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ARTIFICIAL INTELLIGENCE FOR SCIENTIFIC DISCOVERY

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ABSTRACT

Multi-scale coupled physics applications require computational modeling and simulations at large-scale to attain high precision and accuracy. In situations where the quantities of interest are defined in a high dimensional space, the curse of dimensionality pushes the limits of existing high-performance computing (HPC) architectures due to expensive, and sometimes unaffordable, computational requirements.

To alleviate the computational burden of state-of-the-art approaches and facilitate the bridging between multiple scales, artificial intelligence (AI) has been shown to provide significant benefits in several applications ranging from atomic modeling, computational mechanics, computational fluid dynamics, control, topological optimization, drug discovery, and material design.

The benefits of AI for scientific discovery are twofold. On the one hand, deep learning (DL) models accelerate the resolution of forward problem defined in a high dimensional space, where the goal is to predict target properties from a given set of input features. On the other hand, reinforcement learning (RL) and generative models (GM) accelerate the resolution of inverse problems defined in high dimensional spaces, where the goal is to identify the input features that correspond to a desired, prescribed target property.

In this session, we show how AI can be effectively used to accelerate the resolution of forward and inverse problems in several computational sciences and engineering applications and breakthrough existing computational barriers.