

How to Perform Resolution & Noise Analysis on Virtual Microstructures using DREAM.3D

All of the virtual microstructural analysis performed throughout this dissertation used various versions of DREAM.3D [10] (dream3d.bluequartz.net), which has been under constant development for the duration of the research. The link above can be used to download any current or historical version of the software. Note that the analysis for the journal publication associated with section 3.1 in the dissertation [99] was performed using version 2, while the more recent case studies on Inconel 100 and Ti-6Al-4V β grains were completed with version 5. Version 6, the most current version set for release this year, was used for the resolution and noise + cleanup analysis, and it is this most recent version employed herein.

Outlined below is a process by which anyone can perform similar analyses to those presented in this dissertation using DREAM.3D and MATLAB™, including investigating the effects of both resolution and noise (boundary and/or random) by comparing geometric similarity of PDFs and the percentage error in mean values of PDFs for the following microstructural distributions: grain size (equivalent sphere diameter), grain shape (aspect ratio b/a and c/a), and the number-of-nearest neighbor grains. Although the code provided operates within the parameters listed above, it can be easily modified to include additional types of microstructures, sources of error, microstructural parameters, statistical analyses, etc. Much of this modification can be completed through use of these files and/or the DREAM.3D graphical user interface (GUI). Screenshots included in this procedure were taken on a machine using a Windows 7 64-bit operating system, but DREAM.3D is compatible with Windows, Apple, and Linux platforms. Lastly, please note that some code modification will be required, as hard-coded file paths are based on my file structures, and some of the hard-coded character counters in the MATLAB™ files PipelineCreator.m and PipelineRunner.m will need to be modified, as







will the file path hard-coded in ResAndNoise.m. The file paths in Phantom_Build_Stats.json and DownSample.json can be easily updated via the DREAM.3D GUI.

*Feel free to contact the author if you have any questions or comments regarding the use of this analysis code. ~ *Corresponding author. **Email Address: greg.loughnane@gmail.com***

1. **Software Download and File Construction:** Download Version 6 of DREAM.3D and create the files listed below in the appropriate format based on the raw code provided in Appendix B.

1. Phantom_Build_Stats.json
2. Downsample.json
3. PipelineCreator.m
4. ScanPrintLine.m
5. PipelineRunner.m
6. GetCSVs.m
7. ComputeGrainStatistics.m
8. ResAndNoise.m

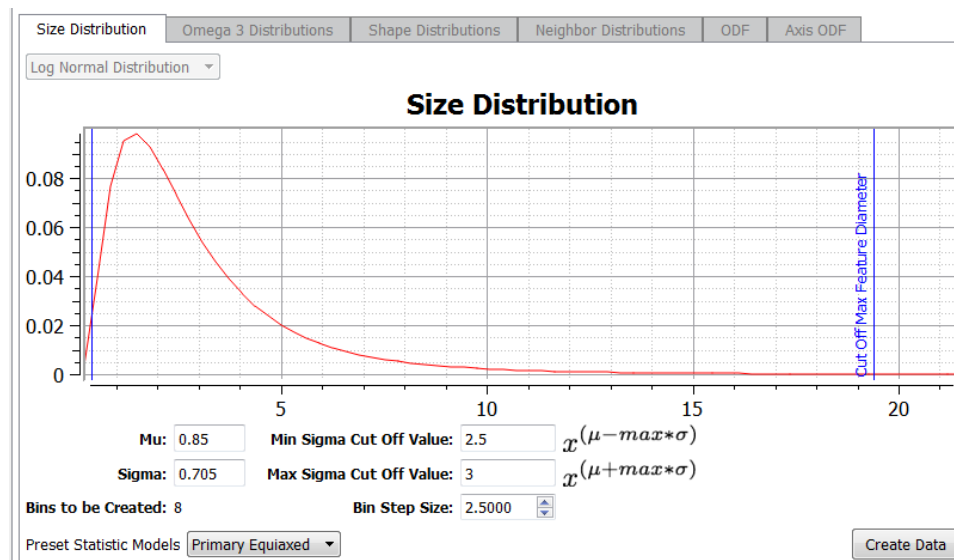
2. **Create Statistical Input Size Distribution:** After downloading DREAM.3D and copying the MATLAB files provided in Appendix B, navigate to the new folder and open StatsGenerator.exe.

	3/1/...	Application	1,457 KB	DREAM3D.exe
	3/1/...	Application	122 KB	PipelineRunner.exe
	3/1/...	Application	671 KB	PluginMaker.exe
	3/1/...	Application	2,847 KB	StatsGenerator.exe
	3/1/...	Application e...	5,215 KB	DREAM3DLib.dll
	3/1/...	Application e...	3,293 KB	DREAM3DWidgetsLib.dll

Choose the microstructure you wish to model by defining an input distribution for grain size.

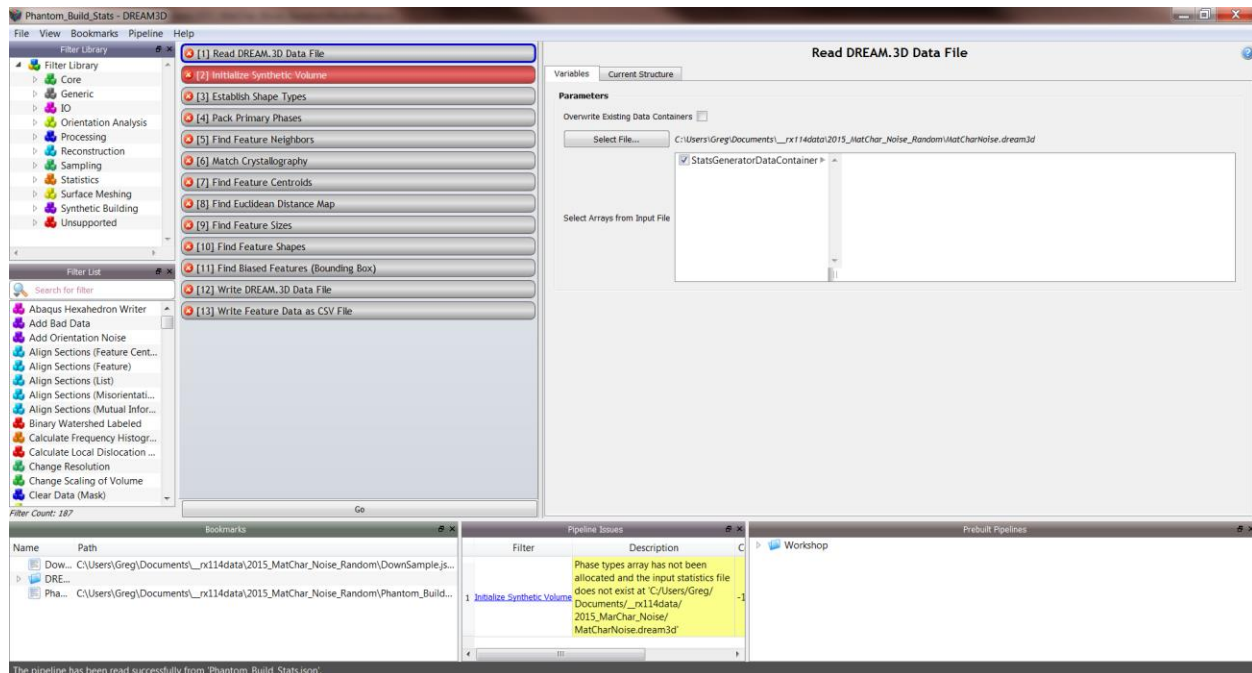
The user can choose to define additional distributions for shape, neighbors, and grain orientation, but based on the grain size input and the Preset Statistical Model, the other distributions will be assigned automatically when “Create Data” is clicked. These other distributions are generated based on microstructural correlations known to exist for the type of Preset Statistic Model (see Ref [87] for an example of these correlations).

After creating the input distributions, save the file in the main DREAM.3D folder.



3. Modify Phantom Build Stats.json & Downsample.json via DREAM.3D GUI: Open DREAM3D.exe and then open Phantom_Build_Stats.json. You will likely be prompted to replace the input statistics file with the one that you just generated. Go through each filter and make sure that there are no remaining red filters like the one shown below. Red denotes

an error that will prohibit DREAM.3D from running the pipeline. Update all file names and file paths so that they are associated with your file structures.



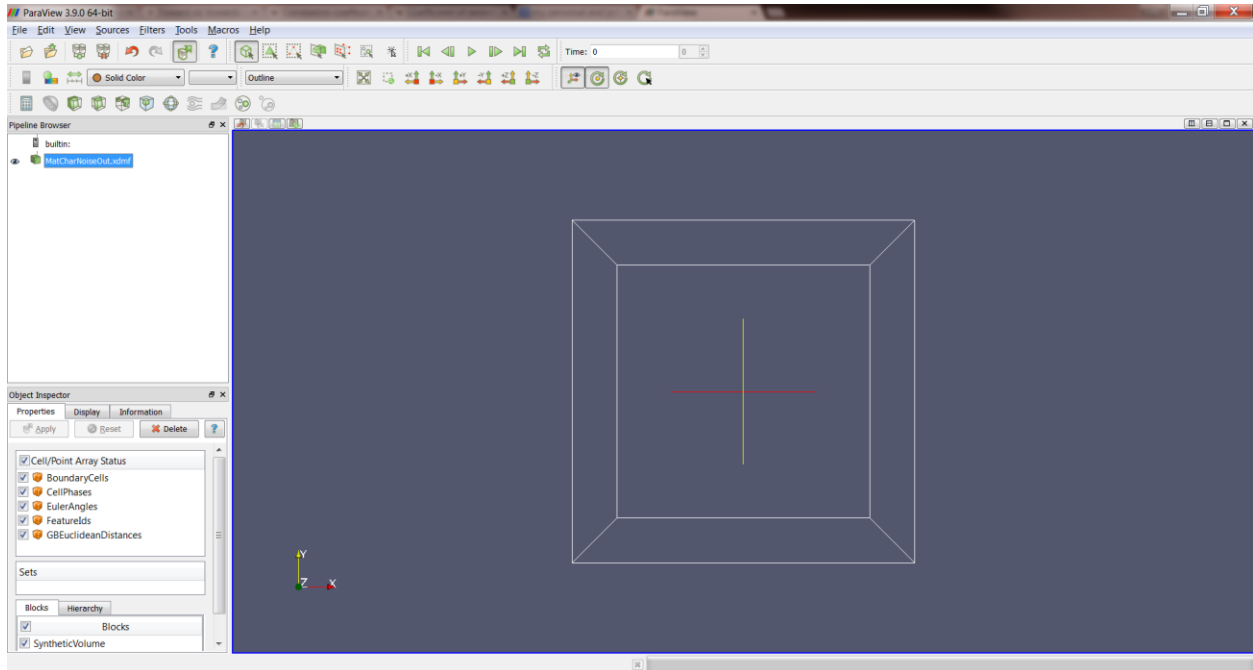
Go through the same procedure with the DownSample.json file. Note that you can also run a single experiment using just these input files and the DREAM.3D GUI. If this is your first time using DREAM.3D this is a good idea, because you can simply click “Go” in the GUI, perform a single phantom build and down-sampling, and then visualize your new microstructures.

4. Download the Latest Version of Paraview to View the Microstructures You Just Created:

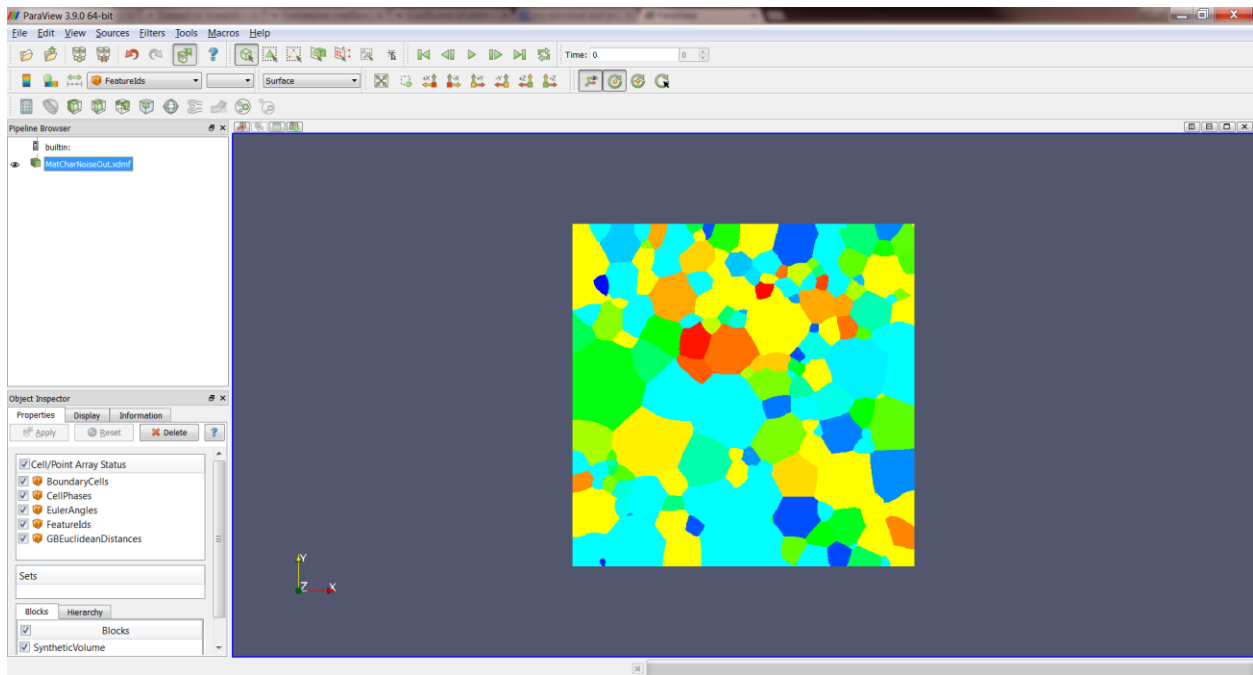
Navigate your web browser to Paraview.org and download the latest version. This software is used to visualize the microstructures that are created with DREAM.3D.

Once downloaded, open the software, navigate to the folder where you are saving your created files (this should be the same DREAM.3D folder that StatsGenerator.exe and DREAM3D.exe are in), and open the phantom reference volume generated from

Phantom_Build_Stats.json in DREAM.3D (.xdmf file type). You should see something like this once the file loads:



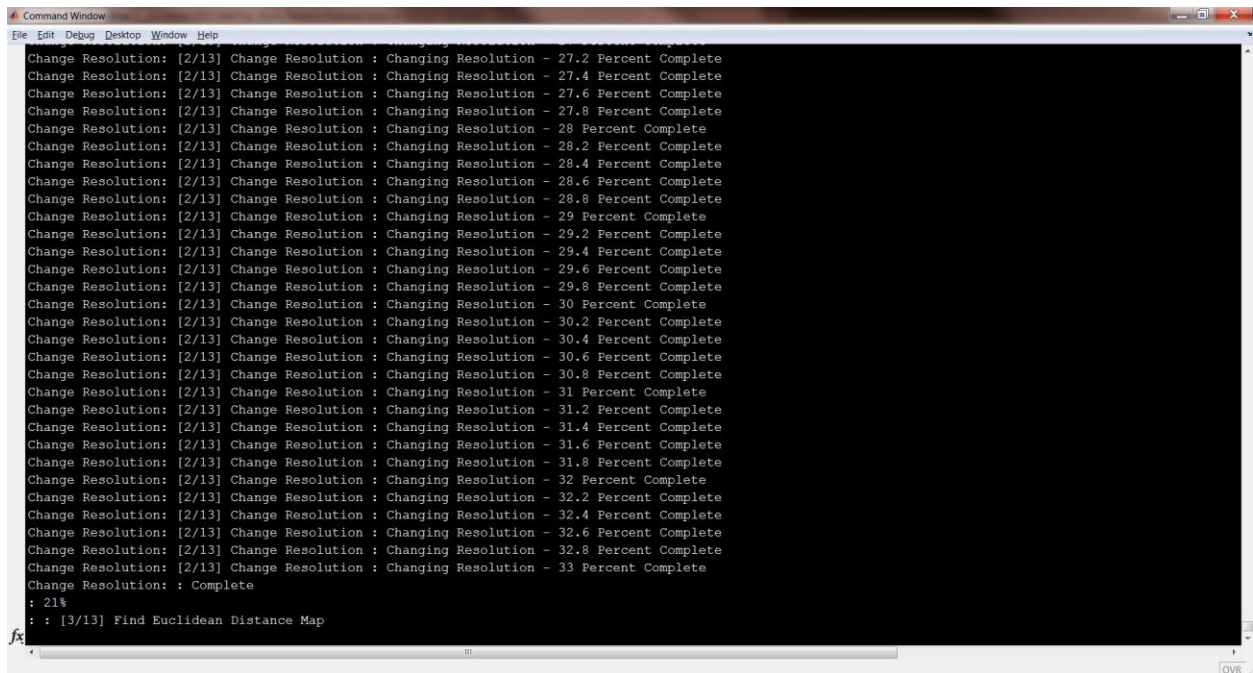
From the drop down menu that reads “Outline,” select “Surface”. Then, from the drop down menu that reads “Solid Color” select “FeatureIds”. You should now be able to see your microstructure and use the mouse to move it as you would with any typical 3D modeling software.



To compare the two visually, feel free to go through these steps with the down-sampled volume as well.

5. *Modify PipelineCreator.m for Your File Structure:* Count the number of characters in the file path string associated with the .dream3d and .csv output files that you created from DownSample.json. Update PipelineCreator.m to reflect these changes in lines 38 and 46, respectively.
6. *Modify ResAndNoise.m for Your Experiment:* Open ResAndNoise.m and modify the file directory, the resolutions desired for analysis, the noise levels to be investigated, the average grains size, and the instantiation number (which represents the number of times you wish to perform each experiment). Assuming that you will only analyze grain size, aspect ratios, and number-of-nearest neighbors as a first cut, there are just a few modifications that you still must make to the ComputeGrainStatistics.m file, which are noted at the top of the code in Appendix B.

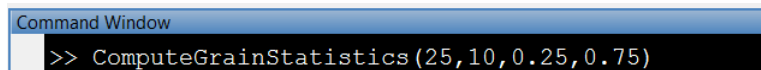
7. Run ResAndNoise.m: Try to run the ResAndNoise.m file. If it is successful, you should see the command window in MATLAB™ doing something like this:



```
Command Window
File Edit Debug Desktop Window Help
Change Resolution: [2/13] Change Resolution : Changing Resolution - 27.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 27.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 27.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 27.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 28 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 28.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 28.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 28.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 28.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 29 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 29.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 29.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 29.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 29.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 30 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 30.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 30.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 30.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 30.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 31 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 31.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 31.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 31.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 31.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 32 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 32.2 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 32.4 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 32.6 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 32.8 Percent Complete
Change Resolution: [2/13] Change Resolution : Changing Resolution - 33 Percent Complete
Change Resolution: : Complete
: 21%
: : [3/13] Find Euclidean Distance Map
```

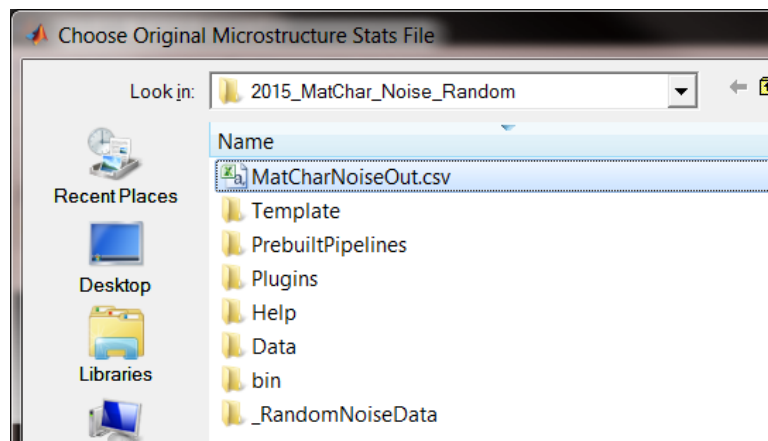
If so, congratulations! If not, then it's time to debug the code. Check that all of your files are located in the DREAM.3D folder that you originally downloaded, check file paths, etc.

8. Compute Statistics from Down-Sampled Volumes: Once you have all of your statistical data following the simulations, run ComputeGrainStatistics.m from the command window using, for example, the following input parameters:

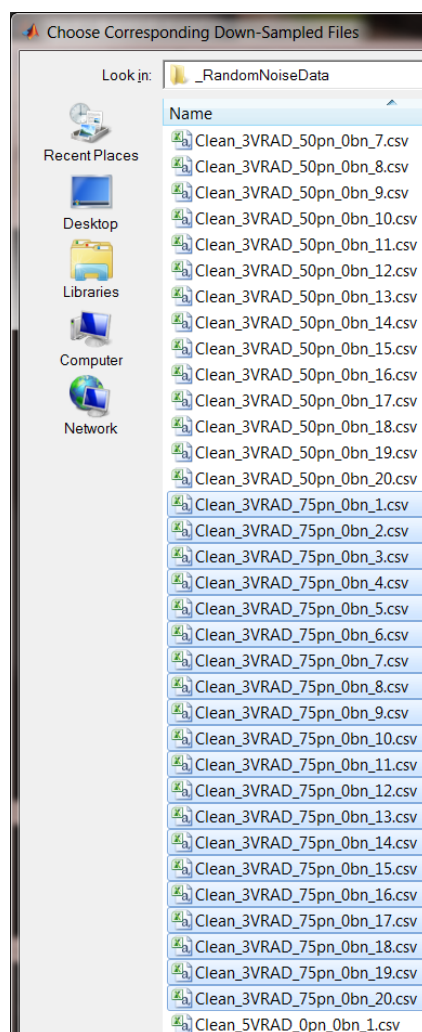


```
Command Window
>> ComputeGrainStatistics(25,10,0.25,0.75)
```

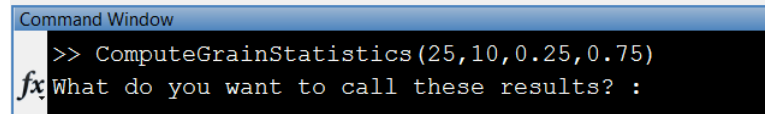
Select the reference volume statistics file for comparison first:



Then choose the down-sampled volume statistics file(s):



You will be prompted to name the output file, and when you do results there will be some select results written to the command window. You can ignore these, as they are saved along with other data automatically in .csv file format.



```
>> ComputeGrainStatistics(25,10,0.25,0.75)
fx What do you want to call these results? :
```

9. View Final Statistics Computed between Reference and Down-Sampled Volumes: Navigate to the files you just created and open “YourFileName_MBCandPercErrMean.csv”. It will appear without descriptive text, however the results correspond to the data shown below, where the numbers in column C correspond to the 95% confidence interval on the answers reported in column B.

Type	Size	Name
File folder		_RandomNoiseData
File folder		bin
File folder		Data
File folder		Help
File folder		Plugins
File folder		PrebuiltPipelines
File folder		Template
Microsoft Exc...	6 KB	3VRAD_0RN_DistData.csv
Microsoft Exc...	1 KB	3VRAD_0RN_MBCandPercErrMeanData.csv
Microsoft Exc...	6 KB	3VRAD_10RN_DistData.csv
Microsoft Exc...	1 KB	3VRAD_10RN_MBCandPercErrMeanData.csv
Microsoft Exc...	7 KB	3VRAD_25RN_DistData.csv
Microsoft Exc...	1 KB	3VRAD_25RN_MBCandPercErrMeanData.csv
Microsoft Exc...	7 KB	3VRAD_50RN_DistData.csv
Microsoft Exc...	1 KB	3VRAD_50RN_MBCandPercErrMeanData.csv
Microsoft Exc...	6 KB	3VRAD_75RN_DistData.csv
Microsoft Exc...	1 KB	3VRAD_75RN_MBCandPercErrMeanData.csv

	A	B	C
1			
2	MBC, ESD	0.29454	0.004274
3	MBC, b/a	0.42878	0.003163
4	MBC, c/a	0.48655	0.002974
5	MBC, NNN	0.13908	0.004856
6		#####	#####
7	Low Quantile MBC, ESD	0.5617	0.002088
8	Low Quantile MBC, b/a	0.35336	0.005442
9	Low Quantile MBC, c/a	0.37728	0.003042
10	Low Quantile MBC, NNN	0.082518	0.00414
11		#####	#####
12	High Quantile MBC, ESD	0.06453	0.005014
13	High Quantile MBC, b/a	0.41474	0.004356
14	High Quantile MBC, c/a	0.22027	0.009691
15	High Quantile MBC, NNN	0.08564	0.001874
16		#####	#####
17	Percent Error in Mean, ESD	21.061	0.38266
18	Percent Error in Mean, b/a	-12.855	0.22519
19	Percent Error in Mean, c/a	-22.326	0.18256
20	Percent Error in Mean, NNN	-0.31048	0.25767
21			

Next open “YourFileName_DistData.csv”. These are the collective distributions, with corresponding error bars for each bin and the percent difference in down-sampled

distribution bins relative to the reference volume. ESD is shown first, followed by number-of-nearest neighbors, aspect ratio b/a , and aspect ratio c/a .

	A	B	C	D	E	F
		Bins	Reference Distribution	Down-Sampled Distribution	95% Confidence Interval For Each Distribution Bin	Percent Difference From Reference Distribution For Each Bin
1						
2	ESD	0.25	0.010681	0	0	1.0681
3		0.75	0.076101	0.0032414	0.00079252	7.286
4		1.25	0.17223	0.020782	0.0019551	15.145
5		1.75	0.17824	0.14369	0.0044843	3.455
6		2.25	0.13818	0.20655	0.0065342	6.8369
7		2.75	0.098798	0.15694	0.0047989	5.8141
8		3.25	0.078099	0.11793	0.0039143	4.3828
9		3.75	0.061415	0.085595	0.0034923	2.418
10		4.25	0.048732	0.061447	0.0025315	1.2716
11		4.75	0.026702	0.045723	0.0019991	1.902
12		5.25	0.024032	0.040726	0.0024344	1.6694
13		5.75	0.016021	0.029464	0.0018614	1.3442
14		6.25	0.012684	0.022574	0.0013139	0.98908
15		6.75	0.015354	0.011328	0.0011483	0.40262
16		7.25	0.011348	0.011386	0.0008595	0.0037177
17		7.75	0.010681	0.013535	0.0011005	0.28536
18		8.25	0.0040053	0.0059755	0.00081244	0.19702
19		8.75	0.0040053	0.0020409	0.0005303	0.19645
20		9.25	0.0040053	0.0040396	0.00066763	0.0034281
21		9.75	0.0033378	0.0061608	0.00074428	0.2823
22		10.25	0.0020027	0.0037292	0.00043004	0.17266
23		10.75	0.0026702	0.0011974	0.00036989	0.14728
24		11.25	0.0020027	0.002101	0.00020018	0.0098306
25		11.75	0	0.0011911	0.00032108	0.11911
26		12.25	0.00066756	0.0014638	0.00033607	0.079628
27		12.75	0.00066756	0.0003496	0.00025679	0.031795
28		13.25	0.00066756	0.0008414	0.00023362	0.017385

	A	B	C	D	E	F
		Bins	Reference Distribution	Down-Sampled Distribution	95% Confidence Interval For Each Distribution Bin	Percent Difference From Reference Distribution For Each Bin
1						
31	NNN	#####	1.00E+100	1.00E+100	1.00E+100	1.00E+100
32		0	0	0	0	0
33		0.04	0	0	0	0
34		0.08	0	0	0	0
35		0.12	0	0	0	0
36		0.16	0	0	0	0
37		0.2	0	0.0005639	0.00040086	0.05639
38		0.24	0	5.77E-05	0.0001207	0.005767
39		0.28	0	0.0054935	0.001071	0.54935
40		0.32	0	0.00039318	0.00030725	0.039318
41		0.36	0	0.0011381	0.00054199	0.11381
42		0.4	0	0.0040694	0.0011494	0.40694
43		0.44	0	0.028574	0.0023598	2.8574
44		0.48	0.0013351	0.018635	0.0023538	1.7299
45		0.52	0.00066756	0.020702	0.0021403	2.0034
46		0.56	0.00066756	0.030931	0.0023675	3.0264
47		0.6	0.0033378	0.057215	0.0039917	5.3877
48		0.64	0.0080107	0.12678	0.0042849	11.877
49		0.68	0.014686	0.06884	0.0043582	5.4153
50		0.72	0.042724	0.09194	0.0045309	4.9216
51		0.76	0.076769	0.1184	0.0050311	4.1629
52		0.8	0.11415	0.096868	0.0045773	1.7284
53		0.84	0.17423	0.091522	0.0038931	8.271
54		0.88	0.24032	0.092118	0.0036156	14.82
55		0.92	0.21762	0.073208	0.002823	14.442
56		0.96	0.10414	0.02848	0.0029358	7.5659
57		1	0.0013351	0.044076	0.0038258	4.274

You have officially completed this tutorial. Have fun plotting the data and identifying trends to inform future microstructural characterization!

Cheers,

Dreg Loughnane

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