Uncertainty Quantification in Computational Fluid Dynamics
26–27 May 2014, Pisa, Italy

Spectral Uncertainty Quantification and Optimal Bayesian Experimental Design of Combustion Reaction Systems using Sparse Adaptive Polynomial Chaos Expansion

***Daesang Kim,*[1,2] *Fabrizio Bisetti,*[1,2] *Quan Long,*[1] *Raul Tempone,*[1] *and Omar Knio*[1,2]**

[1]SRI – Center for Uncertainty Quantification in Computational Science & Engineering, KAUST, Thuwal, Kingdom of Saudi Arabia

[2]Clean Combustion Research Center, KAUST, Thuwal, Kingdom of Saudi Arabia

Key words: uncertainty quantification, polynomial chaos expansion, Bayesian experimental design, and combustion reaction

We have developed a methodology for uncertainty quantification studies of complex combustion systems. The methodology includes analysis of the sensitivity quantities of interest (QoI) to uncertain reaction rate parameters, fast surrogate model construction, optimized Bayesian experimental design, and statistical inference of physical parameters from experiment data.

For sensitivity analyses and surrogate model construction, a sparse adaptive pseudo-spectral projection technique has been developed, and applied to all uncertain input data. This non-intrusive spectral projection (NISP) approach allows convenient reuse of legacy codes for the reaction model simulations. In the sparse pseudo-spectral approach, the expansion coefficients are determined through inner products, defined as weighted quadratures that require repeated simulations on nested sparse grids. The nested quadrature improves the efficiency by allowing reuse of the simulation results computed at the previous adaptation steps. It results in rapidly convergent polynomial chaos (PC) expansions of QoIs. This expansion enables straightforward quantification of variability, correlations, and sensitivities to uncertain inputs. It can also serve as a fast polynomial surrogate model that enables efficient applications of other methods.

The present formalism also includes an optimal experimental design method based on fast estimation of the Kullback-Leibler information gain. The latter is used as a measure of the information gained from an experiment, and the quantity is based on the contrast between the prior and posterior distributions. The new technique based on Bayesian formalism applies the Laplace approximation to the posterior probability density function and this gives a closed-form approximation of the inner integral in the double-loop integration for the expected information gain. Furthermore, sparse quadrature grids are used for the fast calculation of the remaining high-dimensional integration in the parameter. Combined with PC surrogates, the combined approach achieves dramatically fast searches for optimal experimental conditions where the information gain is maximized.

In order to validate the predictions, the experimental design methodology is first applied to an H_2 oxidation experiment in which uncertain parameters to be refined are the pre-exponential factor and the activation energy appearing in the rate expression of the $H+O_2 \Leftrightarrow O+OH$ reaction. In this first experiment, the QoI consists in the peak growth rate of H_2O concentration, whereas the experimental design variables are the initial temperature and initial concentration of O_2. For the present setting, the PC expansion of the peak growth rate of H_2O concentration indicates that the selected reaction has 99% of a sensitivity index while the other 19 reactions share the remaining 1%. The experimental design technique shows that the effect of the initial concentration of O_2 is relatively small, and repeated experiment runs at a low and a high temperature

result in the highest information gain over all other experimental designs including those at temperatures uniform over the temperature range. Up to 124 runs, the optimized information gain grows logarithmically with the number of the experiment runs. To validate and confirm the experimental design result, synthetic experiment data are produced by adding Gaussian errors to computed model predictions. For a design consisting in measurements at fixed temperature intervals, the analysis reveals an average information gain of 4.1, whereas the optimized design gives an improved value of 4.4. The estimated uncertainty in the reaction rate constant is reduced approximately to 5% for the synthetic design exercise.

The methodology is next extended to a more elaborate system describing ionization kinetics during CH_4 oxidation. The reaction mechanism includes 67 reactions from GRI-Mech 3.0, and 22 reactions are selected as uncertain reactions of interest. Specifically, the pre-exponential coefficients these 22 reactions are treated as uncertain independent random variables. The maximum electron concentration and the decay time of the electron concentration are selected as the experimental QoIs, and the initial temperature and initial fuel mixture are the experimental design variables. The adaptive sparse pseudo-spectral scheme enables us to obtain a spectral expansion of the QoIs in terms of polynomials of the design variable and random variables. Analysis of the resulting spectral expansion shows that only a few reactions have sufficiently large sensitivities to affect the predictions. The experimental design methodology is then applied in a similar way as in the hydrogen oxidation example. Computed results reveal that the initial fuel mixture is the more important design variable, and that only reaction parameters having high sensitivity can attain improved statistical inference.