OIM Data Import Tab

1. Input Directory – Directory where the .ang files are located
   1. Code will determine how many .ang files are present
   2. 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
   1. Note that the x and y spacings are automatically read from the .ang files
   2. 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
   1. 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
   1. 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)
   2. 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 choosen.
   1. 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
   1. 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
   1. Like you can choose to not import the entire dataset, you can choose to not reconstruct everything you imported
3. Options – These are all the options that can be set to control the reconstruction
   1. Merge Colonies – this is an option that will reconstruct prior beta grains in an alpha-beta titanium microstructure. It will first identify alpha colonies and then compare neighboring colonies to group colonies form the same prior beta grain
   2. Grains Formed – this is an option to read in a previously reconstructed volume in which the grain ids have already been assigned. Currently it reads the output data from Yoon’s Abaqus analysis and from the FFT code at CMU. I am working to change the format the data is read in and create a standard.
   3. Merge Twins – this is an option similar to Mere Colonies, but when comparing neighboring grains to be merged it uses misorientations linked to twins not colonies from the same beta grain
   4. Cryst. Struct. – this is the crystal structure (i.e. Cubic, Hexagonal, Orthorhombic) of the material being reconstructed. This defines what symmetry operators are used during the misorientation calculations. Note that right now only one crystal structure can be selected at a time, but we are working to allow crystal structures to be assigned to multiple phases that can be present
   5. 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 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.
   6. Ang Orientation – this defines the origin of the ang file.
   7. Min Grain Size – this a clean-up filter that can be set to merge grains below a defined size after grains have been formed. Currently the grains are reset to unassigned and then the region is filled in by a local grain growth algorithm
   8. Disorient. Tol. – this is the orientation difference tolerance allowed between neighboring regions before they are declared different grains
   9. 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
   10. Min. Confidence Index – this is threshold used the same as Min. Image Quaity
   11. 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.
   12. 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.
4. Output Directory – location that all output files will be written to.
5. Optional Output Files – these are all visualization files that can be created.
   1. Reconstruction Visualization - this file contains grain ids and Euclidean distance to grain boundaries
   2. Reconstruction IPF Visualization - this file contains grain ids and Inverse Pole Figure colors
   3. Reconstruction Disorientation Visualization - this file contains grain ids and Kernel Average Misorientations and Grain Average Misorientations
   4. Reconstruction ImageQuality Visualization - this file contains grain ids and Image Qualities
   5. Reconstruction SchmidFactor Visualization - this file contains grain ids and Schmid Factors
   6. Reconstruction DownSampled Visualization - this file contains grain ids for the down-sampled volume
   7. Reconstruction Grains - this file contains each grain with properly defined voxels and their neighbor connectivities
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Synthetic Builder

1. HDF5 Stats File – name and location of the input stats file that can be generated from the reconstruction tab or the stats generator module.
2. Output Directory – location where all the output files will be written
3. Options
   1. Structure Already Formed – this is similar to the option in the reconstruction tab. 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 need any orientation information, just the structural information.
   2. Space Filling Error Weight – this the weight to be applied to the criterion of maximizing space filling during grain placement.
   3. Size Distribution Error Weight – this is the weight to be applied to matching the size distribution during grain placement.
   4. Neighborhood Error Weight – this is the weight to be applied to matching the local neighborhoods during grain placement
   5. 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.
   6. 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 do to memory overload are possible.
   7. Shape Class – this is the type of object 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.
   8. Crystal Structure – this is the crystal structure of the material (i.e. cubic or hexagonal) and is used during the misorientation calculations and orientation matching portion of the builder.
   9. Precipitate Structure – this is an option to place precipitates in the volume on either boundaries or randomly throughout the structure. Currently this option is not useable because neither the reconstruction tab or the stats generator produce statistics for precipitates.
   10. Volume Fraction Precipitates – this defines the amount of precipitates to be placed in the structure
4. Load/Save Preset – this allows the user to save input setting or load previously saved input setting

Surface Meshing Tab

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. It only reads the grain ids block from any of those files.
2. Output Directory – this is the location that all of the output files will be written to
   1. The output file is a .vtk file of poly data
3. 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 is under development with CMU.

Stats Generator Package

1. Size Distribution Tab
   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 number of bins that will be created is displayed in the bottom left corner
   5. Create Default Data – this locks in the values you have entered and populates the other tabs with default values.
2. 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
3. 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 all 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
4. 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
5. ODF Tab
   1. Texture – these are a list of common FCC textures.
   2. Weight – this is the weight in Times Random to be assigned to the texture listed
   3. Sigma – this is the spread to use in blurring out the texture chosen.
   4. Calculate ODF – this builds the ODF and then creates pole figures for the user to inspect.
   5. MDF – this sub-tab will display the baseline MDF for the generated ODF, but is not currently finished.