Enabling Efficient Uncertainty Quantification Using Adjoint-based Techniques

John Shadid[a], Tim Wildey[a], Eric Cyr[a], Paul Constantine[b]
[a]Sandia National Labs, Albuquerque NM 87125. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
[b]Colorado School of Mines, Golden CO 80401
Topic E: Beyond interpretive simulations, No Oral Presentation

Motivation

A critical challenge before the applied/numerical mathematics community is to fully develop, demonstrate and evaluate the promise of extreme-scale computational analysis as a scientific tool for predictive inference, model inversion and design optimization of complex multiphysics plasma systems with uncertainty. Multiphysics plasma systems are strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a large range of length- and time-scales. Models of such full-scale systems are of critical importance to a wide range of impactful plasma-science efforts.

In addressing this challenge, it is important to account for the fact that error and uncertainty are endemic to multiphysics systems. Numerical simulation of complex multiphysics systems in the deterministic regime often requires the use of extreme-scale computing resources to achieve even marginal accuracy. Thus, we are generally limited to at most a few hundred simulations to approximate the probability distributions propagated through the multiphysics systems and to make statistical inferences. Likewise, experimental and observational data on multiphysics systems is expensive to obtain, strictly limited in scope and availability, and subject to significant uncertainty and experimental error. Consequently, truly predictive computational analysis and design for multiphysics scientific and technology systems requires quantifying the effects of as many sources of uncertainty and error as feasible. Achieving this will require the development of (1) new methods for a posteriori error estimates that evaluate contributions of both numerical and stochastic error for statistical information, e.g., probability distributions quantities of interest, (2) new generalized adaptive forward uncertainty quantification algorithms that utilize sensitivity information to determine inactive and slowly varying subsets or subspaces of parameters and reduce the effective dimension of the parameter space, (3) innovative generalized adaptive algorithms based on a posteriori error estimates that efficiently distribute computational resources balancing all sources of stochastic and deterministic errors.

Critical to achieving this overarching goal will be the development, analysis and evaluation of a set of mathematical and algorithmic advances for propagating and estimating numerical error on extreme-scale architectures:

- New methods for a posteriori error estimates that evaluate contributions of both numerical and stochastic error for statistical information, e.g., probability distributions quantities of interest,
- Efficient and reliably accurate extreme-scale algorithms for sampling probabilities and surrogate model construction,
- Local and global sensitivity analysis to enable effective reduction of stochastic dimension using active subspace techniques[1],
- Efficient adaptive algorithms based on a posteriori error estimates that efficiently distribute computational resources balancing all sources of stochastic and deterministic uncertainty/errors.

Approach

We believe that the model derivative computed using adjoint problems is a key algorithmic enabling technology approach for successful development of these fundamental tools. Derivative information about multiphysics operators is crucial, in part, because of the practical limitations on the number of simulations that can be computed, which makes maximizing the information provided by each simulation essential. Adjoint calculations provide N additional pieces of information, where N is the dimension of the parameter space, for approximately the same cost of computing the QoI. Additionally, derivatives provide a mechanism for understanding the sensitivity of output quantities of interest to input parameters and provide a means to determine active subspaces of parameters. Recent work has also shown that the deterministic errors introduced through the use of response surface approximations in UQ can be estimated and adaptively controlled using adjoint-based error estimates[2,3,4]. Finally, the computational power of extreme-scale architectures makes the use of these adjoint-based techniques a tractable approach to achieving efficient forward propagation for multiphysics systems.

One of the major computational burdens in the application of adjoint techniques to time-dependent nonlinear problems is the backwards in time storage and access of the full forward approximate solution required to form the adjoint problem. This results in both large storage costs but also frequent and expensive access to disk when solving the adjoint problem. Check-pointing methods are one approach to mitigating these issues[5]. These techniques store the forward solution at carefully selected times and the forward solution is recomputed during an adjoint computation. However, the cost of re-computing the forward solution may be too great to justify the use of the adjoint methods. A promising new approach uses data compression techniques to store and reconstruct the forward solution when solving the adjoint problem[6], but this approach has not been demonstrated on complex multiphysics systems.

Another challenge is efficient implementation for treating multiple QoI. It is often the case that multiple QoI are required from a model simulation, implying that a different adjoint problem must be solved for each QoI. One approach would be to exploit next generation architectures to take advantage of the fact that this set of problems is equivalent to solving a linear problem with multiple right-hand sides, thereby minimizing the cost of adjoint-based error estimation and sensitivity analysis for multiple QoI.

The mathematical models that are used to describe such multiple-time-scale multiphysics plasma systems are varied and include, continuum MHD approximations, kinetic descriptions, particle-in-cell type methods, integral-equations, and others. Adjoints for many of these models have yet to be developed. Another challenge is the issue of dealing with discontinuous solutions, however in the case of continuum CFD, recent work on adjoint techniques for hyperbolic systems with shocks appears promising[6].

Impact

This research would make significant progress towards achieving predictive simulations for complex fusion devices. New approaches are needed to understand the effect of propagating uncertainty between heterogeneous models, through the component models at each scale, and through the inter-scale transfer operators. The proposed work on error estimation and UQ for multi-physics, multi-scale, multi-model simulations would provide a path towards understanding these issues.

References

[1] P. Constantine. Active subspaces: Emerging ideas for dimension reduction in parameter studies. SIAM, 2015.

[2] T. Butler, C. Dawson, and T. Wildey. A posteriori error analysis of stochastic spectral methods. *SIAM J. Sci. Comput.*, 33:1267–1291, 2011.

[3] T. Butler, C. Dawson, and T. Wildey. Propagation of uncertainties using improved surrogate models. SIAM/ASA Journal on Uncert. Quant. 1 (1), 164-191, 2013.

[4] J. Jakeman and T. Wildey. Enhancing adaptive sparse grid approximations and improving refinement strategies using adjoint-based a posteriori error estimates. J. Comp. Phys. 280, 54-71, 2015.

[5] A. Griewank and A. Walther. Algorithm799: Revolve: an implementation of checkpointing for the reverse or adjoint mode of computational differentiation. *ACM Trans. Math. Softw.*, 26(1):19– 45, March 2000.

[6] E. Cyr, J. Shadid, and T. Wildey. Towards efficient backward-in-time adjoint computations using data compression techniques. Comp. Meth. Appl. Mech. Engrg., 288, 24-44, 2015.

[7] M. Giles and S. Ulbrich. Convergence of Linearized and Adjoint Approximations for Discontinuous Solutions of Conservation Laws Part 1, SIAM J. Numer. Anal. 48(3), 2010.