The Evolving Landscape of AI for Science and Engineering: Bridging Simulation, Experiment, and Multi-scale Dynamics

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**Friday, March 6, 2026
3pm, Reception 2:45pm
66-110**

Recent advances in large-scale scientific datasets are creating new opportunities for machine learning (ML) methods to more effectively capture scientific phenomena with greater accuracy and reach. In this talk, I will discuss how these advances are both shifting ML design paradigms and enabling new scientific inquiries. This includes investigations into understanding if neural networks can autonomously discover fundamental physical relationships from data, and demonstrating how more flexible machine learning modeling design choices enable capturing dynamics across multiple scales. I will also explore how generative modeling approaches rooted in statistical physics can be applied to accelerate the sampling of dynamic pathways, and as a framework to align and bridge the gap between simulated data and experimental observations.

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