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MODEL TUNING FOR MULTIFIDELITY SAMPLING IN DAKOTA

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Computational simulation continues to advance in its predictive capability through the development of high-fidelity multi-physics/multi-scale simulation models, with unprecedented resolution enabled by the latest high-performance computers. Uncertainty quantification (UQ) methodologies are challenged in this environment, both by the prohibitive cost of computing high-fidelity ensembles and by the increasing number of uncertainty sources that is often induced by this model complexity. One strategy to address these challenges is to harness the utility that exists within an ensemble of model forms and/or resolution levels in order to control multiple sources of error while optimizing the allocation of simulation resources. By relaxing the need for exclusive reliance on the most expensive models, high-fidelity UQ studies can become tractable.

An important challenge that commonly arises in realistic application deployments is the need to identify the set of low-fidelity approximations that can be the most effective within a multifidelity setting. A priori assumptions about this set are often proven to be inaccurate, as the correlation versus cost trade-offs can be complex and non-intuitive, leading to potentially significant losses in multifidelity performance. In this talk, we focus on *model tuning* to address this challenge. Given a set of hyper-parameters that govern the balance of accuracy versus cost for one or more low fidelity models, one can formulate an optimization problem to identify the model settings that provide the greatest utility for the context of interest. We propose performing this optimization within the context of a particular statistical estimator and employing an all-at-once approach to minimizing the estimator's variance. Our initial demonstrations will focus on sampling methods, especially multifidelity Monte Carlo and approximate control variates, where we will leverage trust-region surrogate-based optimization for efficiently navigating hyper-parameter trade-offs. Application demonstrations of interest include tunable model problems as well as production deployments in plasma physics and thermal battery analysis.

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