Learning-based predictive models: a new approach to integrating large-scale simulations and experiments

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Large-scale scientific endeavors are often focused on improving predictive capabilities by challenging theory-driven simulations with experimental data. Today, these challenges, or tests of predictive capability, are done mainly by subject matter expert scientists using small subsets of available data and simplified low-order models. Yet, both simulation and experiment have become very data-rich with a complex of observables including scalars, vector-valued data, and various images. Traditional approaches developed by science practitioners can omit much of this information, making the resulting models less accurate than they otherwise could be. Across applications, laboratory scientists need new methods to improve predictive capabilities – ones that amplify the scientist's ability to incorporate both simulation and experimental results without being forced to eliminate large amounts of data in the process.

We will describe a large research effort at Lawrence Livermore National Laboratory (LLNL) aimed at using recent advances in deep learning, computational workflows, and computer architectures to develop an improved predictive model – the learned predictive model. Our goal is to first train deep neural network models on simulation data to capture the theory implemented in advanced simulation codes. Later, we improve, or elevate, the trained models by incorporating experimental data. The training and elevation process both improves our predictive accuracy and provides a quantitative measure of uncertainty in such predictions. We will present work using inertial confinement fusion research and experiments at the National Ignition Facility (NIF) as a testbed for development. We will describe advances in machine learning architectures and methods necessary to handle the challenges of ICF science, including rich, multimodal data (images, scalars, time series) and strong nonlinearities. We will also cover state-of-the-art tools that we developed to steer both physics simulation and model training. We have used these tools to produce 100 million ICF simulations, including 4.8 billion multi-view and multi-channel images using the Sierra supercomputer. We will describe our ongoing efforts to exploit the GPU-rich architecture of Sierra to develop a learned predictive models based on this massive data set.