2015 UCSB Workshop on Collection and Analysis of Big Data in 3D Materials Science Software Guide

Software List and Brief Description

SPPARKS (Stochastic Parallel PARticle Kinetic Simulator) – An open-source grain growth/microstructure evolution code package from Sandia National Laboratory.

DREAM.3D (Digital Representation Environment for Analyzing Microstructure in 3D) – An open-source suite of microstructural analysis tools to visualize, reconstruct, quantify, mesh and instantiate microstrucutal datasets developed at Air Force Research Laboratory with BlueQuartz Software.

CTEMSoft (Conventional Transmission Electron Microscopy Software) – An open-source code package for simulating (or forward modeling) data/images generated by electron microscopy.

FIJI (Fiji Is Just ImageJ) – An open-source image processing toolset built upon ImageJ developed at a number of institutes, but primarily Univ. of Wisonsin-Madison and MPI-CBG in Dresden, Germany.

FFT (Full-Field Fast Fourier Transform) – A pseudo-open-source software package for simulating the response of material microstructures developed at Los Alamos National Laboratory.

Paraview – An open-source data analysis and visualization application developed at Los Alamos National Laboratory and maintained by Kitware, Inc.

HDFView – A free-ware visual tool for browsing and editing HDF4 and HDF5 files developed and supported by HDFGroup.org.

Notes for Obtaining Software

SPPARKS – http://www.cs.sandia.gov/~sjplimp/spparks.html See separate document for full build notes for SPPARKS.

DREAM.3D – DREAM.3D is a built for Windows, OSX and Linux. The precompiled binaries can typically be found at http://dream3d.bluequartz.net/?page_id=32 HOWEVER, for this workshop, we will be using a pre-release, beta-version that can be found at http://dream3d.bluequartz.net/binaries/experimental/ When visiting the experimental page, look for the most recently dated folder and then the operating system you wish to download. There is no installation necessary for DREAM.3D, simply unpack the downloaded file and open the DREAM.3D executable.

CTEMSoft – The source code can be found at https://github.com/marcdegraef/CTEMsoft The code is written in Fortran90 (some Fortran77), so a Fortran compiler will be necessary. There is a README file in the source code that explains the building procedure.

FIJI – A precompiled executable can be found at http://fiji.sc/Downloads and no installation is necessary to use FIJI, simply unpack the download and begin. For development or modification of FIJI, the source code can be obtained at https://github.com/fiji/fiji/

FFT – The FFT package is currently "by request only" and can be inquired about by emailing its developer at lebenso@lanl.gov.

Paraview – A precompiled binary can be found at http://www.paraview.org/download/ and no installation is necessary, simply unpack the download and begin using. The source code can be obtained from https://gitlab.kitware.com/paraview/paraview

HDFView – A precompiled binary is located at http://hdfgroup.org/products/java/release/download.html

Comments about Software Tutorials

SPPARKS – Being a simulation tool, the examples that will be shown may not be realistic to run in real-time during the tutorial. The tutorial will cover how to use SPPARKS and details of the input and output files, but will not be a truly "hands-on" tutorial. As such, building the code prior to the workshop is not a necessity to participate in the tutorial.

DREAM.3D – DREAM.3D will be used/highlighted in a number of the tutorials as the main focus or as a pre- or post-processor of the data for other tools. There will be a brief, high-level overview of how to use DREAM.3D that will be more "hands-on". Some of the tutorials will have "follow along" examples and others will have more pre-worked examples. It is recommended though that DREAM.3D is acquired prior to the workshop to be able to follow along where appropriate.

CTEMSoft – The computations in CTEMSoft are somewhat lengthy and will be demoed during the tutorial as pre-worked examples. Attendees are welcome to download the source code and compile the package in advance, but the tutorial will not be run as a "hands-on" demo. There is a precompiled Mac binary that will be made available at the time of the tutorial for those using OSX.

FIJI – The FIJI demo will be more "hands-on" than many of the other tutorials. There will be time spent on the location of tools within the package and how to apply them. The tutorial will be worked on data that will not be supplied to the attendees, so if you would like to follow

along, bring some images of your own. The tutorial will mainly focus on the thought processes that should be employed when using the tool, but functional use of the code will also be explained. It is recommended that the attendees obtain FIJI prior to the workshop.

FFT – The FFT package is a simulation tool and while significantly faster than Finite Element, is not practical to run in real-time during the tutorial. The tutorial will cover how to set up simulations and visualize the results. The tutorial will focus on the sensitivities and subtleties of the tool. It is not necessary for the attendees to obtain the FFT package prior to the workshop to participate in the tutorial.

Paraview – Paraview will be used as a visualization tool associated with many of the tutorials. There will be some overview of the layout of the software and how to perform various simple actions. Users are encouraged to download Paraview prior to the workshop.

HDFView – HDFView will be briefly covered in association with the DREAM.3D tutorials. The use and layout of the tool will be quickly overviewed, but is not critical to follow along. Attendees will be able to follow along with HDFView demos to gain comfort, but is not critical to the tutorial participation. Users are recommended to obtain HDFView prior to the workshop if desired.