**DREAM.3D User Manual**

***Software Authors***

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**D**igital **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 EBSD (TSL. ang and HKL .ctf) 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**

**EBSD Import Tab**

**EBSD Import.tif**

* ***Input Directory*** – Directory where the EBSD (.ang or .ctf) files are located
  + ***Total EBSD Files Found*** - Code will determine how many EBSD files are present.
  + Currently only .ang and .ctf files are supported.
* ***Output File*** – Name and location of desired output .h5ebsd file
* ***Z spacing*** – This is the spacing between z slices
  + Note that the x and y spacing are automatically read from the EBSD files.
  + If the x and y spacing values change, the ones in the first section are used.
* ***File Prefix, Suffix and File Extension*** – Variables that are combined to generate the list of file names
  + These values should all be automatically determined, but should be checked if there are weird prefixes or suffixes.
* ***Start Slice, End Slice and Total Digits*** – More variables that are combined to generate the list of file names
  + Start slice and end slice define the range of data to be included in the .h5ebsd file (i.e. you don’t have to import the entire dataset).
  + Total digits control the number of leading zeros that are present in the filename.
* ***File List*** – This lists all the files that will be included in the .h5ebsd file based on the inputs chosen.
  + 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**

**Reconstruction - Input.tif**

* ***EBSD HDF5 File*** – This is the name and location of the .h5ebsd file you wish to reconstruct
  + The ***minimum and maximum slice*** numbers will be automatically displayed with the ***x, y, and z dimensions and resolutions (or spacings).***
* ***Input Parameters***
  + ***Start Slice and End Slice*** – This defines the range of sections you wish to reconstruct
    - Like you can choose to not import the entire dataset, you can choose to not reconstruct everything you imported.
  + ***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.
  + ***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.
  + ***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.
  + ***Reference Frame Origin*** – this defines the location of the origin in the EBSD file(s). 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 (corner of the scan) 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/z coordinates of the scan are all consistently modified (in conjunction with the reference z-direction) by the code during reconstruction and not changed in the .h5ebsd file (which means the origin needs to be set every time the dataset is reconstructed).
  + ***Reference Z Direction*** – this defines the positive z-direction relative to the EBSD file(s). This does two things, first it sets the order of stacking of the sections (into the slice means the first slice is on the bottom of the stack and out of slice means the first slice is the top of the stack) and second it defines the x and y directions of the scan because the setting the origin only places the origin, while defining the positive z-direction sets x and y by the right-hand rule. Note that the box itself is always placed in the positive (x, y and z) quadrant.
  + ***Merge Twins*** – this is an option that will identify 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.
  + ***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.
  + ***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).

Reconstruction - PhasesQualityMetrics.tif

* ***Phases|Quality Metrics***
  + ***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.
  + ***Voxel Quality Metrics*** – this is a bank of threshold values that are used to define whether a voxel is of good quality. Any metric stored by the EBSD collection software to define the quality, perfection or confidence in the orientation pattern or its indexing can be selected and threshold on. A voxel will only be considered a good quality voxel if it meets all of the threshold values entered in this bank. Bad quality voxels are used to define the outer boundary of a sample if that alignment method is chosen and are used to terminate the segmentation algorithm once all good quality voxels have been assigned. Bad quality voxels are then assigned via cleanup processes. The “plus” and “minus” buttons allow the user to add or subtract threshold values.
* ***Outputs*** 
  + ***Output Directory*** – location that all output files will be written to.
  + ***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.
  + ***Voxel Data File*** – this file is written automatically and is a HDF5 formatted file that is the input into the Microstructure Statistics Tab.
  + ***Optional Output Files*** – these are visualization or data files that can be created. The formats of the files vary and are listed next to the file name.
    - ***HDF5 Grains File*** - this file contains each grain’s geometry and a list of its neighbor connectivity. This file is a binary HDF5 format of VTK polydata, which can be viewed in ParaView with a special plugin.
    - ***Down Sampled Visualization File*** - this file contains (at each voxel) grain ids for the down-sampled volume
      * ***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’.
    - ***DX Voxel Data File*** - this file is similar to the HDF5 voxel data file that is automatically written, but in a slightly different format. It holds the grain ids of each voxel.
    - ***PH Voxel Data File*** - this file is also similar to the HDF5 voxel data file that is automatically written, but in a slightly different format. It holds the grain ids of each voxel.
    - ***Visualization File*** - this file is a VTK rectilinear grid format and contains (at each voxel) grain ids and potentially other attributes based on selected options:

Reconstruction - VTKOptions.tif

* + - * ***VTK Options***
        + ***Phase Ids*** – writes phase number at each voxel
        + ***IPF Colors*** – writes Inverse Pole Figure colors at each voxel
        + ***Binary VTK*** – writes the file in binary instead of ASCII
* ***Load/Save Preset*** – this allows the user to save input settings or load previously saved input settings

**Grain Generator Tab**

**Grain Generator.tif**

* ***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.
* ***Options***
  + ***Structure Already Formed*** – If a volume has already been created, this option will read the grain ids from a VTK rectilinear grid file or HDF5 voxel data file. It enters the synthetic builder right before the orientation assignment and matching, so it does not read 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.
  + ***X, Y, Z Dims and Spacing*** – these are the dimensions (number) and resolutions (spacing) of the voxels in the generated volume. The user should be aware of the size distribution when selecting these values as it will affect the number of grains in the volume.
    - ***Estimated Number of Grains*** – this is an estimate of the number of grains that will be in the volume given the size of the volume entered by the user. The final number may not be this exact value, but should be close. If the number of grains is of more critical concern than the size of the box, then the box size can be iteratively changed until the number of grains desired is reached. Note though that the box then may be too large to build due to memory issues.
  + ***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.
  + ***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.
  + ***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.
  + ***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.
  + ***Shape Types*** – this is the type of object(s) being placed during grain placement. The user can choose ellipsoids, superellipsoids, cylinders or truncated octahedra. Ellipsoids do not need the omega3 value, but the other two options require omega3 to be defined. Note that each phase can be assigned a different shape type.
* ***Outputs***
  + ***Output Directory*** – location where all the output files will be written
  + ***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.
  + ***Grain Angles File*** – this file is written automatically and is a CSV formatted file that lists the orientations (as Bunge Euler angles) of the grains in the volume.
  + ***Voxel Data File*** – this file is written automatically and is a HDF5 formatted file that is the input into the Microstructure Statistics Tab.
  + ***Optional Output Files*** – these are visualization or data files that can be created. The formats of the files vary and are listed next to the file name.
    - ***HDF5 Grains File*** - this file contains each grain’s geometry and a list of its neighbor connectivities. This file is a binary HDF5 format of VTK polydata, which can be viewed in ParaView with a special plugin.
    - ***PH Voxel Data File*** - this file is also similar to the HDF5 voxel data file that is automatically written, but in a slightly different format. It holds the grain ids of each voxel.
    - ***Grain Data File*** – this file is a CSV formatted file that lists the orientation (as Bunge Euler angles), equivalent sphere diameter, b/a, c/a, and Omega3 value of the each grain in the volume. Note that these sizes and shapes are those of the grains before packing and may be different that the sizes and shapes of the grains after the packing process (though the goal of the packing process is to retain these values).
    - ***Visualization File*** - this file is a VTK rectilinear grid format and contains (at each voxel) grain ids and potentially other attributes based on selected options:

Grain Generator - VTKOptions.tif

* + - * ***VTK Options***
        + ***Surface Voxels*** – writes the number of adjacent voxels with different neighbors at each voxel
        + ***Phase Ids*** – writes phase number at each voxel
        + ***IPF Colors*** – writes Inverse Pole Figure colors at each voxel
        + ***Binary VTK*** – writes the file in binary instead of ASCII
* ***Load/Save Preset*** – this allows the user to save input setting or load previously saved input settings.

**Surface Meshing Tab**

**Surface Mesh.tif**

1. ***Inputs***
   1. ***VTK File*** – name and location of the .vtk file that will be used in the surface meshing
      1. 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.
2. ***Options***
   1. ***Smooth Surface Mesh*** – this option allows the user to choose to run a moving finite element smooth procedure over the resulting marching cubes surface mesh.
3. ***Output Files***
   1. ***Output Directory*** – this is the location that all of the output files will be written to
   2. ***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.
   3. ***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 a threshold of the data, the grains will appear to having ‘missing’ triangular patches.
   4. ***Binary VTK File*** – This option allows the user to choose whether the output visualization file is in binary or ASCII format.
   5. ***Write STL Files*** – this option allows the user to choose to write a binary STL format triangle surface mesh for each grain in the volume.
   6. ***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.

**Stats Generator Utility Package**

**Size Distribution Tab**

**SG Size Dist Tab.tif**

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.

SG Phase Edit Popup.tif

* 1. ***Select Crystal Structure*** – this allows the user to specify the crystal structure of the phase. Currently, the two options are Cubic and Hexagonal.
  2. ***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).
  3. ***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.
  4. ***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.

1. ***Mu*** – this is the average value of the lognormal grain size distribution
2. ***Sigma*** – this is the standard deviation of the lognormal grain size distribution
3. ***Sigma Cut Off Value*** – this allows the user to truncate the distribution to remove very large grains
4. ***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.
   1. Note that the ***Bins to be Created*** is displayed in the bottom left corner
5. ***Preset Statistic Models*** – this allows the user to select a ‘morphological-type’ of microstructure to populate the default data.
   1. ***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.
   2. ***Equiaxed*** – this populates the statistic tabs with data that is designed to generate a random equiaxed microstructure.
   3. ***Rolled*** – this populates the statistic tabs with data that is designed to generate a rolled microstructure with elongated grains with user defined aspect ratios.

SG Rolled Preset Popup.tif

* + 1. ***Aspect Ratio 1*** – this is the aspect ratio between the dimensions of the grains in the rolling direction and transverse direction, respectively.
    2. ***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.

1. ***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**

**SG Omega3 Tab.tif**

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)**

**SG Shapes Tab.tif**

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**

**SG Neighbors Tab.tif**

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**

**SG ODF Tab.tif**

1. ***Weights and Spreads Sub-Tab***
   1. ***Euler 1-3*** – these are the Euler angles that define an orientation that the user would like to increase in weight.
   2. ***Weight*** – this is the weight in MRD (multiples of random) to be assigned to the orientation listed
   3. ***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).
   4. ***Calculate ODF*** – this builds the ODF and then creates pole figures (PFs) for the user to inspect.
2. ***Pole Figure (PF) Sub-Tabs***
   1. 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).

SG ODF 001 PF Tab.tif

1. ***MDF Sub-Tab*** 
   1. 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.

SG ODF MDF Tab.tif

* + 1. ***Angle*** – this is the angle of the misorientation to increase in weight.
    2. ***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.
    3. ***Weight*** – this is the weight in units of MRD (multiples of random) of the entered misorientation.

**Axis ODF Tab**

**SG Axis ODF Tab.tif**

1. ***Weights and Spreads Sub-Tab***
   1. ***Euler 1-3*** – these are the Euler angles that define an orientation that the user would like to increase in weight.
   2. ***Weight*** – this is the weight in MRD (multiples of random) to be assigned to the orientation listed
   3. ***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).
   4. ***Calculate ODF*** – this builds the ODF and then creates pole figures (PFs) for the user to inspect.
2. ***Pole Figure (PF) Sub-Tabs***
   1. 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).

SG Axis ODF A Axis Tab.tif