On Model Error and Statistical Calibration of Physical Models

Habib N. Najm[*], Khachik Sargsyan[†], Roger G. Ghanem[††]

[*†]Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov, ksaragsy@sandia.gov

[††] University of Southern California
Los Angeles, CA, USA
ghanem@usc.edu

ABSTRACT

Existing methods for representation of model error in the statistical calibration of computational models typically rely on convolving model predictions of select observables with statistical data and model error terms. This strategy is successful in providing a statistical correction to model predictions in a manner that interpolates observations with meaningful uncertainty estimation between points. However, this approach faces a number of challenges when applied in the context of calibration of physical models, where, e.g. auxiliary physical constraints are in force, the model is intended for use outside the calibration regime, and other non-observable model output predictions are of interest.

We have developed a calibration strategy that addresses these challenges. We define constraints of interest as regards uncertain predictions, for example we require that the mean prediction is centred on the data, and that the predictive uncertainty is consistent with the range of discrepancy between the means of the prediction and the data. We embed statistical model error terms in select model components, where, e.g. specific phenomenological model assumptions are in force. We then formulate the problem as a density estimation problem and solve it using approximate Bayesian computation methods.

We demonstrate this construction on simple model problems, and for calibration of a simplified chemical model for methane-air kinetics against another, more complex, model. Select parameters of the simple model are encumbered by model error. We show how this uncertainty translates to model output uncertainty, and how the desired constraints on the uncertain prediction are achieved,