

Instructions for reading the rectilinear grid vtk file in PRISMS-PF

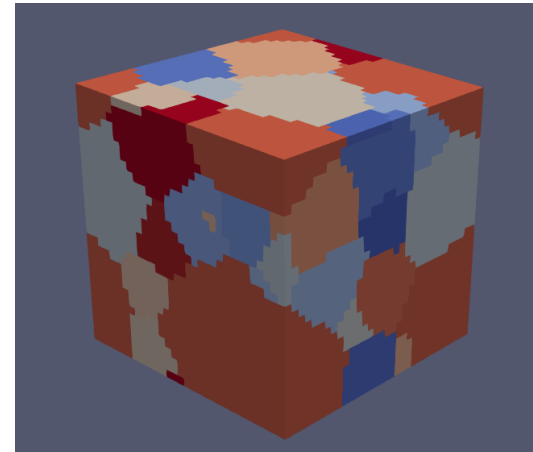
Input polycrystalline microstructure

1. Create a Dream3D microstructure **with the desired resolution** (e.g. if you want to run the PF code with 128^3 grid then create microstructure with 128^3 in Dream3D)
2. write a **rectilinear legacy vtk** output file from Dream3D
3. The output file should look like this (example with 32^3 grid):

```
# vtk DataFile Version 2.0
Data set from IO Version 6.4.197.9a0dee2
ASCII

DATASET RECTILINEAR GRID
DIMENSIONS 33 33 33
X_COORDINATES 33 float
0.500000 0.500000 1.500000 2.500000 3.500000 4.500000 5.500000 6.500000 7.500000 8.500000 9.500000 10.500000 11.500000 12.500000
13.500000 14.500000 15.500000 16.500000 17.500000 18.500000 19.500000
20.500000 21.500000 22.500000 23.500000 24.500000 25.500000 26.500000 27.500000 28.500000 29.500000 30.500000 31.500000
Y_COORDINATES 33 float
-0.500000 0.500000 1.500000 2.500000 3.500000 4.500000 5.500000 6.500000 7.500000 8.500000 9.500000 10.500000 11.500000 12.500000
13.500000 14.500000 15.500000 16.500000 17.500000 18.500000 19.500000
20.500000 21.500000 22.500000 23.500000 24.500000 25.500000 26.500000 27.500000 28.500000 29.500000 30.500000 31.500000
Z_COORDINATES 33 float
-0.500000 0.500000 1.500000 2.500000 3.500000 4.500000 5.500000 6.500000 7.500000 8.500000 9.500000 10.500000 11.500000 12.500000
13.500000 14.500000 15.500000 16.500000 17.500000 18.500000 19.500000
20.500000 21.500000 22.500000 23.500000 24.500000 25.500000 26.500000 27.500000 28.500000 29.500000 30.500000 31.500000
CELL_DATA 32768
SCALARS FeatureIds int 1
LOOKUP_TABLE default
26 26 26 26 26 26 26 17 17 17 17 17 30 30 30 30 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 17
17 17 17 17 17 17 30 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 17 17 17 17 17 17 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 17 17 17 17 17 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 20 17 17
17 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 20 17 17 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 20
20 18 18 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 20 18 18 18 18 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 18 18 18 18 18 18 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 18 18 18
18 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 18 18 18 18 18 18 18 18 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 14 14 14
14 14 14 14 18 18 18 18 18 18 26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 18
```

We will not read this file directly to PRISMS-PF
(we want point data instead of cell data)



Input polycrystalline microstructure

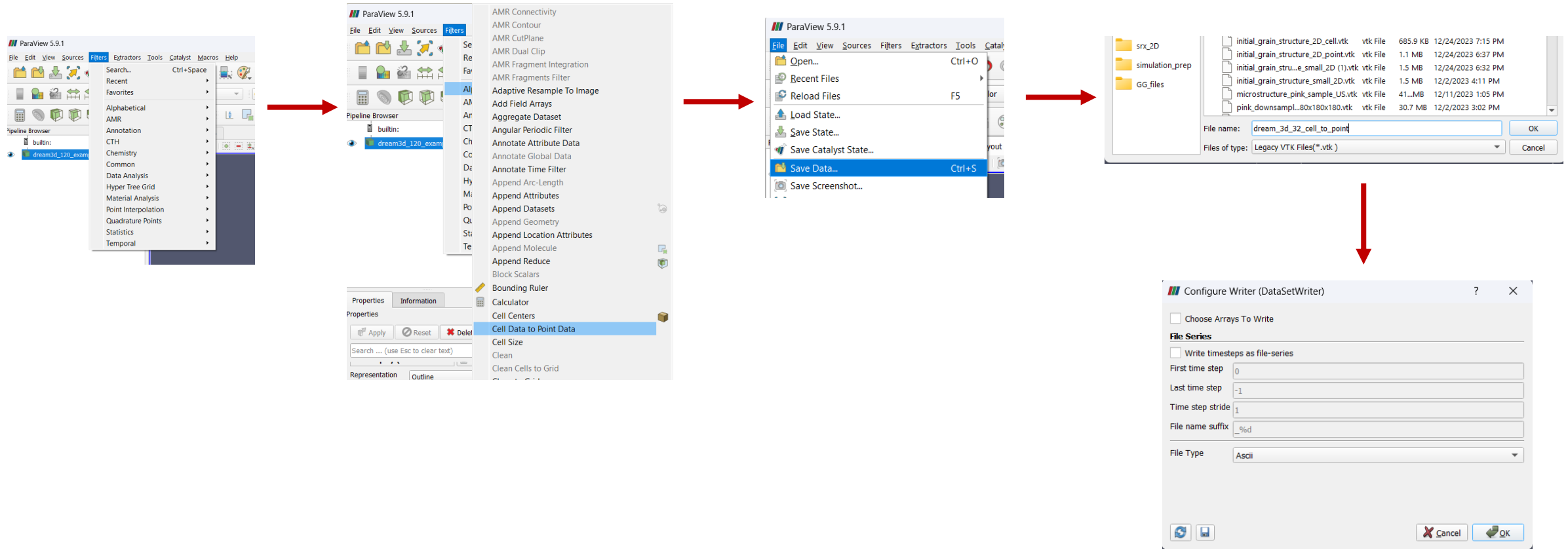
4. Convert the Dream3D file to rectilinear point data vtk file

Using paraview (filter: cell data to point data)

OR

Using visit or **resample_vtk_RL.py** code given with the graingrowth app (which calls visit from the terminal)

Paraview flowchart for cell data to point data:



Input polycrystalline microstructure

5. Converted paraview file looks like this:

```
# vtk DataFile Version 5.1
vtk output
ASCII
DATASET RECTILINEAR_GRID
DIMENSIONS 33 33 33
X_COORDINATES 33 float
-0.5 0.5 1.5 2.5 3.5 4.5 5.5 6.5 7.5
8.5 9.5 10.5 11.5 12.5 13.5 14.5 15.5 16.5
17.5 18.5 19.5 20.5 21.5 22.5 23.5 24.5 25.5
26.5 27.5 28.5 29.5 30.5 31.5
METADATA
INFORMATION 0

Y_COORDINATES 33 float
-0.5 0.5 1.5 2.5 3.5 4.5 5.5 6.5 7.5
8.5 9.5 10.5 11.5 12.5 13.5 14.5 15.5 16.5
17.5 18.5 19.5 20.5 21.5 22.5 23.5 24.5 25.5
26.5 27.5 28.5 29.5 30.5 31.5
METADATA
INFORMATION 0

Z_COORDINATES 33 float
-0.5 0.5 1.5 2.5 3.5 4.5 5.5 6.5 7.5
8.5 9.5 10.5 11.5 12.5 13.5 14.5 15.5 16.5
17.5 18.5 19.5 20.5 21.5 22.5 23.5 24.5 25.5
26.5 27.5 28.5 29.5 30.5 31.5
METADATA
INFORMATION 0

POINT_DATA 35937
SCALARS FeatureIds int
LOOKUP_TABLE default
26 26 26 26 26 26 26 26 22 17
17 17 17 24 30 30 30 28 26
26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26
26 26 26 26 22 17 17 17 17
20 24 27 29 27 26 26 26 26
26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26
26 22 17 17 17 17 17 17 23
27 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 24 19
```

6. But it still writes the coordinates starting from negative values. Translate the X,Y and Z coordinates to start from 0

You can do the translation using visit/paraview or **just by copying and pasting a series of floats starting from 0**

For translation using paraview, checkout the filter : Transform

Input polycrystalline microstructure

7. The final file will look like this (example 32^3):

```
# vtk DataFile Version 5.1
vtk output
ASCII
DATASET RECTILINEAR_GRID
DIMENSIONS 33 33 33
X_COORDINATES 33 float
0.000 1.000 2.000 3.000 4.000 5.000 6.000 7.000 8.000 9.000
10.000 11.000 12.000 13.000 14.000 15.000 16.000 17.000 18.000
19.000 20.000 21.000 22.000 23.000 24.000 25.000 26.000 27.000
28.000 29.000 30.000 31.000 32.000
METADATA
INFORMATION 0

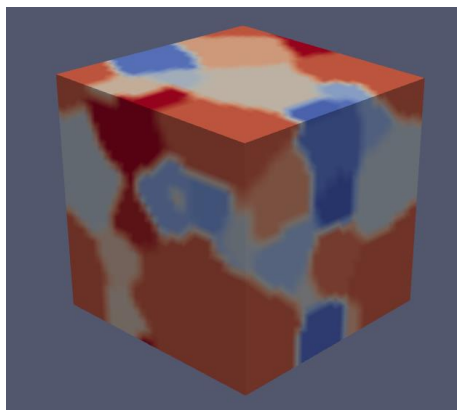
Y_COORDINATES 33 float
0.000 1.000 2.000 3.000 4.000 5.000 6.000 7.000 8.000 9.000
10.000 11.000 12.000 13.000 14.000 15.000 16.000 17.000 18.000
19.000 20.000 21.000 22.000 23.000 24.000 25.000 26.000 27.000
28.000 29.000 30.000 31.000 32.000
METADATA
INFORMATION 0

Z_COORDINATES 33 float
0.000 1.000 2.000 3.000 4.000 5.000 6.000 7.000 8.000 9.000
10.000 11.000 12.000 13.000 14.000 15.000 16.000 17.000 18.000
19.000 20.000 21.000 22.000 23.000 24.000 25.000 26.000 27.000
28.000 29.000 30.000 31.000 32.000
|
METADATA
INFORMATION 0

POINT_DATA 35937
SCALARS FeatureIds int
LOOKUP_TABLE default
26 26 26 26 26 26 26 26 22 17
17 17 17 24 30 30 30 28 26
26 26 26 26 26 26 26 26 26
26 26 26 26 26 26 26 26 26
```

This file can be used as input in the PRISMS-PF as rectilinear grid. The rectilinear grid file is significantly smaller than unstructured grid and file reading is also more efficient.

Nonetheless, you still have a choice to use the unstructured grid as input.



Running the modified code:

Code location : /anvil/projects/x-dmr110007/prisms_pf_supriyo/phaseField_US_RL/phaseField_US_RL_working_code

Pull request to merge with release version will be done soon

Parameters.prm file:

```
# =====  
# Set the number of dimensions (2 or 3 for a 2D or 3D calculation)  
# =====  
set Number of dimensions = 3  
  
# =====  
# Set the length of the domain in all three dimensions  
# (Domain size Z ignored in 2D)  
# =====  
# Each axes spans from zero to the specified length  
set Domain size X = 32  
set Domain size Y = 32  
set Domain size Z = 32
```

set the maximum length (Lx, Ly, Lz) as used in the microstructure

Switch between unstructured mesh and rectilinear mesh:

Rectilinear grid file reading:

```
set Load grain structure = true  
set Load as unstructured grid = false  
set Grain structure filename = RL_converted_paraview  
set Grain structure variable name = FeatureIds  
set Number of smoothing cycles after grain structure loading = 0  
set Minimum radius for loaded grains = 0.0
```

keep “set Load as unstructured grid” as false

Unstructured grid file reading:

```
set Load grain structure = true  
set Load as unstructured grid = true  
set Grain structure filename = microstructure_US  
set Grain structure variable name = FeatureIds  
set Number of smoothing cycles after grain structure loading = 0  
set Minimum radius for loaded grains = 0.0
```

keep “set Load as unstructured grid” as true

Comparison of current release version and modified version:

Graingrowth_dream3d APP:

Dimension: 120x120x120 μm^3

Refine factor: 5

#grainids: 118

#Order parameter : 15

Anvil : wholenode

Node:1, cpus: 32

It takes more time to read the file

Release version : unstructured grid (279 MB file)

Total wallclock time elapsed since start				18.1s	
Section	no. calls	wall time	% of total		
matrixFreePDE: computeRHS	1	0.00424s	0%		
matrixFreePDE: initialization	1	17.9s	99%		
matrixFreePDE: output	2	0.116s	0.64%		
matrixFreePDE: save_checkpoint	2	0.0759s	0.42%		
matrixFreePDE: setNonlinearEqInitialGuess	1	1.84e-05s	0%		
matrixFreePDE: solve	1	0.202s	1.1%		
matrixFreePDE: solveIncrements	2	0.00445s	0%		

modified version : rectilinear grid (5.5 MB file)

Total wallclock time elapsed since start				9.37s	
Section	no. calls	wall time	% of total		
matrixFreePDE: computeRHS	1	0.00347s	0%		
matrixFreePDE: initialization	1	9.05s	97%		
matrixFreePDE: output	2	0.148s	1.6%		
matrixFreePDE: save_checkpoint	2	0.153s	1.6%		
matrixFreePDE: setNonlinearEqInitialGuess	1	1.64e-05s	0%		
matrixFreePDE: solve	1	0.313s	3.3%		
matrixFreePDE: solveIncrements	2	0.00364s	0%		

Comparison of current release version and modified version :

Dimension: 120x120x120 μm^3

Refine factor: 5

#grainids: 118

#Order parameter : 15

Anvil: wholenode

Node:1, cpus: 64

Release version : unstructured grid

```
Currently Loaded Modules:
 1) gmp/6.2.1      4) zlib/1.2.11      7) numactl/2.0.14    10) modtree/cpu
 2) mpfr/4.0.2     5) gcc/11.2.0       8) openmpi/4.0.6
 3) mpc/1.1.0      6) libfabric/1.12.0 9) xalt/2.10.45 (S)

Where:
  S: Module is Sticky, requires --force to unload or purge

mkdir: cannot create directory '/anvil/scratch/x-chakraborty/release_newcode': File exists
slurmstepd: error: Detected 1 oom_kill event in StepId=4283314.0. Some of the step tasks have been OOM Killed.
srun: error: a974: task 47: Out Of Memory
```

```
Construct PField 'FeatureIds'
done
done
done
Construct PField 'FeatureIds'
done
Construct PField 'FeatureIds'
done
done
done
done
done
```

modified version : rectilinear grid

Total wallclock time elapsed since start		19.3s	
Section	no. calls	wall time	% of total
matrixFreePDE: computeRHS	1	0.00285s	0%
matrixFreePDE: initialization	1	17.9s	93%
matrixFreePDE: output	2	0.431s	2.2%
matrixFreePDE: save_checkpoint	2	0.95s	4.9%
matrixFreePDE: setNonlinearEqInitialGuess	1	1.93e-05s	0%
matrixFreePDE: solve	1	1.4s	7.2%
matrixFreePDE: solveIncrements	2	0.003s	0%