APS Scientific Computation Seminar Series

Speaker:
Weijian Zheng, Postdoctoral Appointee, Data Science & Learning Division

Title:
AI-Driven Approaches for X-ray Diffraction: Rapid Plastic Deformation Detection and Scalable ML Infrastructure

Date:
March 17, 2025

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:
This presentation will highlight two research efforts—fast anomaly detection for X-ray diffraction and M2ML's scalable machine learning infrastructure. Both contribute to advancing AI-driven automation and computational efficiency in large-scale scientific research, supporting next-generation facilities like APS-U. Advancements in high-energy X-ray diffraction and machine learning are transforming materials research by enabling faster detection of plastic deformation events in metallic polycrystals. Tracking these deformation events is crucial for understanding material behavior under stress and improving the design of structural materials. Our automated anomaly detection method achieves up to 50× speedup, efficiently identifying these events. We also present a preliminary study on pinpointing individual grains responsible for plastic deformation, leveraging MIDAS simulations for further investigation. At the same time, the growing complexity of machine learning models and expanding data volumes demand scalable solutions. We introduce M2ML, a high-performance framework that streamlines data transfer, model training, fine-tuning, and inferencing across experimental facilities, HPC centers, and edge devices. By integrating Globus services, M2ML automates complex workflows and optimizes distributed computing resources.