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EFFECTIVE UNCERTAINTY QUANTIFICATION USING ADJOINT-BASED ERROR ESTIMATES AND SURROGATE MODELS

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Uncertainty and error are ubiquitous in predictive modeling and simulation due to unknown model parameters and various sources of numerical error. Consequently, there is considerable interest in developing efficient and accurate methods to quantify the uncertainty in the outputs of a computational model. Monte Carlo techniques, including the Latin Hypercube variants, are the standard approach to quantify the uncertainty in a computational model. The general appeal of these methods can be attributed to their relative ease of implementation and the fact that they often circumvent the *curse of dimensionality*. Unfortunately, the number of samples required to accurately estimate certain probabilistic quantities, especially the probability of high-risk, low-probability events, may be prohibitively large for high-fidelity computational models. Improvements such as importance sampling can greatly reduce the computational cost, but often the number of high-fidelity model evaluations is still unacceptably large.

In general, the accuracy to which uncertainty can be quantified is limited by the computational resources available to resolve the governing equations. Many applications require vast amounts of computational effort and thus the number of model evaluations that can be used to interrogate the uncertainty in the system behaviour is limited. Therefore, any approximation of a probabilistic quantity contains both deterministic (discretization) and stochastic (sampling) errors. Producing a reliable estimate of a probabilistic quantity requires that each of these sources of error be reduced to an admissible level. A number of recently developed methods for uncertainty quantification (UQ) have focused on constructing surrogates of expensive simulation models using only a limited number of model evaluations. The fact that a very large number of samples may be efficiently computed using the surrogate effectively reduces the statistical component of the error. However, the deterministic component of the error may be quite large for each sample due to the standard sources of discretization error as well as the interpolation of the surrogate model. The accumulation of these deterministic errors may significantly affect the accuracy of the probabilistic quantity of interest.

Recently, a posteriori error estimation has arisen as a promising approach to estimate the deterministic error in surrogate-based approximations of input-output relationships. Adjoint-based techniques are commonly used to estimate error in numerical approximations of deterministic PDEs (see e.g., [1]), but recent modifications, introduced in [3] and further analyzed in [2, 4], allow similar ideas to be used to estimate error in surrogate approximations of quantities of interest from PDEs with uncertain parameters.

In this presentation, we show how adjoint-based techniques can be used to efficiently estimate the error in a quantity of interest computed from a sample of a surrogate model. We then show how these error estimates can be combined with adaptive sparse grid approximations to provide enhanced convergence, new adaptive strategies, and a means to avoid over-adapting the sparse grid beyond the accuracy of the spatial discretization. Finally, we demonstrate that these a posteriori estimates can also be used to guide adaptive improvement of a surrogate model with the specific goal of accurately estimating probabilities of events. This final demonstration is similar to the approach considered in [5] where a hybrid strategy was defined to limit the number of high-fidelity model evaluations. Our approach improves upon this hybrid strategy in several ways and results in an accurate approximation of the probability of the event of interest with far fewer evaluations of the high-fidelity model.

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