Materials Science and Engineering Department

Spring Seminar Series

My PI is an AI: How Collaborations Between Human and Artificial Intelligence are Enabling New Experiments at Large Scale User Facilities

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As new and upgraded x-ray light sources are established alongside advances in detector technology, the data generation rates at beamlines are skyrocketing. Data collected in fractions of a second to minutes at such facilities may take weeks to months to process and understand. Such a dramatic mismatch in measurement-to-analysis times can, in part, be attributed to a lagging effort towards modernizing data analysis methods. The lack of available real-time feedback during an experiment can force beamline users into 'flying blind', leading to missed opportunities and mistakes. New streaming analysis methods, particularly those employing Artificial Intelligence (AI), have demonstrated the ability to expedite data analysis to the speed and scale required for the light source community. As these tools mature, the capability to utilize them at the beamline as first-pass analysis methods becomes viable. While there is still significant research required to determine both the efficacy and accuracy of AI-based analysis tools, we are quickly approaching the day where these tools may form the basis of a new experimental modality at x-ray light sources.

Beyond the ability to accelerate researchers real-time understanding of their ongoing experiment at the beamline, these methods offer the potential to run fully automated experiments that are driven by directed scientific inquiry; for example, searching for a boundary in a phase-map or tuning synthesis conditions to maximize product. Bringing these methods to bear at large-scale user facilities has the potential to increase scientific output. At such facilities, however, this level of automation does not need to be limited to a single measurement. Increasingly, the use of multimodal characterization is required to fully understand the structure and function of complex materials. The inherent information content from one measurement can be used to inform and drive others, such as using relatively fast total scattering measurements to drive slower, but equally critical, spectroscopy studies. Just as human researchers can look at the full range of available information on a material to inform their understanding, we have begun to use AI-methods that leverage multifaceted data from different measurement techniques.

Daniel Olds is a beamline scientist on the Pair-Distribution Function (PDF) beamline at the National Synchrotron Light Source II at Brookhaven National Laboratory. His research focuses on developing real-time AI-driven analysis during in situ and high throughput studies of complex materials to discover the underlying atomic origins of the relevant material properties such as reaction pathways, synthesis, decomposition mechanisms, phase-transitions, and material passivation/poisoning. By leveraging advanced computational methods in both the data analysis and experimental control, he hopes to both accelerate the pace of discovery and expand access to a broader community of light source users.

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