Digital Representation Environment for Analysis of Microstructure in 3D

dream3d.bluequartz.net

Mr. Michael A. Jackson
Owner
BlueQuartz Software
Acknowledgements

Mike Groeber (AFRL)

• Funding (AFRL & NRL)
  • Contract FA8650-07-D-5800
  • Contract FA8650-10-D-5210
  • Contract N00173-07-C-2068

• Code, Ideas, Vision
  • The Ohio State University
  • Carnegie Mellon University

• Anyone who has
  • Tested
  • Provided Feedback
  • Bug Reports
  • Data
  • Corrections
  • Discussions
Development Team
Development Team

Dr. Mike Groeber
Development Team

Mr. Mike Jackson

Dr. Mike Groeber

Algorithms
Topics

- What is DREAM3D?
- What DREAM3D is NOT
- Examples
  - 2D/3D reconstruction & analysis
  - Surface Meshing Algorithms
  - Synthetic Microstructure Generation
What is it?

Environment that integrates algorithms in such a way as to allow those algorithms to communicate inputs and outputs between them.
The Motivation for DREAM.3D

Understanding, accounting for and/or utilizing anisotropy and inhomogeneity in materials is critical in the engineering design process.

Each processing step affects μ/s, properties & performance.

Must control processing & predict microstructure across scale of component.

Each μ/s feature contributes to properties & performance.

Must understand microstructure effects & predict response for gambit of microstructures.

Adapted from Semiatin & Woodward, 2011

Adapted from Larsen & Woodward, 2011
The Evolution to DREAM.3D

Significant, isolated work completed by multiple researchers on different programming platforms and with different data formats.
What DREAM3D is NOT?

- Direct Visualization
- Use another more capable package
  - ParaView
  - Avizo Fire
  - MATLAB
  - IDL
Data Representation
The Backbone of DREAM.3D

Hierarchy of microstructure features/gradients accounted for in extensible digital data structure
Getting Data Into DREAM3D

- Input Data
  - TSL, HKL, HEDM for Orientation Data
  - Raw Binary Files
    - You describe it, DREAM3D can read it
  - H5Ebsd for archived Orientation Data
  - Ph, Dx with Grain Ids
- Pre-Segmented Images ***
Getting Data Out of DREAM3D

- Voxel Based Export Formats
  - VTK Rectilinear Grids and Polydata (.vtk)
  - Xdmf file wrappers (.xdmf)
  - Avizo Rectilinear Grids (.am)
  - CSV File for Statistical data
  - Ph and Dx* files (CMU Legacy)
  - FFT Simulation Codes (Los Alamos)
  - Tif, Bmp, Png for Misc Images (IPF Color Maps)

- Triangle Based Exports
  - STL
  - VTK PolyData
  - XDMF
  - Nodes/Triangles/Edges Ascii Files
  - Abaqus File (Experimental)
HDF5

- Open Source & Free
- Built for LARGE quantities of data
- 100s GB to TB sizes
- Fully self describing
- Rich meta data attachment
- User selects how to organize the data
- Free HDFView to visualize and export data

www.hdfgroup.org
XDMF

- Small XML wrapper file
- Describes the grids used in DREAM3D
- ParaView has native support
- User can selectively load data
- Store BOTH Voxel and Triangle based representations
- HIGHLY recommended to use this file type instead of the .vtk files
Caution !!

- DREAM3D is just a Tool
- Understand your data
  - Degrees or Radians?
  - Phases? Crystal Symmetry?
- Understand the algorithms
- Is it appropriate for my data?
- GIGO:
  - Garbage In, Garbage Out
So, what does it look like?
Filter Groups, Prebuilt & Favorites
Errors & Warnings
Basics
Basics

Right Click to show Help for filter
Basics

Click to show DREAM3D Help
Red Filter outline mean errors in the pipeline setup
Basics: Favorites

Show in Finder

Drag filters here to build up a pipeline
Basics: Favorites

Click to show Favorite Pipelines

Drag filters here to build up a pipeline
Basics: Favorites

Click to show Favorite Pipelines

Right click favorite for options

Drag filters here to build up a pipeline
Basics: Favorites

Click to show Favorite Pipelines

Right click favorite for options

- Save Pipelines to text files
- Share Pipelines with colleagues
Read H5Ebsd File

Group (Subgroup)

I/O Filters (Input)

Description

This Filter reads from the "*.h5ebsd" file that was generated with the Import Orientation File(s) to H5Ebsd filter. The user can use the checkboxes under the "**Voxel Data**" tab to select which specific data arrays they are interested in processing. Different pipelines may require different arrays to be read and this advanced interface allows the user to be selective in the data that is read into memory for processing. The user can select a subset of the slices if they do not wish to process the entire volume of data. The type of transformations that are recommended based on the manufacturer of the data are also listed with a checkbox that the user can check to make sure the data is transformed into the proper Euler and Spatial reference frame.

If the processing pipeline is going to process phase based data for crystallographic information the user should enable the reading of the CrystalStructure _**Ensemble Data**_ array.

Example:

```
EBSD HDF5 File: /ers/Shared/Data/Ang_Data/Small_IN100_Output/Small_IN100_h5ebsd

X Dim: 189  X Res: 0.25  Minimum Slice: 1  EBSD Manufacturer: TSL
Y Dim: 201  Y Res: 0.25  Maximum Slice: 117  Sample Transformation(Recommended): 180 @ <010>
Z Dim: 117  Z Res: 0.25  Stacking Order: Low To High  Euler Transformation (Recommended): 270 @ <001>
Start Slice: 1  End Slice: 117  Use Recommended Transformations: 
```
Example Pipelines

- Archiving Data
- EBSD Reconstruction
- Microstructure Statistics
- Synthetic Microstructure Generation
Archiving Data

- 3D Data has multiple files
- Meta data scattered throughout extra files
- Keep all the data in a single location
- DREAM3D archives the raw data into HDF5 based files
- EBSD: Watch your Reference Frames!!!
### Table View - Image Quality

<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>235.8</td>
</tr>
<tr>
<td>2</td>
<td>226.4</td>
</tr>
<tr>
<td>3</td>
<td>219.9</td>
</tr>
<tr>
<td>4</td>
<td>217.2</td>
</tr>
<tr>
<td>5</td>
<td>201.1</td>
</tr>
</tbody>
</table>

### Table View - Phi

<table>
<thead>
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<th>0</th>
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</thead>
<tbody>
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<td>1.97701</td>
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<tr>
<td>2</td>
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<td>4</td>
<td>1.44902</td>
</tr>
<tr>
<td>5</td>
<td>1.43330</td>
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</table>

### Table View - Confidence Index

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</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>2</td>
<td>2.3883</td>
</tr>
<tr>
<td>3</td>
<td>2.3831</td>
</tr>
<tr>
<td>4</td>
<td>12.56637</td>
</tr>
<tr>
<td>5</td>
<td>0.714</td>
</tr>
</tbody>
</table>

### Text View - OriginalHeader

```plaintext
# TEM_PIXperUM   1.000000
# x-star         0.372300
# y-star         0.689300
# z-star         0.970100
# WorkingDistance 5.000000
#
# Phase 1
# MaterialName   Nickel
# Formula        Ni
# Info
# Symmetry       43
# LatticeConstants 3.520 3.520 3.520 90.000 90.000 90.000
# NumberFamilies 4
# hkIFamilies    1 1 1 0.000000
# hkIFamilies    2 0 0 1.000000
# hkIFamilies    3 3 0 1.000000
```
3D Reconstruction
Overview - EBSD

- Import the data
- Align slices
- Segment the grains
- Cleanup the data
ParaView Visualization

1. Select the 'Surface' option.
2. Adjust the 'Magnitude' setting.
3. Utilize the 'Search' feature for color customization.
4. Set the 'Opacity' to 1 and the 'Interpolation' to Couraud.

2013 Aug 20. Materials in 3D: Modeling and Imaging at Multiple Length Scales
Monday, August 26, 13
Small IN100

- “The” IN100 3D data (Uchic et. al.)
- 117 Slices
- EBSD, IISE, 4x SE Tilts
- Pt Cap on sample
- Available on DREAM3D Web Site
Small IN100

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As Imported

- Doesn’t look too bad?
- What could be wrong?
Slice Volume (X Axis)

- Several Slices badly out of alignment
What are Good Voxels?

Confidence Index

Image Quality
After Defining Good Voxels
After Alignment Step
After Clean Up Filters
Categories of Reconstruction Filters

- Clean up, Conversion, Thresholds
- Alignment, Grouping, Segmentation
- Cropping, Cutting, Rotation, Resolution
- See DREAM3D User manual for more
EBSD Reconstruction

Nickel Super Alloy—Data Courtesy of M. Uchic AFRL

Nickel Super Alloy with Internal Pore—Data Courtesy of M. Uchic AFRL

2 Phase Steel Alloy. Data courtesy of Colette Rey and Thierry Auger, ECP/MSSMAT, UMR CNRS 8579, France
Other Data Sources

- HKL .ctf files (EBSD)
- HEDM (from APS)
- Pre-Segmented gray scale Images
EulerAngles (17799956)
32-bit floating-point, 4444713 x 3
Number of attributes = 2
NumComponents = 3
ObjectType = DataArray<float>
Calculating Statistics
Categories of Stats

• Crystallographic
• Avg Orientation...
• Morphological
  • Grain Size, Num Neighbors
• Ensemble Stats
• To Feed into StatsGenerator
• Export Data as CSV File
Computed Statistics
5 Parameter GBCD

- Rohrer, Rowenhorst, Rollett, DeGraef
- Experimental in 4.2.97
- Still in development

Small IN100 60Deg @ <111>
Surface Meshing
Two Algorithms

- MultiMaterial Marching Cubes
  - Initially Smoother Structure
  - Slow to run
  - Inconsistent triangle winding
- Quick Mesh
  - Follows exact voxel boundary
  - Very fast to run
  - Consistent Triangle Winding
2D View Comparison

M3C: White
Quick: Black
Meshing Comparison

M3C

Quick
Export Mesh

- Write STL file PER grain
- Write raw nodes & triangles file
- Write an Abaqus file
  - Experimental currently
- Write VTK polydata
- Write a DREAM3D file
MFE Smoothing

- Donated by A.D. Rollet @ CMU
- Moving Finite Element Method
- Compute intensive
- Guarantees triangle aspect ratios
- Algorithm needs some updating
- Volunteers?

Laplacian Smoothing

- Iterative Process
- Node positions changed
- Topology not changed
- Tends to shrink the mesh
- Input Lambda values range 0 to 1.0


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Filters Applied to Mesh

- Centroids, Normals, Areas
- IPF Colors, Misorientation Colors
- Grain Face Curvature
Generating Synthetic Microstructures
Generating Synthetic Micros

• Need a set of statistics that describe your microstructure

• Compute or Create

• Distributions
  • Grain Sizes
  • Shapes
  • Neighbors

• Texture
  • ODF, MDF
Generating Synthetic Micros

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Generating Synthetic Micros

- Single Phase Equiaxed
- Single Phase Rolled
- Fiber Composite
Synthetic Summary

- Define Statistics
- StatsGenerator
- DREAM3D itself (Compute Ensemble Statistics)
- Use DREAM3D to generate the structure
- Mesh and Export to modeling program
Real World Uses
• CMU (rollett@andrew.cmu.edu)

• Synthetic microstructures that represent complex 2-phase titanium alloys.

• Synthetic microstructures that represent nano-twinned copper

• Extract microstructural data (volume fractions etc) from multiphase microstructures for fuel cells.
ARL and UCSB

- ARL
  - Synthetic microstructures that represent pearlitic steel alloys.

- UCSB
  - Analyze Femto-Second LASER ablated Ti-6-4

Image courtesy of B. Anglin (ARL)
Arizona State Univ.

- Manual Reconstruction
- 2 weeks effort
- Inconsistent grain numbering

- DREAM3D/Avizo Fire
- Initial 3D Reconstruction
- Surface Mesh
- 1.5 Hours

Adding Plugin to DREAM3D
Layers of DREAM3D
Layers of DREAM3D

- C/C++ Compilers
- CMake
- Doxygen
- Git
Layers of DREAM3D

Qt  Qwt  Boost  HDF5  Eigen  TBB
C/C++ Compilers  CMake  Doxygen  Git
Layers of DREAM3D

Qt  Qwt  MXA  DREAM3DLib  H5Lite  EBSDLib
  Boost  HDF5  Eigen  TBB
C/C++ Compilers  CMake  Doxygen  Git
Layers of DREAM3D

- DREAM3D & StatsGenerator
- Plugins
- Qt
- Qwt
- MXA
- DREAM3DLib
- H5Lite
- EBSDLib
- Boost
- HDF5
- Eigen
- TBB
- C/C++ Compilers
- CMake
- Doxygen
- Git
Why a Plugin?

- Proprietary Codes
  - Company does not want to release sources
  - Protect Intellectual Property
- Internal development
- Incompatible source codes
  - Codes will not compile on all platforms
- Introduce External Library dependencies
Create a Plugin

• Use the “PluginMaker” application.

• Compiled with DREAM3D

• Generates all the basic code and support files

• Allows you to concentrate on your filter

• Group all your filters into a single plugin
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• Generates all the basic code and support files
• Allows you to concentrate on your filter
• Group all your filters into a single plugin
• Will Lenthe @ UCSB writing Plugins!!
Getting Help

- http://dream3d.bluequartz.net
- Email DREAM3D@bluequartz.net
- User Manual on Web Site
- Several Tutorials in the User Manual
Ideas for the Future

• Process Images
• Improved FEM Workflows
• Pole Figures for Texture Analysis
  • Currently Testing
• Python Access to DREAM3D Algorithms
• More Parallelization
  • OpenCL (CUDA)
Ideas for the Future

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Cost & License

• BSD Licensed

• http://opensource.org/licenses/BSD-3-Clause

• What you have today is FREE to use.
Availability

- [http://dream3d.bluequartz.net/downloads/](http://dream3d.bluequartz.net/downloads/)
- Version 4.2.x available NOW.
- System Requirements
  - Windows 32/64 bit
  - OS X 64 Bit (10.6.8/10.7/10.8)
  - Linux RHEL 6.3
- Reasonable Graphics card for Visualization
Source Code

- Hosted at GitHub.com
  - http://github.com/DREAM3D
- Anyone can get the source code
- Track Issues, Report Bugs, Wiki
- Follow development of DREAM3D
- Work in your own area then request your changes to be merged into DREAM3D
Users*

DoD and DoE Laboratories
Air Force Research Lab, OH+FL, USA
Los Alamos National Lab, NM, USA
Naval Research Lab, VA, USA
Idaho National Lab, ID, USA
NASA Langley, VA, USA
Army Research Lab, MD, USA
Sandia National Lab, NM, USA

OEMs/Industry
GE Global, NY, USA
GE Aviation, OH, USA
HRL Laboratories LLC, CA, USA

International
Ghent University, Belgium
Univ. Paul Verlaine-Metz, France
Queens Univ., Canada
Seoul National Univ., S. Korea
Univ. of Manchester, UK
Univ. Lorraine, France
Salzgitter Mannesmann Forschung GmbH, Germany
Deakin University, Australia
King Abdullah Univ., Saudi Arabia
University College, Ireland
Riso/DTU, Denmark
Pohang Univ., Korea

U.S. Academia
Ohio State Univ., OH, USA
Carnegie Mellon Univ., PA, USA
Cornell, NY, USA
Univ. of Michigan, MI, USA
Drexel Univ., PA, USA
Lehigh Univ., PA, USA
Iowa State Univ., IA, USA
Northwestern Univ., IL, USA
Purdue Univ., IN, USA
Georgia Tech, GA, USA
Univ. of North Texas, TX, USA
Johns Hopkins Univ., MA, USA
Boise State Univ., ID, USA
Univ. of Dayton, OH, USA
Univ. of Pittsburgh, PA, USA
Vanderbilt Univ., TN, USA
Univ. of Kentucky, KY, USA
Univ. of California Santa Barbara, CA, USA
Univ. of Florida, FL, USA
Univ. of Texas at San Antonio, TX, USA
Wright State Univ., OH, USA
Case Western Univ., OH, USA
Univ. South Carolina, SC, USA
Mississippi State Univ., MS, USA