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PREDICTIVE MACHINE LEARNING AND GENERATIVE ARTIFICIAL INTELLIGENCE FOR SCIENTIFIC DISCOVERY AND DESIGN

MASSIMILIANO LUPO PASINI[*]

[*] Oak Ridge National Laboratory
1 Bethel Valley Road, Mail Stop 6085,
P.O. Box 2008, Oak Ridge, TN, 37831, USA

lupopasinim@ornl.gov
https://www.ornl.gov/staff-profile/massimiliano-lupo-pasini

ABSTRACT

Computational physics applications require computational modeling and simulations at large-scale to attain high precision and accuracy. When 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) is supporting several applications such as atomic modeling, computational mechanics, computational fluid dynamics, control, topological optimization, drug discovery, and material design. The computational advantages of AI for scientific discovery and design are twofold. On the one hand, predictive machine learning (ML) accelerates the resolution of forward problems 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, generative AI (GenAI) accelerates 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 illustrate how predictive ML and GenAI models can accelerate the resolution of forward and inverse problems in several computational sciences and engineering applications and breakthrough existing computational barriers.