

APS Scientific Computation Seminar Series

Speaker:

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Title:

Operating scientific facilities with foundation models and teachable agents

Date: July 14, 2025

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

Location:

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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract:

Advanced scientific user facilities, such as next generation X-ray light sources and self-driving laboratories, are revolutionizing scientific discovery by automating routine tasks and enabling rapid experimentation and characterizations. However, these facilities must continuously evolve to support new experimental workflows, adapt to diverse user projects, and meet growing demands for more intricate instruments and experiments. This continuous development introduces significant operational complexity, necessitating a focus on usability, reproducibility, and intuitive human-instrument interaction. In this work, we explore the integration of agentic AI, powered by Foundation Models, as a transformative tool to achieve this goal. We present our approach to developing a human-in-the-loop pipeline for operating advanced instruments including an X-ray nanoprobe beamline and an autonomous robotic station dedicated to the design and characterization of materials. Specifically, we evaluate the potential of various LLMs as trainable scientific assistants for orchestrating complex, multi-task workflows, which also include multimodal data, optimizing their performance through optional human input and iterative learning. We demonstrate the ability of AI agents to bridge the gap between advanced automation and user-friendly operation, paving the way for more adaptable and intelligent scientific facilities.