A Digital Twin for Spatiotemporal Experiments*

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Abstract

The need for a physically-informed strategy for offline design and optimization of these experiments is emerging as a grand challenge for SUFs. The rapid advancement in AI/ML algorithms, improved shared workflows and the advent of exascale computational resources now make it possible to create a physically-informed virtual platform to augment and guide spatiotemporal experimental trials. This talk will discuss our ongoing efforts to embrace these advancements to tackle this SUF challenge by creating a virtual platform or “Digital Twin”, wherein the users can exhaustively explore experimental controls and obtain reliable synthetic read-outs. We take advantage of the fact that most experimental spatiotemporally-resolved measurements at SUFs in real or reciprocal space can be derived from the accurate prediction of atomic configurations and their dynamical evolution across time- and space. The key challenges to realize the Digital Twin are (i) information extraction from spatiotemporal experiments to serve as model input, (ii) physically accurate, flexible and efficient models across multiple time and length-scales, and (iii) seamless information exchange between models and experiments. We plan to integrate and build on the key complementary AI/ML tools developed by the multi-disciplinary PIs from the various DOE SUFs for solving the inverse problem, multi-fidelity simulation scale bridging, and shared workflows to successfully create the Digital Twin platform.

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