DREAM.3D User Manual

Software Authors

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Digital **R**epresentation **E**nvironment for **A**nalyzing **M**icrostructure in **3D** (**DREAM.3D**)

Overview of Software Scope

Core Software Package:

The core software package has four (4) major functionalities. First, a series of TSL .ang files can be read and packed into a single HDF5 binary data in order to reduce data size and clutter. Second, the sections can be aligned, cleaned, reconstructed, segmented and statistically characterized. Third, the statistics can be read in and used to generate statistically-equivalent, synthetic microstructures. Fourth, the reconstructed volumes and the synthetic volumes can be surfaced meshed.

Stats Generator Utility Package:

The stats generator utility package is used to generate statistics to be used in the core software package to generate statistically-equivalent, synthetic microstructures. This utility is especially useful when the user has no 3D statistics from a previously reconstructed volume. This utility can be used to generate many volumes with combinations of statistics for sensitivity studies.

Core Software Package

OIM Data Import Tab

1. ***Input Directory*** – Directory where the .ang files are located
   a. ***Total Ang Files Found*** - Code will determine how many .ang files are present.
   b. Currently only .ang files are supported.

2. ***Output File*** – Name and location of desired output .h5ang file
3. ***Z spacing*** – This is the spacing between sections
    a. Note that the x and y spacings are automatically read from the .ang files.
    b. If the x and y spacing values change, the ones in the first section are used.
4. ***File Prefix, Suffix and File Extension*** – Variables that are combined to generate the list of file names
    a. These values should all be automatically determined, but should be checked if there are weird prefixes or suffixes.
5. ***Start Slice, End Slice and Total Digits*** – More variables that are combined to generate the list of file names
    a. Start slice and end slice define the range of data to be included in the .h5ang file (i.e. you don't have to import the entire dataset).
    b. Total digits controls the number of leading zeros that are present in the filename.
6. ***File List*** – This bank lists all the files that will be included in the .h5ang file based on the inputs chosen.
    a. The files in the list will have a green light if they are present in the directory selected and a red light if they are not present.

Reconstruction Tab

1. ***OIM HDF5 File*** – This is the name and location of the .h5ang file you wish to reconstruct
   a. The ***minimum and maximum slice*** numbers will be automatically displayed with the ***z resolution or spacing.***
2. ***Start Slice and End Slice*** – This defines the range of sections you wish to reconstruct

a. Like you can choose to not import the entire dataset, you can choose to not reconstruct everything you imported.

3. ***Phase Types*** – these are required descriptors to classify the 'type' of phase each phase in the EBSD scan. These classifications are used when moving the data to the Synthetic Builder Tab, but are not critical to the reconstruction itself – only the statistics calculations.

4. ***Options*** – These are all the options that can be set to control the reconstruction

   a. ***Merge Twins*** – this is an option that will indentify neighboring grains that have a twin relationship (Σ3, Σ5, Σ9) and merge them together. Effectively, this is a second burn algorithm (performed on the identified grains, rather than the individual voxels) using the specific twin misorientations as a joining criterion rather than the misorientation tolerance used for forming the grains.

   b. ***Merge Colonies*** – this is an option that is similar to the ***Merge Twins*** option, but will reconstruct prior beta grains in an alpha-beta titanium microstructure. It will first identify grains (which would be alpha colonies in a transformed beta microstructure) and then perform a burn algorithm on neighboring grains/colonies, using the specific misorientations between alpha variants from the same beta grain as the joining criterion.

   c. ***Rectangularized Sample*** – this option will fix the sample to look like a perfect rectangular sample by determining the smallest rectangular box that fits around the reconstructed volume and coarsening the structure to fill in the empty space within the rectangular box. Note that the box is created with axes along x, y and z. This option is generally not used unless the reconstruction needs to be used in a program that cannot handle having 'empty space' outside of the sample (i.e. possibly a Finite Element simulation).

   d. ***Alignment Method*** – this allows the user to choose the method used to align neighboring sections. Outer Boundary simply tries to align the area identified as sample on each section. Minimum Disorientation moves the sections until there is a minimum value of disorientation between all voxels in one section and the voxel directly above it in the next section. Mutual information segments each section independently and then performs a mutual information analysis on the grain ids.

   e. ***Ang Orientation*** – this defines the origin of the ang file. Note that TSL and HKL define different locations on an EBSD scan as the origin. Additionally, the origin may be defined differently for the Euler angles and the morphological features. This setting allows the user to define what location in the 2D EBSD map they want to be the origin for both the Euler angles and morphological features. The Euler angles and x/y coordinates of the scan are all consistently modified by the

code during reconstruction and not changed in the .h5ang file (which means the origin needs to be set every time the dataset is reconstructed.

    f. ***Min Grain Size*** – this a clean-up filter that can be set to merge grains below a defined size after grains have been formed. The voxels of the removed grains are reset to unassigned and then the region is filled in by a local grain growth algorithm.

    g. ***Disorient. Tol.*** – this is the orientation difference tolerance allowed between neighboring voxels before they are declared to belong to different grains. Neighboring voxels with misorientations lower than the tolerance are joined during a burn algorithm.

    h. ***Min. Image Quality*** – this is a threshold value that is used to define the outer border of the sample and terminate grain formation during segmentation. Image Quality is a metric used by TSL to define the quality or perfection of the orientation pattern at a data point. Generally when serial sections are collected, there is some extra area collected around the sample and this data usually has 'much' lower values of Image Quality. This tolerance thresholds the outer area and also ends the grain formation burn algorithm, because it is not desirable to begin formation of a grain with a 'very' low value of pattern quality.

    i. ***Min. Confidence Index*** – this is threshold used the same as Min. Image Quaity, but using another TSL data metric that defines the confidence in the orientation determined from the orientation pattern.

    j. ***Down-sample Res.*** – this a factor used to down-sample the 3D volume if desired. If the value is set to 1, then nothing happens, but any other value will scale the resolution by that value. A new grid is created and laid over the original data grid. This option is usually only used if the dataset is too large to transfer into some other program(s) and needs to be 'coarsened'.

    k. ***Bin Step Size*** – this is the step size used in correlating statistical descriptors to grain size. The value is set in microns, so for example, if the maximum grain size is 50 microns, a value of 5 would create 10 size bins in which grains would be segregated to create shape, no. of neighbors, etc. distributions as a function of grain size. This value should be selected by balancing each of the following: how quickly are other statistics likely to vary with size and how many grains are needed in each size bin to describe grains of that size. Creating size bins too small will result in not enough grains in a bin and creating size bins too large may miss identifying correlations.

5. ***Output Directory*** – location that all output files will be written to.

6. ***Output File Prefix*** – this option allows the user to define a prefix to place on the output data files (which have a fixed 'base' name). The full names of the files will update in real-time on the list of output files.

7. ***Write Binary VTK Files*** – This option allows the user to choose whether the output visualization files are in binary or ASCII format.

8. ***Optional Output Files*** – these are all visualization files that can be created. The output files are .vtk files of structured grid type.

   a. ***Reconstruction Visualization*** - this file contains (at each voxel) grain ids, phase ids and the number of neighboring voxels that have grain ids different from the reference voxel.

   b. ***Reconstruction IPF Visualization*** - this file contains (at each voxel) grain ids and Inverse Pole Figure colors

   c. ***Reconstruction Disorientation Visualization*** - this file contains (at each voxel) grain ids and Kernel Average Misorientations and Grain Average Misorientations

   d. ***Reconstruction ImageQuality Visualization*** - this file contains (at each voxel) grain ids and Image Qualities

   e. ***Reconstruction SchmidFactor Visualization*** - this file contains (at each voxel) grain ids and Schmid Factors

   f. ***Reconstruction DownSampled Visualization*** - this file contains (at each voxel) grain ids for the down-sampled volume

   g. ***Reconstruction Grains*** - this file contains each grain with properly defined voxels and their neighbor connectivities. This file is a binary HDF5 format of vtk poly data. Additionally, all the attributes listed in the other files are all contained in this one file.

9. ***Load/Save Preset*** – this allows the user to save input settings or load previously saved input settings
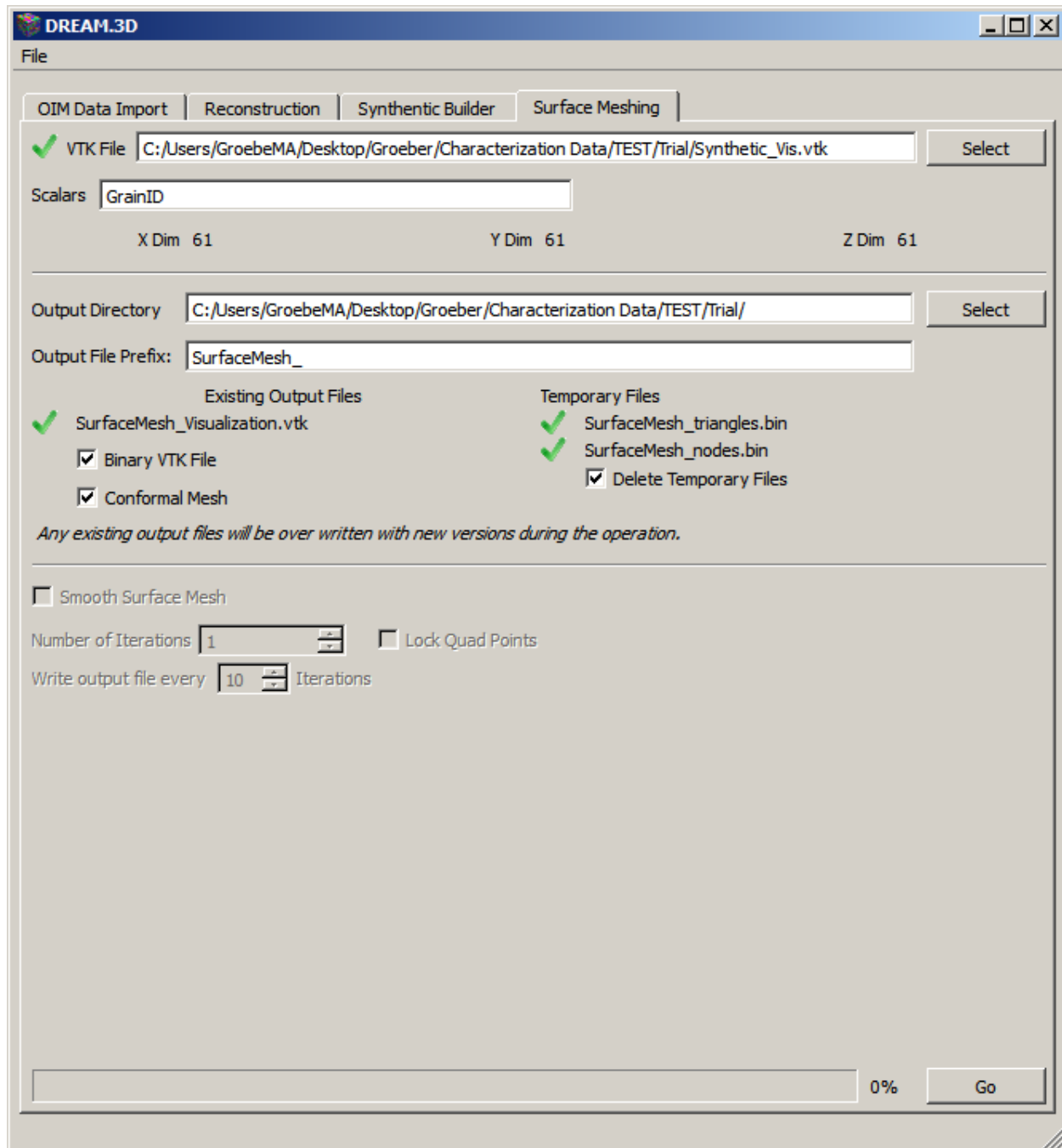
Synthetic Builder Tab

1. ***HDF5 Stats File*** – name and location of the input stats file that can be generated from the reconstruction tab or the stats generator utility package.
2. ***Options***
   a. ***Structure Already Formed*** – If a volume has already been created, this option will read the .vtk file with grain ids. It enters the synthetic builder right before

the orientation assignment and matching, so it does not readd any orientation information, just the structural information. This file must be accompanied by a HDF5 stats file that contains the ODF and MDF that will be matched after reading the previously formed structure.

b. ***Number of Grains*** – this is the target desired number of grains. The final number may not be this exact value, but should be close. This defines the size of the volume generated, which is not defined by the user. Generally, the number of grains is of more critical concern than the size of the box and that is the reason it is the input variable. If the size of the box is more important, then the number of grains that will produce the desired box size can be estimated by dividing the desired box volume by the average grain volume.

c. ***Shape Class*** – this is the type of object(s) being placed during grain placement. The user can choose ellipsoids, superellipsoids or truncated octahedra. Ellipsoids do not need the omega3 value, but the other two options require omega3 to be defined.

d. ***Periodic Boundaries*** – this option allows the user to specify whether the grains being packed can 'wrap' from one side of the volume to the opposite size. This option should be turned on if the volume is being imported into a program that requires periodic boundary conditions (i.e. some Finite Element simulations). Turning this option off will make the volume look more like a volume cut out of a 'real' microstructure.

e. ***X, Y, Z Spacing*** – this is the resolution of the voxels in the generated volume. The user should be aware of the size distribution when selecting this value and the number of grains. If attention is not paid to these values in conjunction, crashes due to memory overload are possible. Typically, a resolution that results in ~10 voxels across the diameter of the average grain is a good value to select.

f. ***Space Filling Error Weight*** – this is the weight to be applied to the criterion of maximizing space filling during grain placement. This weight should generally be set to 1.0, because if space is not 'well-filled' during the packing step, the grains will have to change size and shape to fill in the gaps during the filling in step.

g. ***Size Distribution Error Weight*** – this is the weight to be applied to matching the size distribution during grain placement. This weight should be left at 1.0, unless the size distribution is not critical to match.

h. ***Neighborhood Error Weight*** – this is the weight to be applied to matching the local neighborhoods during grain placement. This weight is the most likely to be reduced from 1.0, especially if the local neighborhoods are not known well.

3. ***Output Directory*** – location where all the output files will be written
   a. The output file is a .vtk file of structured grid type.

4. ***Output File Prefix*** – this option allows the user to define a prefix to place on the output data files (which have a fixed 'base' name). The full names of the files will update in real-time on the list of output files.

5. ***Write Binary VTK Files*** – This option allows the user to choose whether the output visualization files are in binary or ASCII format.

6. ***Optional Output Files*** – these are all visualization files that can be created. The output files are .vtk files of structured grid type.

    a. ***GrainGenerator Visualization*** - this file contains (at each voxel) grain ids, phase ids and the number of neighboring voxels that have grain ids different from the reference voxel.

    b. ***GrainGenerator IPF Visualization*** - this file contains (at each voxel) grain ids and Inverse Pole Figure colors

    c. ***GrainGenerator Grains*** - this file contains each grain with properly defined voxels and their neighbor connectivities. This file is a binary HDF5 format of vtk poly data. Additionally, all the attributes listed in the other files are all contained in this one file.

7. ***Load/Save Preset*** – this allows the user to save input setting or load previously saved input settings

Surface Meshing Tab

1. ***VTK File*** – name and location of the .vtk file that will be used in the surface meshing
   a. This can be any of the volumes created in the reconstruction tab or the synthetic builder tab. The ***XDim***, ***YDim*** and ***ZDim*** are the size of the volume (in voxels), read from the input .vtk file.

2. ***Scalars*** – name of the block of data to read from the input .vtk file. If the volume is from either of the Reconstruction or Synthetic Builder Tab, then this should generally be set to GrainID.

3. ***Output Directory*** – this is the location that all of the output files will be written to
   a. The output file is a .vtk file of poly data

4. ***Output File Prefix*** – this option allows the user to define a prefix to place on the output data files (which have a fixed 'base' name). The full names of the files will update in real-time on the list of output files.

5. ***Options***
   a. ***Binary VTK File*** – This option allows the user to choose whether the output visualization file is in binary or ASCII format.
   b. ***Conformal Mesh*** – this option creates a copy of every triangular surface patch if turned on. This option is useful for visualization because when writing poly data in a .vtk file, only one attribute is assigned to each triangle, which negates that two grains actually 'share' a triangle. If this option is on, then each triangle will be written twice and one will be assigned to one grain and the other to the second grain. If turned off, when the user visualizes one grain at a time by thresholding the data, the grains will appear to having 'missing' triangular patches.
   c. ***Delete Temporary Files*** – this option will delete the temporary nodes and triangles files between all the individual sections once the full volume has been meshed. This option should usually be on since the temporary files are binary and generally not of use to the user after-the-fact.

6. ***Smooth Surface Mesh*** – this is an option to smooth the surface mesh that is output from the marching cubes portion of the tab. Currently this option is not functional and is under development with CMU.

Stats Generator Utility Package

Size Distribution Tab
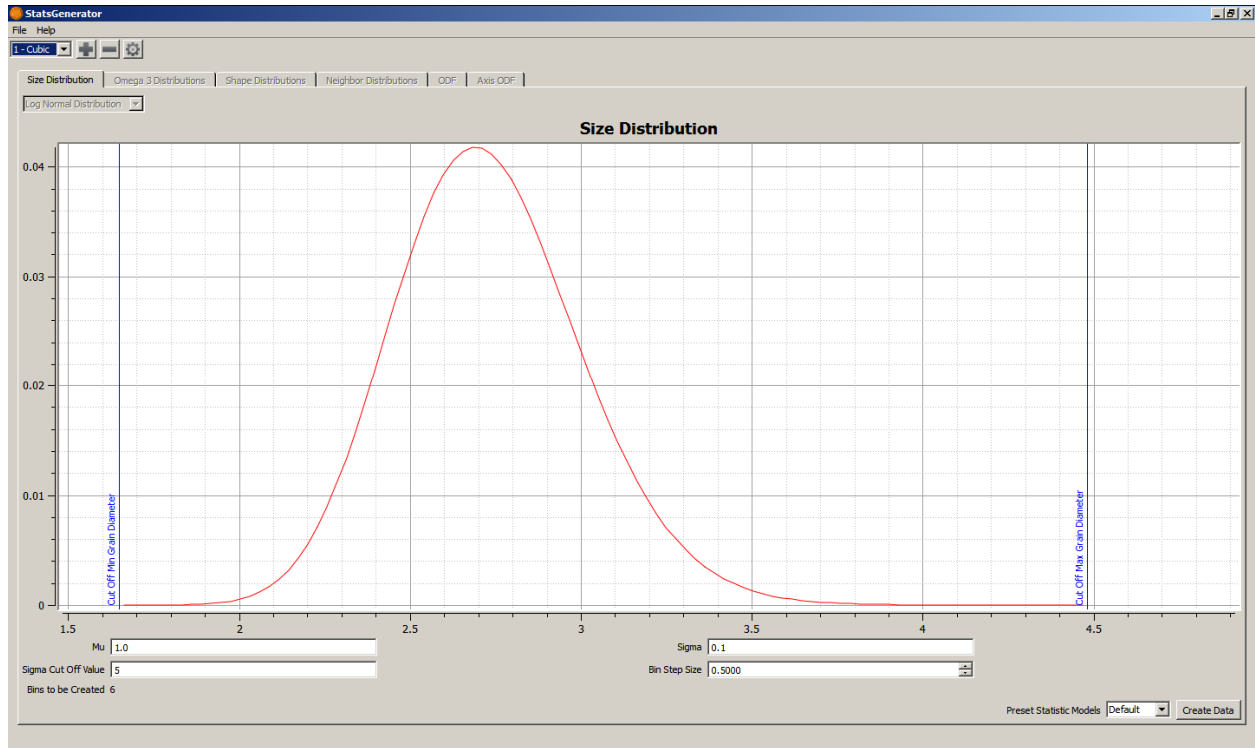
1. ***Phase Bank*** – this is the area where the user can enter information about the phase for which statistics are currently being generated. The ***Plus Button*** allows the user to add a phase, the ***Minus Button*** allows the user to remove a phase and the ***Wheel Button*** allows the user to edit the currently selected phase.

a. ***Select Crystal Structure*** – this allows the user to specify the crystal structure of the phase. Currently, the two options are Cubic and Hexagonal.

b. ***Fraction*** – this is the volume fraction of the phase. The ***Calculated Phase Fraction*** is updated as more phases are added, by scaling the current total of all the phases fractions to 1 (in case the user's total is not equal to 1 when finished).

c. ***Select Phase Type*** – this specifies the type of the phase. Currently, the two types of phases are Primary and Precipitate. Note that there must be at least one Primary phase before any Precipitate phase can be created or the Synthetic Builder will fail.

d. ***Fraction of Precipitate on Boundary*** – if the phase type is set to Precipitate, then the user must specify the number fraction of the precipitates that are located on grain boundaries of the primary phase. This value will be scaled to 1 if the user's value is larger than 1. The value is keyed to -1 for Primary phases.

2. ***Mu*** – this is the average value of the lognormal grain size distribution

3. ***Sigma*** – this is the standard deviation of the lognormal grain size distribution

4. ***Sigma Cut Off Value*** – this allows the user to truncate the distribution to remove very large grains

5. ***Bin Step Size*** – this is the size of bin to use in segregating the grains into size classes for correlating other statistics to grain size.

   a. Note that the ***Bins to be Created*** is displayed in the bottom left corner

6. ***Preset Statistic Models*** – this allows the user to select a 'morphological-type' of microstructure to populate the default data.

   a. ***Default*** – this populates the statistic tabs with generic random data that may not create a 'buildable' microstructure. This option should only be used if the user is going to enter the values on all the statistics tabs themselves.

   b. ***Equiaxed*** – this populates the statistic tabs with data that is designed to generate a random equiaxed microstructure.

   c. ***Rolled*** – this populates the statistic tabs with data that is designed to generate a rolled microstructure with elongated grains with user defined aspect ratios.
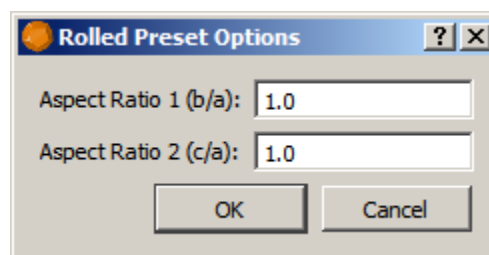
      i. ***Aspect Ratio 1*** – this is the aspect ratio between the dimensions of the grains in the rolling direction and transverse direction, respectively.

      ii. ***Aspect Ratio 2*** – this is the aspect ratio between the dimensions of the grains in the rolling direction and normal direction, respectively. This value must be larger than ***Aspect Ratio 1*** or the default values will be wrong.

7. ***Create Default Data*** – this locks in the values the user has entered and populates the other tabs with default values. The user can move through the other tabs and change any default values if desired.
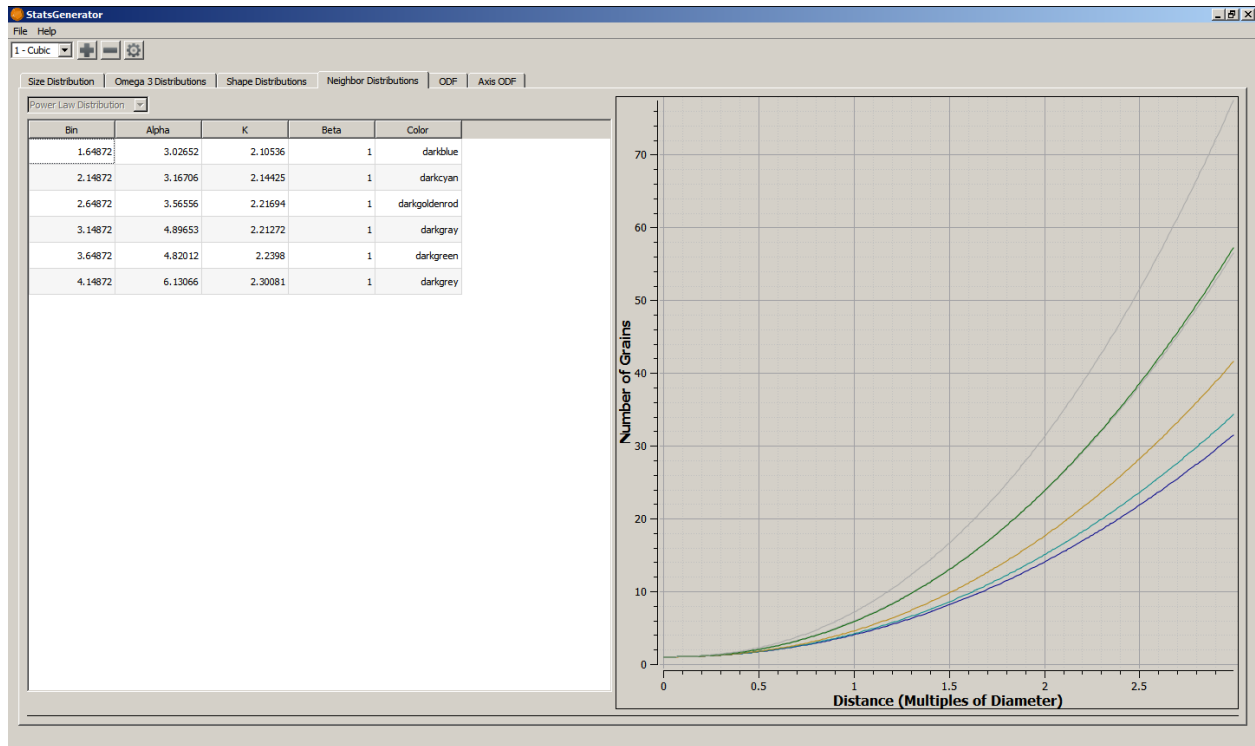
Omega 3 Tab
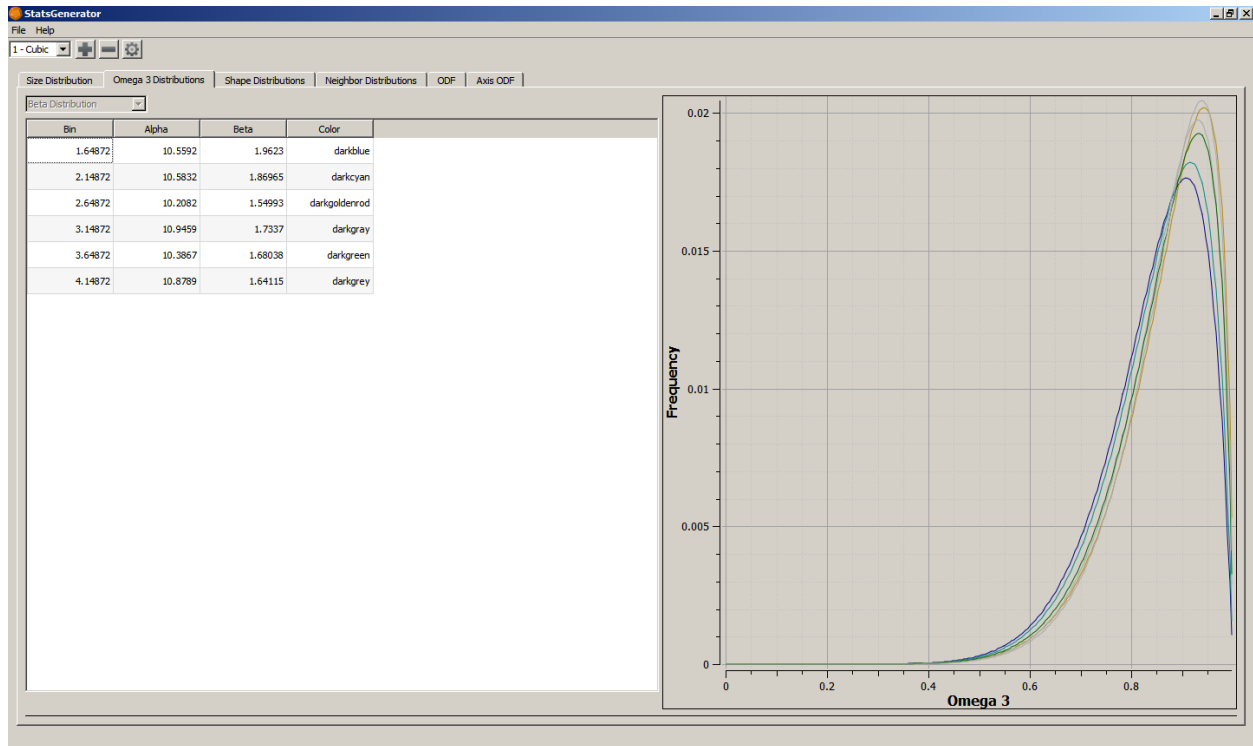
1. **Bin** – this column is calculated from the size distribution and cannot be changed.
2. **Alpha** – this is the alpha parameter of a Beta distribution. Omega 3 is normalized and can only be between 0 and 1, so the Beta distribution is a good fit
3. **Beta** – this is the beta parameter of the Beta distribution.
4. **Color** – this allows the user to change colors of the curves for image creation or easier identification during stats generation

Shape Distributions Tab (there are 3 aspect ratio combinations)
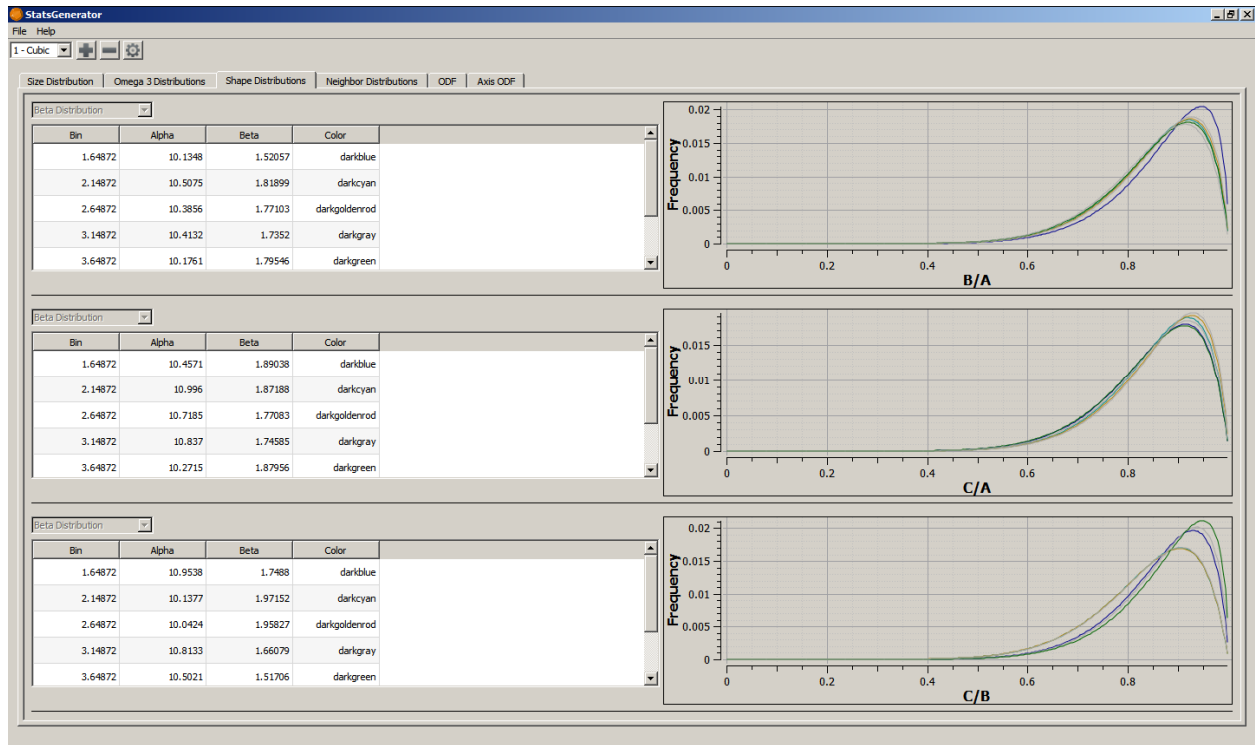
1. **Bin** – this column is calculated from the size distribution and cannot be changed.
2. **Alpha** – this is the alpha parameter of a Beta distribution. B/A, C/A and C/B are normalized and can only be between 0 and 1, so the Beta distribution is a good fit
3. **Beta** – this is the beta parameter of the Beta distribution.
4. **Color** – this allows the user to change colors of the curves for image creation or easier identification during stats generation

Neighbor Distributions Tab

1. **Bin** – this column is calculated from the size distribution and cannot be changed.
2. **Alpha** – this is the alpha parameter of a Power Law distribution.
3. **K** – this is the exponent of a Power Law Distribution
4. **Beta** – this is the beta parameter of a Power Law distribution.
5. **Color** – this allows the user to change colors of the curves for image creation or easier identification during stats generation

ODF Tab

1. ***Weights and Spreads Sub-Tab***
   a. ***Euler 1-3*** – these are the Euler angles that define an orientation that the user would like to increase in weight.
   b. ***Weight*** – this is the weight in MRD (multiples of random) to be assigned to the orientation listed
   c. ***Sigma*** – this is the spread to use in blurring out the orientation chosen. The value corresponds to the number of bins in Rodrigues (orientation) space it takes for the MRD value entered in the ***Weight*** column to reduce to 0.0 (decreasing quadratically from the bin of the entered orientation).
   d. ***Calculate ODF*** – this builds the ODF and then creates pole figures (PFs) for the user to inspect.
2. ***Pole Figure (PF) Sub-Tabs***
   a. There are three PFs formed for each of the crystal structures that can be chosen (though they are of different directions for the different crystal structures).
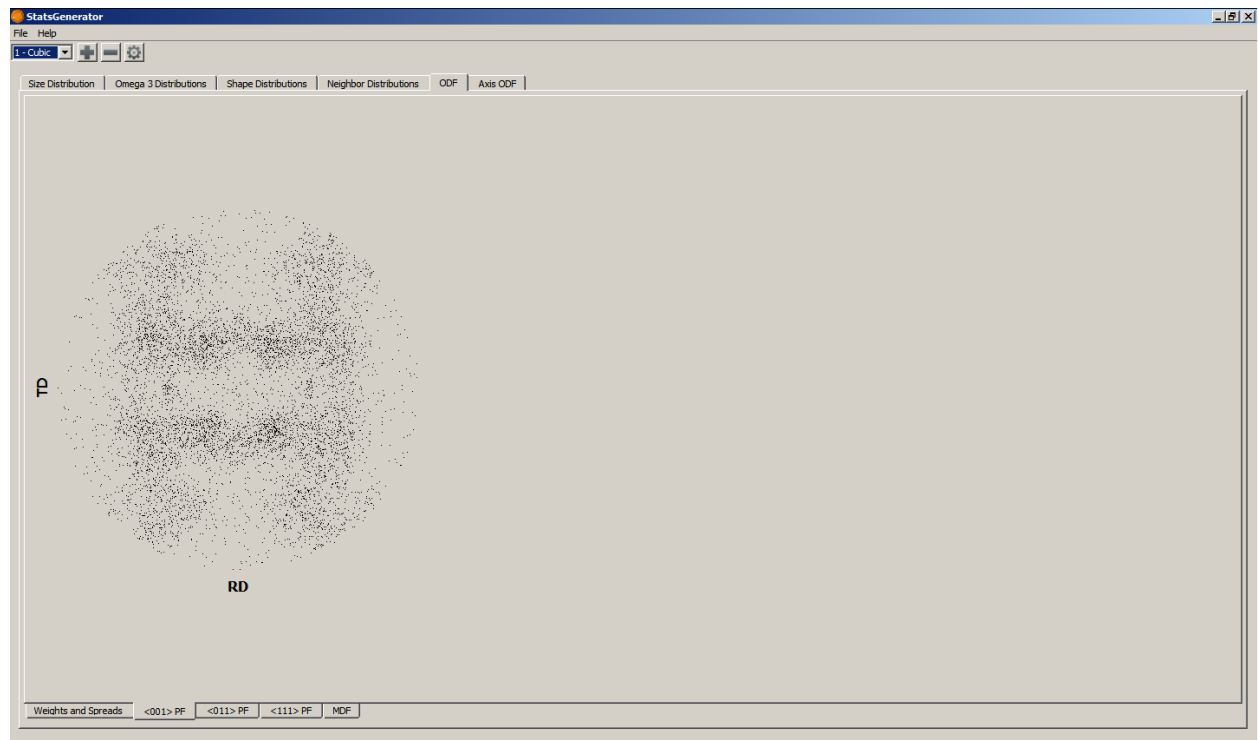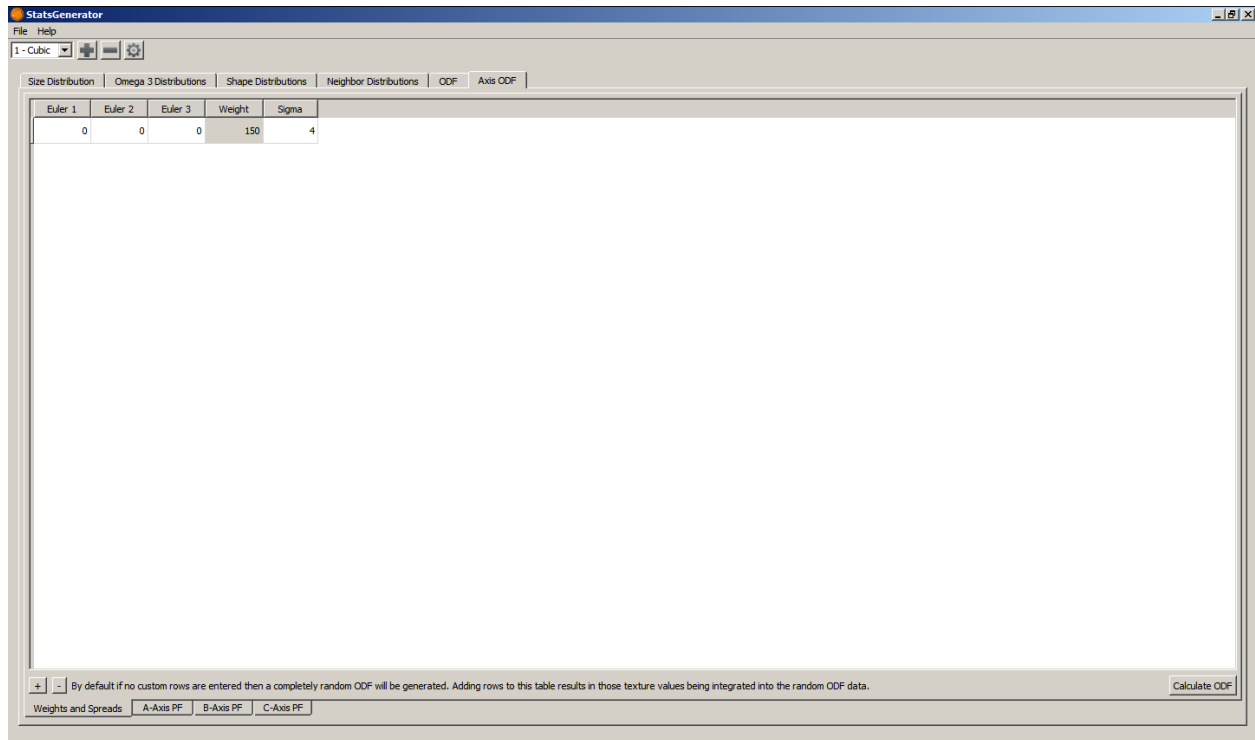
3. *MDF Sub-Tab*

    a. This sub-tab will display the baseline MDF for the generated ODF. This is done by randomly sampling pairs of orientations from the ODF and calculating the misorientation (axis-angle only). Only the angle is plotted in the misorientation distribution plot. The user can also add axis-angle pairs to increase in weight.
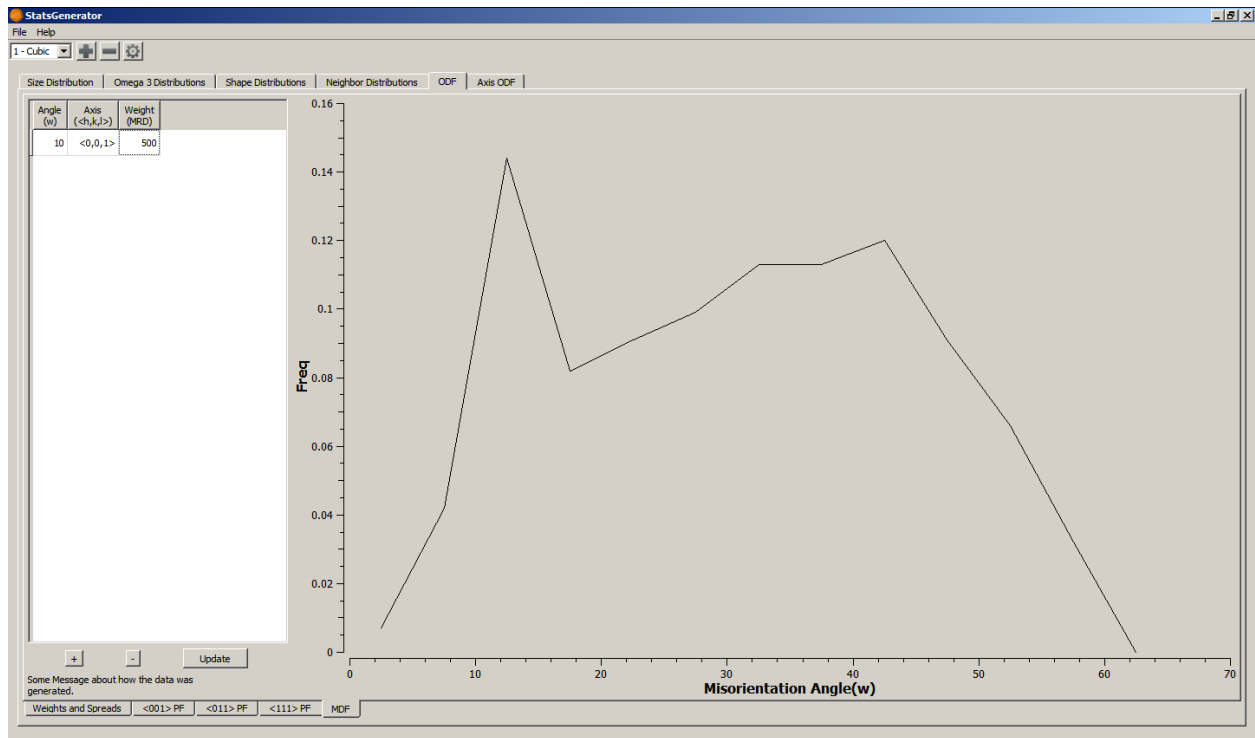
i. ***Angle*** – this is the angle of the misorientation to increase in weight.

ii. ***Axis*** – this is the axis of the misorientation to increase in weight. If the crystal structure being used for the phase is Hexagonal, then this axis is in the 3-index, orthogonal convention, not the true (hkil) convention.

iii. ***Weight*** – this is the weight in units of MRD (multiples of random) of the entered misorientation.

Axis ODF Tab

1. ***Weights and Spreads Sub-Tab***
   a. ***Euler 1-3*** – these are the Euler angles that define an orientation that the user would like to increase in weight.
   b. ***Weight*** – this is the weight in MRD (multiples of random) to be assigned to the orientation listed
   c. ***Sigma*** – this is the spread to use in blurring out the orientation chosen. The value corresponds to the number of bins in Rodrigues (orientation) space it takes for the MRD value entered in the ***Weight*** column to reduce to 0.0 (decreasing quadratically from the bin of the entered orientation).
   d. ***Calculate ODF*** – this builds the ODF and then creates pole figures (PFs) for the user to inspect.
2. ***Pole Figure (PF) Sub-Tabs***
   a. There are three PFs formed, which correspond to the location of the 3 principal axes of the grains to be generated (i.e a > b > c).