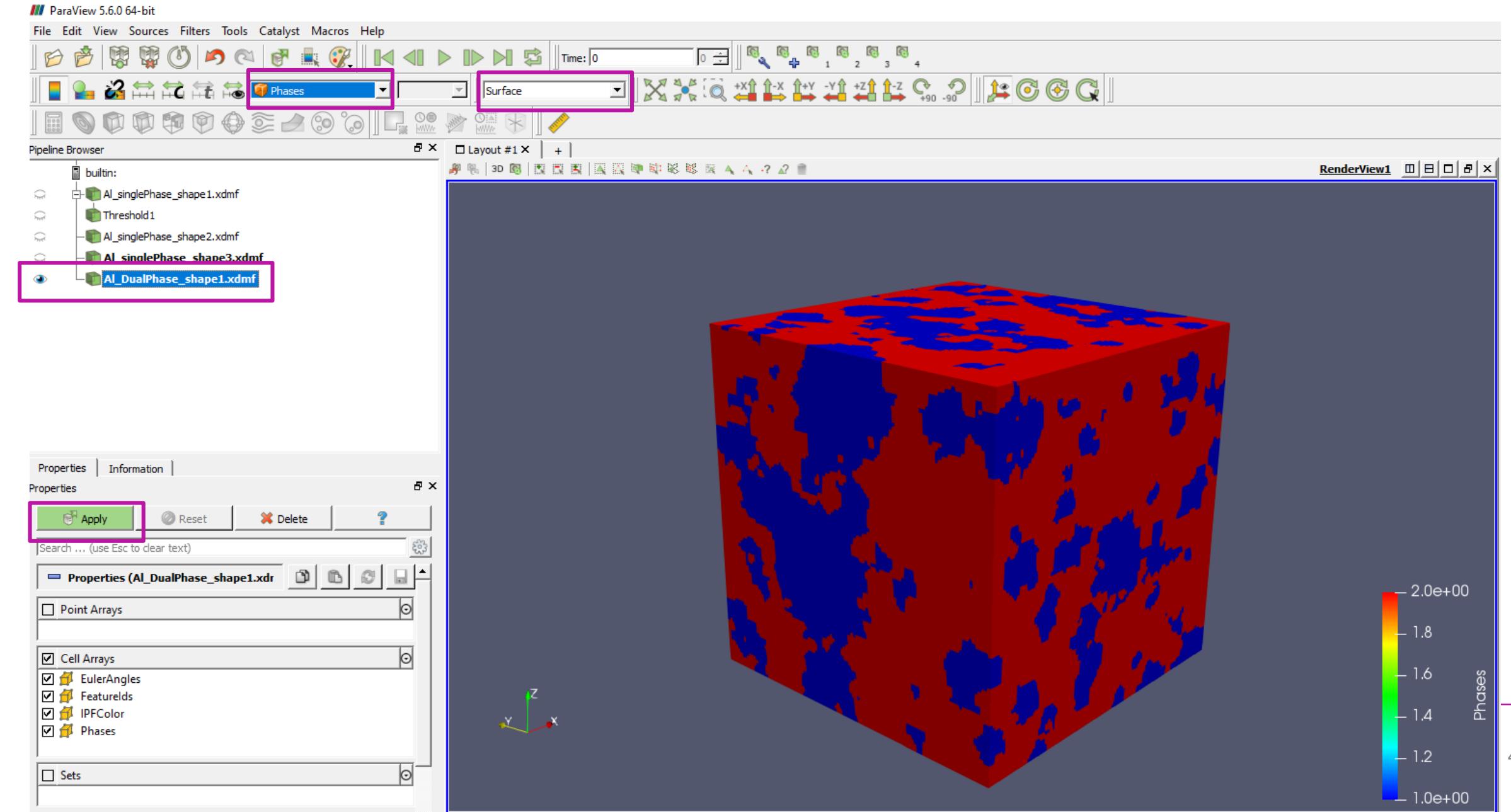
Filter Library

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

Phases

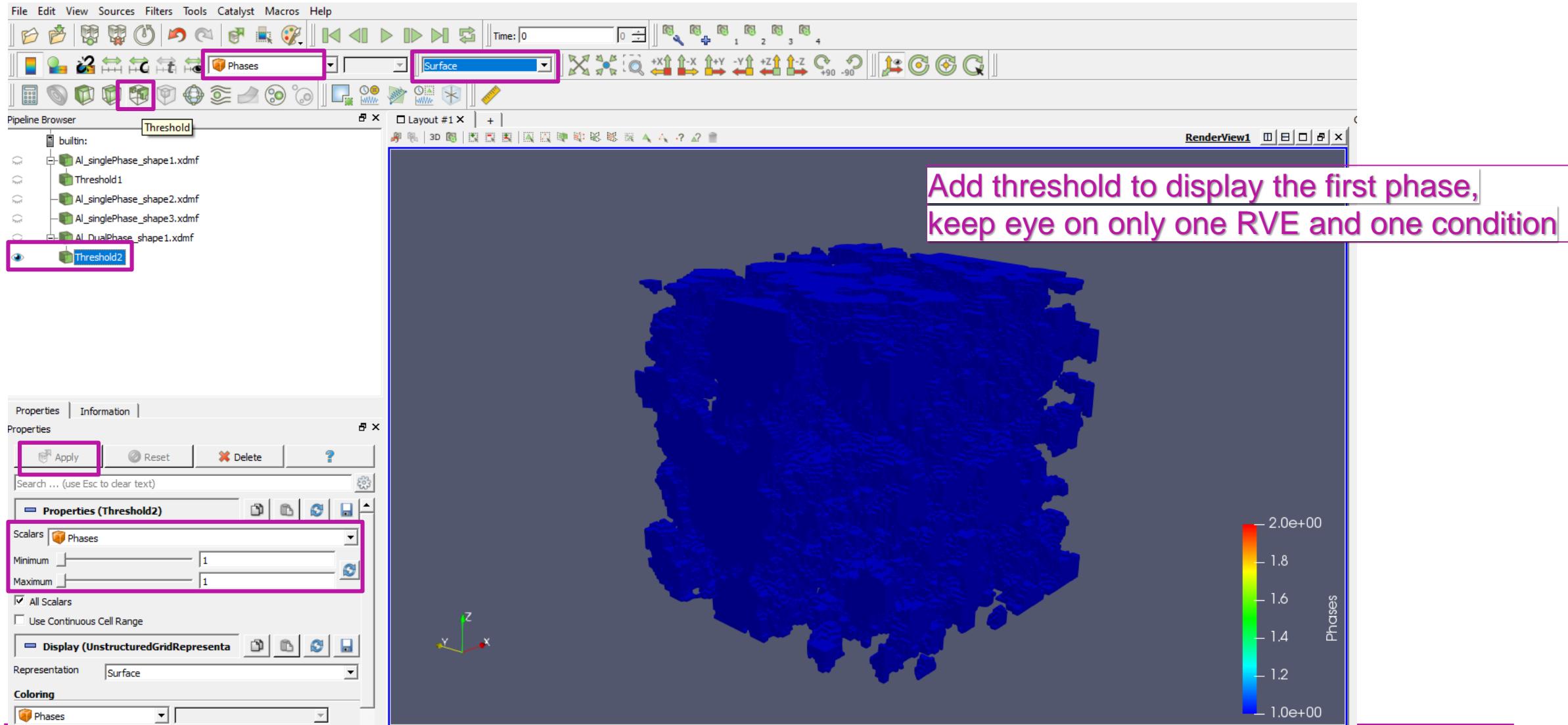
46

ParaView - Dual-phase structure



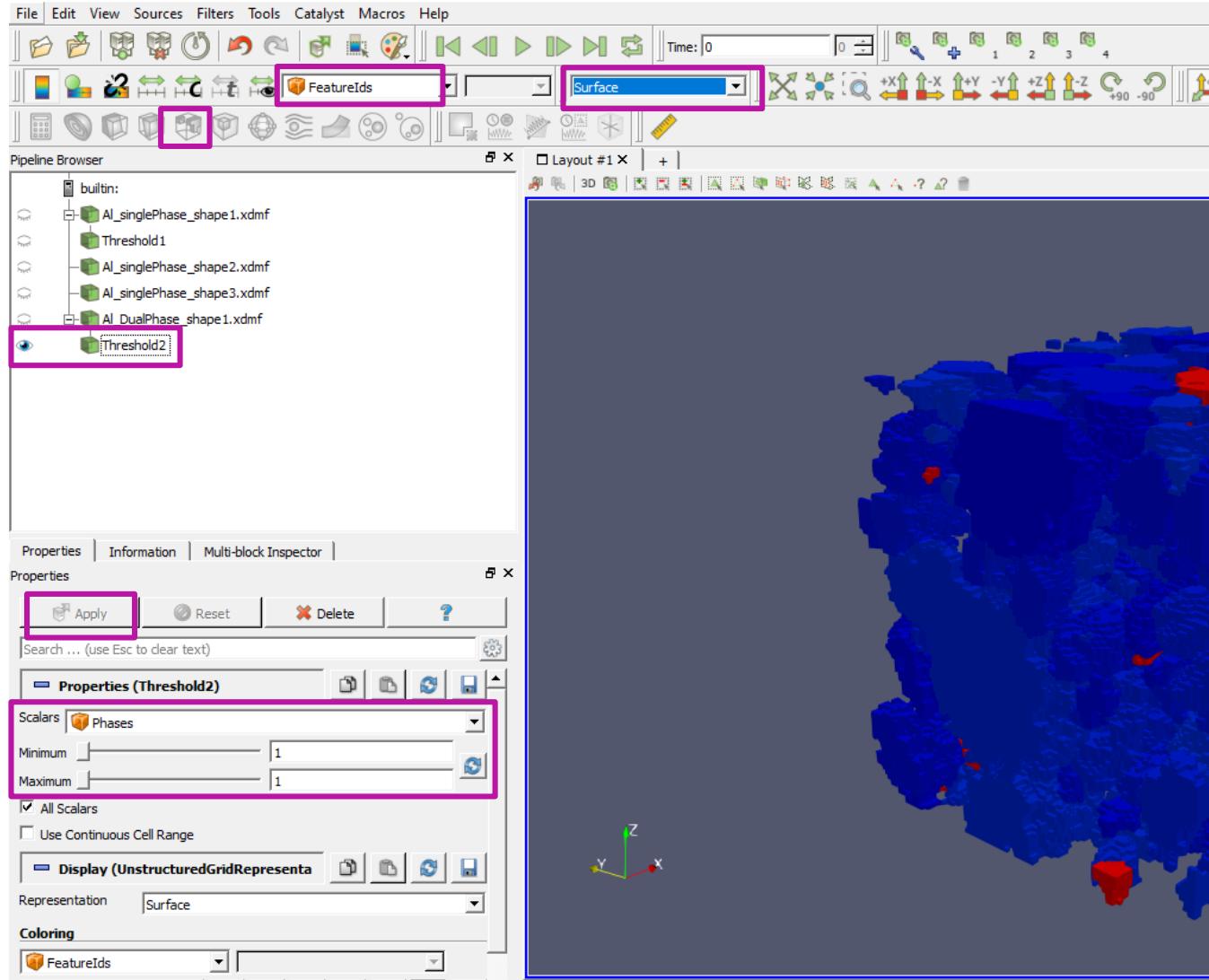
ParaView - Dual-phase structure

ParaView 5.6.0 64-bit



ParaView - Dual-phase structure

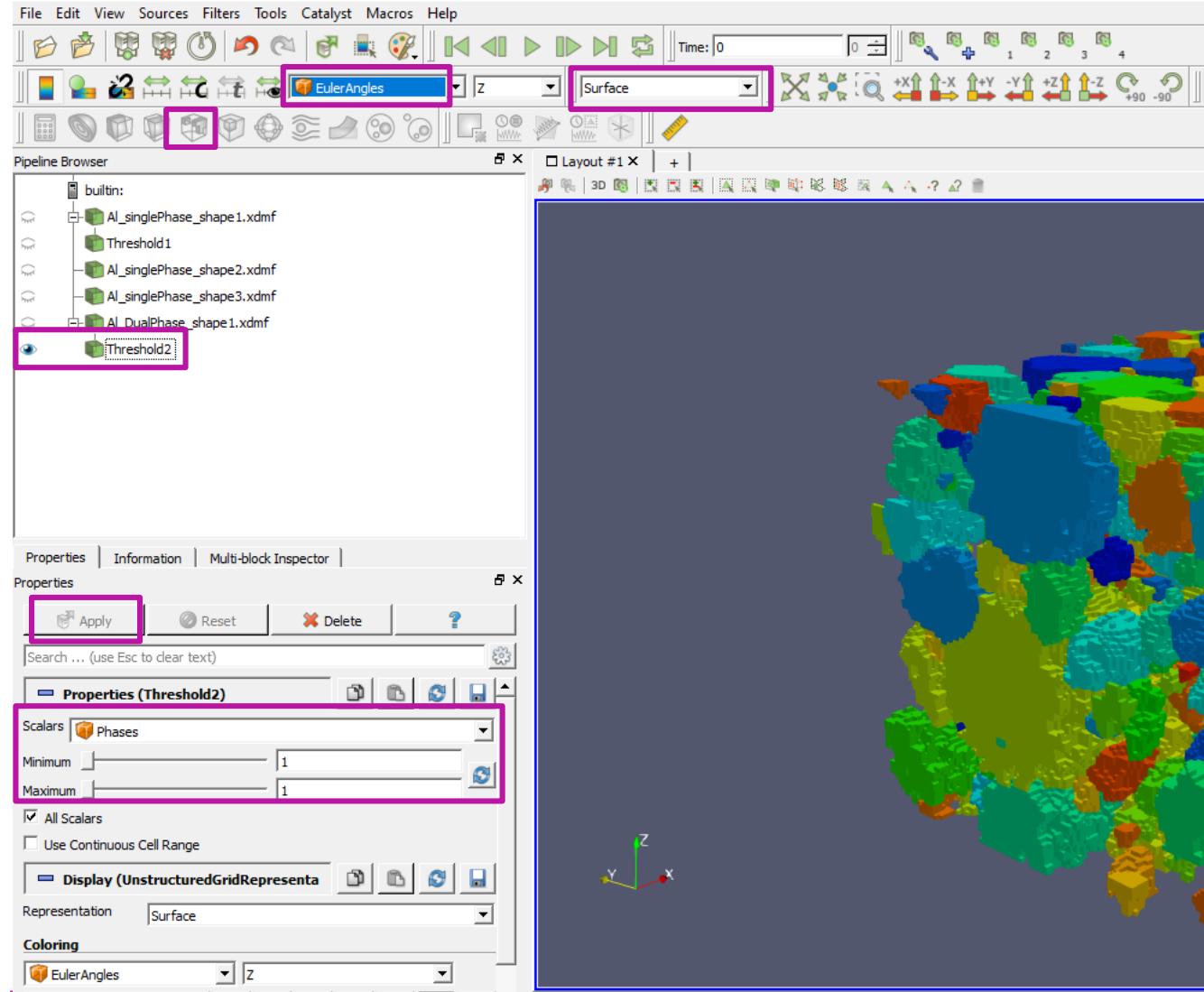
ParaView 5.6.0 64-bit



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

ParaView - Dual-phase structure

ParaView 5.6.0 64-bit

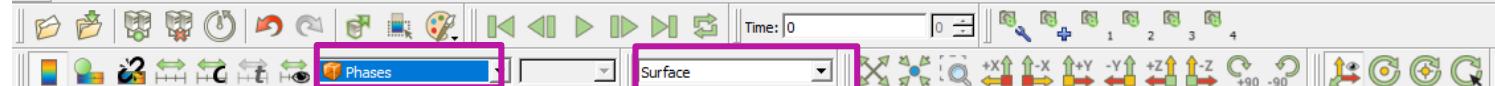


Change to coloring by FeatureIds, i.e. grain ID
but the grain ID is ordered according to phase,
the color code is too closed for grains in one
phase. -> Try to coloring by EulerAngles

ParaView - Dual-phase structure

ParaView 5.6.0 64-bit

File Edit View Sources Filters Tools Catalyst Macros Help



Properties | Information | Multi-block Inspector |

Properties



Search ... (use Esc to clear text)

Properties (Threshold2)

Scalars



Minimum

2

Maximum

2

All Scalars

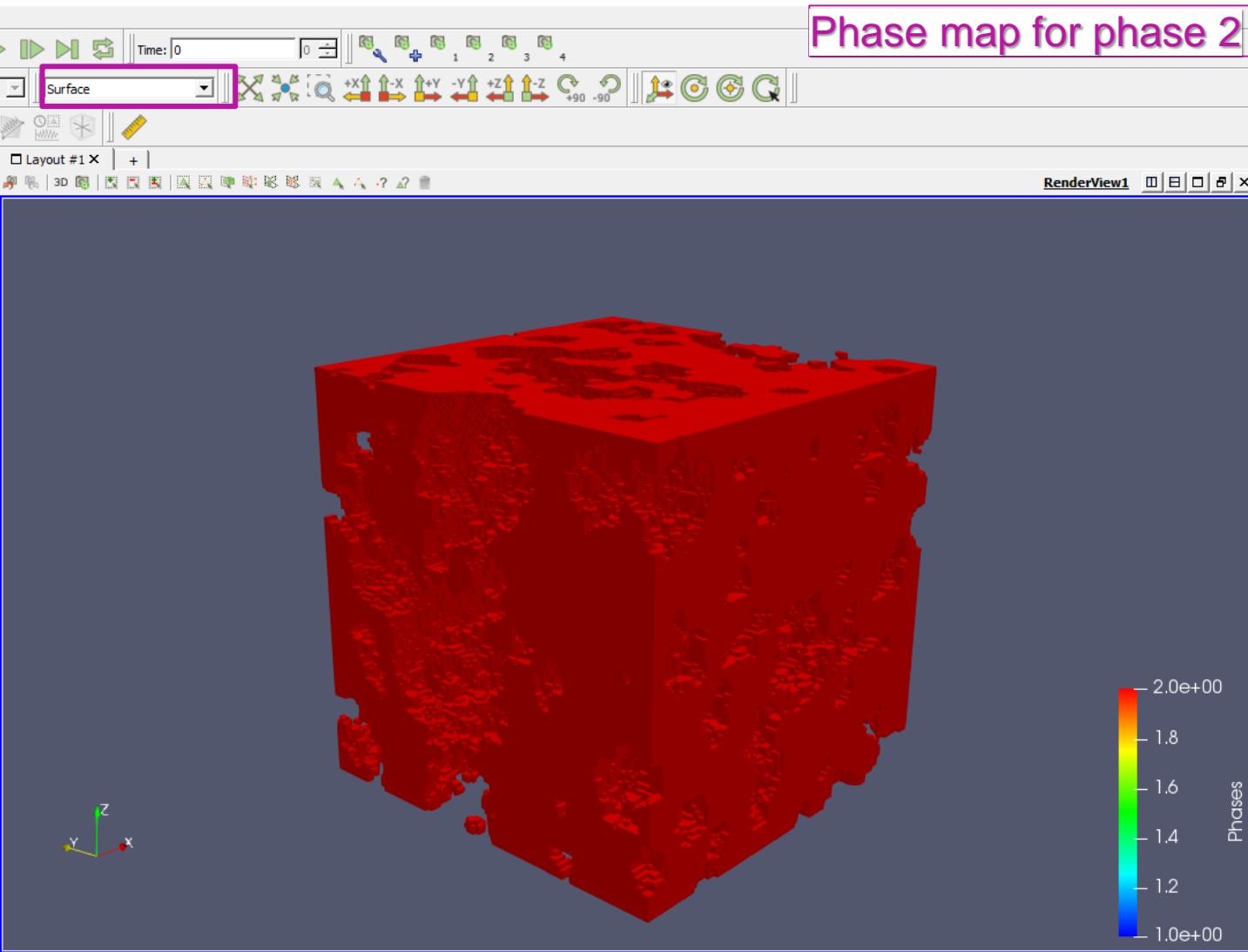
Use Continuous Cell Range

Display (UnstructuredGridRepresen

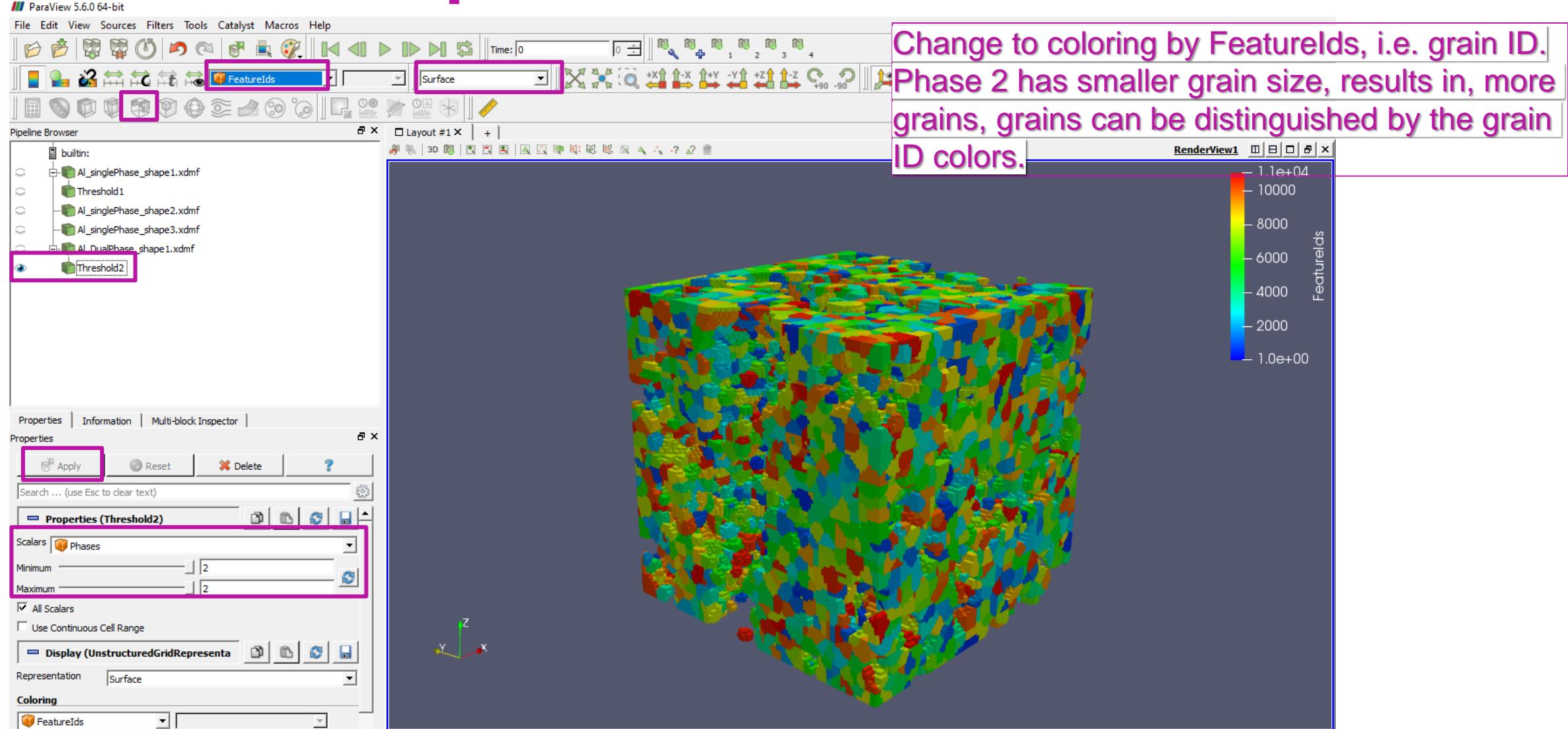


Coloring

Phases



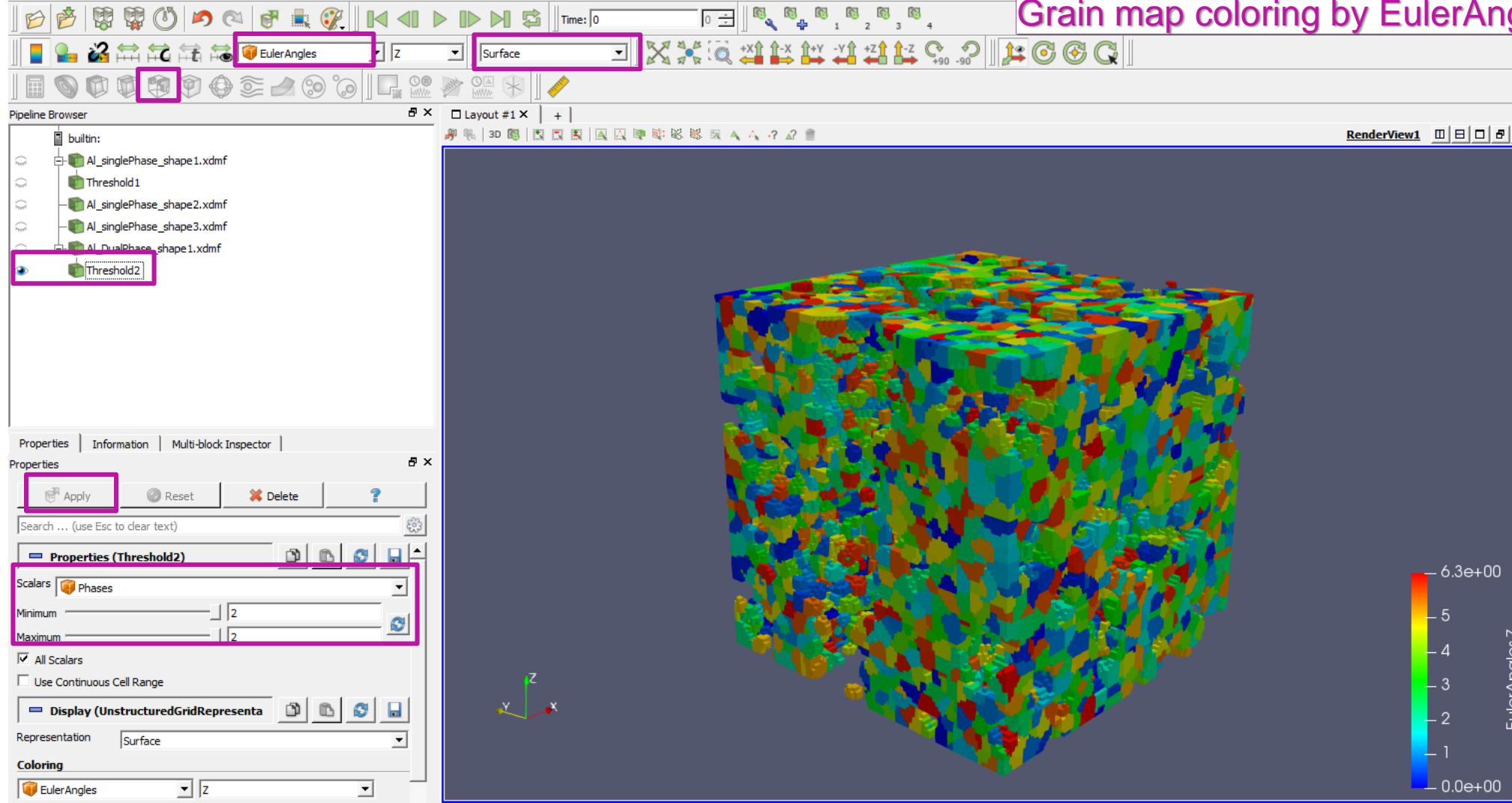
ParaView - Dual-phase structure



ParaView - Dual-phase structure

ParaView 5.6.0 64-bit

File Edit View Sources Filters Tools Catalyst Macros Help



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.