

APS Scientific Computation Seminar Series

Speaker: Patrick Avery, Senior R&D Engineer, Kitware

Title: Analyzing X-ray Diffraction Data Using the Open-Source HEXRDGUI Application

Date: May 15, 2023

Time: 1:00 p.m. (Central Time)

Location: Join ZoomGov Meeting

<https://argonne.zoomgov.com/j/1601444470?pwd=N1phbHZVdCtmcVR5cGh0c1Zhc0orZz09>

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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract: HEXRDGUI is a cross-platform open-source application for analyzing and visualizing X-ray diffraction image data. Built upon the Highly Extensible X-Ray Diffraction (HEXRD) Python library along with several scientific Python libraries, HEXRDGUI provides many interactive workflows for visualizing and processing diffraction images using the generic multi-detector instrument model in HEXRD. HEXRDGUI supports several diffraction modalities: powder, Laue, and multi-grain rotation (a.k.a. 3DXRD, HEDM). Robust instrument calibration workflows are available for each modality. Whole powder pattern fitting (WPPF) methods such as the LeBail and Rietveld analyses are also available. This talk will demonstrate how different interactive visualization techniques have been invaluable for analyzing X-ray diffraction data from a wide array of experimental platforms. A few additional open-source scientific applications that may be of interest will be briefly mentioned as well.