APS Scientific Computation Seminar Series

Speaker: Vivek Thampy, Project Scientist

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Title: X-Dart: A GUI tool for XRD data visualization and analysis based on pyFAI and pyGIX

Date: Monday, March 14, 2022

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

Location: Join ZoomGov Meeting

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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract: The increased use of area detectors to collect x-ray scattering data over the last several

years has positively impacted user science by increasing data collection efficiency, and enabling more complex in-situ/operando experimentation. However, the concomitant increase in data rates has led to significantly increased complexity of data analysis. In this talk, I will present a graphical tool, X-Dart, based on the powerful pyFAI and pyGIX packages, that we've been developing to perform both rudimentary data handling functions (i.e., calibration, reciprocal space transformation, and integration), as well as data interpretation (i.e feature identification, fitting and real space modelling) so as to be applicable to the majority of scattering users. The more advanced data interpretation functions such as feature identification, unit cell determination will be implemented using ML-based algorithms that are also being developed. These tools are meant to provide users with data handling tools that enable them to both make informed decisions while they are running experiments, as well as perform detailed analysis of their data upon returning to their home institution in a timely fashion.