APS Scientific Computation Seminar Series

Speaker:
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Title:
Accelerating Diffraction Analysis Using the MAUD Interface Language Kit (MILK)

Date:
March 11, 2024

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

Location:
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Abstract:
Diffraction experiments often result in tens to thousands of patterns from which information can be extracted ranging from microstructure to equation of state. The extraction happens by fitting models of the diffraction process which describe the instrument (e.g. sample-to-detector distances and angles), the sample's crystal structure (e.g. crystallographic space group and lattice parameters), and the microstructure (e.g. phase fractions and texture). Finding the set of parameters that best describes a measurement is hard to do in a robust way without expert intervention and in a way that leverages parallel resources (critical for real-time analysis). Benchmark examples of the open-source Python scripting framework for MAUD Rietveld software (MILK) will be presented with the Python Rietveld optimization and uncertainty quantification package (Spotlight) which together enable the scalable Rietveld optimization strategy for large datasets and advanced analysis workflows (e.g. sampling uncertainty in key parameters).