

NSF Meta-Workshop: AI to Accelerate Science and Engineering Discover
(AI2ASED)

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AI for Science in Quantum, Atomistic, and Continuum Systems

Monday 2 October 2023 11:30 (8 minutes)

In this talk, I will provide an overview of research on developing AI methods to understand the natural world from the subatomic (wavefunctions and electron density), atomic (molecules, proteins, materials, and interactions), to macro (fluids, climate) scales. My talk will focus on how to capture symmetries in physical systems using equivariant models. I will also touch on a few other technical challenges, including explainability, out-of-distribution generalization, and knowledge transfer with foundation and large language models. My talk will be a summary of our recent review paper on AI for science available at <https://arxiv.org/abs/2307.08423>

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Session Classification: Lightning talk I