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PHYSICS INFORMED MACHINE LEARNING FOR SCIENTIFIC APPLICATIONS

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ABSTRACT

Data-driven surrogate models have recently gained a lot of attention in the scientific community as they provide a promising path to accelerate computationally expensive multi-scale physics models in several applications ranging from atomic modeling, computational mechanics, computational fluid dynamics, and systems engineering. In particular, machine learning (ML) models have been shown to provide surrogate models that effectively capture complex non-linear dependencies of a physical system from high-dimensional parameters.

Once it is deployed in production codes, besides being accurate, the surrogate model needs also to be (1) generalizable, in order to reliably handle physical scenario with configurations different from the ones explored during the training, and (2) transferable across multiple sizes of the physical system in order to accommodate scale bridging. We call robust, surrogate models that satisfy these three properties simultaneously.

To ensure robustenss, ML models need to be cognizant of the physics in order to ensure self-consistency between different target properties that need to be simultaneously predicted. Usually physics information is injected into the ML models either by extracting physical correlations among different target properties described in the data or by complementing the ML model with additional physics laws.

In this session, we will focus on showing how physics-informed ML leads to robust predictions of target properties in scientific and engineering applications.

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