ANOVA, DERIVATIVE-BASED SENSITIVITY, AND APPLICATIONS TO A PLASMA-COMBUSTION SYSTEM

Kunkun Tang*, Jonathan B. Freund

The Center for Exascale Simulation of Plasma-coupled Combustion (XPACC) University of Illinois at Urbana-Champaign, Urbana IL 61801, USA.

Key words: Sensitivity Analysis, UQ, Validation, Combustion, High-dimensional Problems

Sobol' and Kucherenko [1, 2] introduced two first-order derivative-based sensitivity indices (DSI) and have shown a link with global sensitivity indices (GSI). Even though GSI are considered superior to DSI for importance ranking since they contain more model information (e.g. higher-order and mixed derivatives), they are often impractical due to their high cost [2]. Monte Carlo (MC) algorithms for DSI and GSI have been developed and compared, and DSI are particularly attractive since their MC convergence can be much faster than GSI in applications with relatively little derivative variation. The approach proposed by Sudret and Mai [3] aims to estimate the DSI [1] based on a polynomial chaos expansion. However, the extension of this for other DSI [2] seems difficult because of additional terms in the integrand. In the paper, we will introduce two and new derivative-based measures for inputs of arbitrary probability distribution that can be efficiently estimated using an adaptive Analysis of Variance (ANOVA) surrogate, and we use them in a multi-physics application with hundreds of uncertain parameters. We will compare our DSI formulation to standard approaches [1, 2], both theoretically and numerically, together with their relation to GSI. The cost advantage of our DSI will be shown from both viewpoints of Monte Carlo algorithms and spectral polynomial expansions. A simple extension of DSI for dependent inputs will also be presented to account for the high correlation often encountered in reaction models. The overall methodology will be demonstrated for large-scale supersonic combustion simulations in jet-in-crossflow configurations with corresponding experiments. This involves models of laser-induced breakdown phenomena in non-equilibrium plasma, nozzle inlet/outlet conditions, combustion kinetics, and transport. Multiple time and/or space scales, complex physics, high-dimensionality, and computational cost make the Uncertainty Quantification (UQ) particularly challenging, even with the state-of-the-art computing facilities. We will also show for this application how an ANOVA representation can be employed for fast optimization and calibration of important model parameters using experimental data.

Acknowledgment. This material is based in part upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number DE-NA0002374.

References

- [1] I.M. Sobol' and S. Kucherenko. Derivative based global sensitivity measures and their link with global sensitivity indices. *Mathematics and Computers in Simulation*, 79(10):3009–3017, 2009.
- [2] I.M. Sobol' and S. Kucherenko. A new derivative based importance criterion for groups of variables and its link with the global sensitivity indices. *Computer Physics Communications*, 181(7):1212–1217, 2010.
- [3] B. Sudret and C.V. Mai. Computing derivative-based global sensitivity measures using polynomial chaos expansions. *Reliability Engineering & System Safety*, 134:241–250, 2015.