EMBEDDED FRAMEWORK FOR MODEL ERROR QUANTIFICATION AND PROPAGATION

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ABSTRACT

Model error estimation remains one of the key challenges in uncertainty quantification and predictive science. While accounting for data noise and parametric uncertainties has become routine in the uncertainty quantification context, the same cannot be said about model errors, also known as model structural error, model inadequacy, or model misspecification. In fact, for computational models of complex physical systems, model error is often the largest contributor to the overall predictive uncertainty. Nevertheless, model calibration often ignores model errors by assuming that the computational model replicates the exact physics behind data generation. As a result, calibrated model parameters are often biased, leading to reduced predictive skill. Conventional external methods [1] of augmenting model outputs with statistical correction terms may remove the predictive bias, but they can violate physical laws, make the calibrated model ineffective for predicting non-observable quantities, and experience identifiability challenges in distinguishing between data noise and model error.

This work will present a Bayesian framework for representing, quantifying, and propagating uncertainties due to model structural errors by *embedding* statistical representations in the model instead of external corrections [2]. The physical inputs and correction parameters are then simultaneously inferred within a Bayesian paradigm via surrogate-enabled Markov chain Monte Carlo sampling. With a polynomial chaos characterization of the correction term, the approach allows for efficient propagation and decomposition of uncertainty that includes contributions from data noise, parameter posterior uncertainty, and model error. The embedded approach ensures physical constraints are satisfied and renders calibrated model predictions meaningful with respect to structural errors over multiple, even unobservable, quantities of interest.

Further, we will recast the methodology and draw parallels to model uncertainty quantification for neural networks, specifically methods employing approximate Bayesian computation and functional variational inference. Throughout the talk, key strengths and challenges of the embedded model error quantification method will be demonstrated on synthetic examples and practical applications ranging from chemical modeling to climate science.

REFERENCES

[1] Kennedy, M.C. and O'Hagan, A., "Bayesian calibration of computer models". Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63: 425-464. 2001.

[2] K. Sargsyan, X. Huan, H. N. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", International Journal of Uncertainty Quantification, 9:4, pp. 365–394, 2019.