

APS Scientific Computation Seminar Series

Speaker: Christopher Fancher, Oak Ridge National Laboratory
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Title: Real-Time Reduction of Time-of-Flight Neutron Diffraction Data at the SNS

Date: August 29, 2022

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

Location: <https://argonne.zoomgov.com/j/1615356746>

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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract: Time-of-flight (TOF) neutron diffraction is an energy-dispersive technique that exploits the temporal dispersion of pulsed neutrons to resolve their energy. When coupled with large, pixilated area detectors, the resulting data provides simultaneous access to extensive volumes in reciprocal space. This data is especially potent when applied to studies of real-world materials with complex sample textures and anisotropic strains. However, the resultant computational processing necessary to remove instrumental artifacts is significant. The slow data reduction pipelines have become a critical issue on the brightest TOF instruments at the Spallation Neutron Source (SNS) at ORNL, whose data rates heavily stress existing frameworks for data reduction. Much of the computational complexities arise from the “event” data structure that maintains a timestamp for detected neutrons. The underlying event structure is beneficial as this data streamline time-resolved and stroboscopic measurements by storing synchronized neutron and metadata within a single file. The challenge is perhaps most keenly felt by the VULCAN and SNAP diffractometers, which focuses on real-time *in situ* measurements and demand instant access to and visualization of the reduced neutron data. Alternative data reduction approaches are needed to facilitate AI/ML accelerated experiments. In this talk, we will summarize the current state of play and touch on some of the key priorities and strategies relating to data reduction at the SNS.