APS Scientific Computation Seminar Series

Speakers:
Ayana Ghosh, Research Scientist, Oak Ridge National Laboratory, Tennessee
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Title:
HPC-driven autonomous experiments in action

Date:
February 17, 2025

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

Location:
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Hosts:
Mathew Cherukara and Nicholas Schwarz

Abstract:
Recent advancements in algorithms and electron microscopy offer the potential to integrate theoretical models with experiments for solving material science challenges. AI methods excel in extracting atomic features from images, predict physical properties, while being useful to find regions of interest to perform next set of measurements. However, challenges remain in creating an autonomous instrument-computing system, particularly around deployment, novel physics exploration, while refining experimental and theoretical parameters. Issues include instrument specificity, implementation complexity, managing the different latencies of imaging with simulations. This presentation will focus on the development of a multi-surrogate framework on two-dimensional materials that combines deep kernel learning, tree-based models, with Gaussian Mixture Models (GMM) for material property prediction, alongside an autoencoder-decoder for structural reconstruction. In addition, we shall demonstrate how a common metadata framework (CMF) can provide improved model performance via continuous training with dynamic parameter adjustments. The framework is aimed at bringing us closer to time-to-solution by advancing autonomous laboratories through the integration of computational insights with real-time experiments.