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Data-Driven Methods of Accelerating Physical Simulations and Their Applications

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A surrogate model is built to accelerate computationally expensive physical simulations, which is useful in multi-query problems, such as inverse problem, uncertainty quantification, design optimization, and optimal control. In this talk, two types of data-driven surrogate modeling techniques will be discussed, i.e., the black-box approach that incorporates only data and the physics-informed approach that incorporates the physics information as well as data within the surrogate models. The advantages and disadvantages of each method will be discussed. Furthermore, several recent developments at LLNL of data-driven physics-informed surrogate modeling techniques will be introduced in the context of various physical simulations. For example, the time-windowing reduced order model overcomes the difficulty of shock propagation phenomenon, achieving a speed-up of $O(4\sim10)$ with a relative error less than 1% for relatively small Lagrangian hydrodynamics problems. The space-time reduced order model accelerates large-scale Neutron transport simulations by a factor of 2,700 with a relative error less than 1%. The nonlinear manifold reduced order model shows perfect marriage between machine learning and physics-informed surrogate modeling and also solves the challenge imposed by the advection-dominated physical simulations. Finally, successful application of these surrogate models in design optimization problems will be presented.