Uncertainty Quantification in Computational Models of Fusion Systems*

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1 Motivation

Progress in fusion science relies to a large degree on the availability of predictive computational models and tools for analysis and design of fusion devices and experiments. Given the rich array of physical processes involved in fusion systems, these computations rely on numerous underlying models of physical phenomena. As a result, computations of fusion systems necessarily involve a range of model parameters that are measured experimentally or estimated from targeted simulations at smaller scales. In both cases, these parameters are only known up to a certain degree of uncertainty. At the same time, other significant sources of uncertainty exist, including model error, as well as discretization errors in unresolved mesh-based solutions of governing equations. Accordingly, to be truly predictive; to enable model validation, comparison, and selection; and to provide means for robust design optimization and decision support, it is necessary that computational predictions of fusion devices provide for adequate quantification of uncertainty. Predictive computations need to account for important sources of input uncertainty, and to allow for propagation of these uncertainties to quantities of interest (QoIs) based on model output predictions [1–4]. Further, assimilation of data for parameter estimation, model validation/comparison, and hypothesis testing, needs to be done in a framework that allows for accurate handling of uncertainty.

While it is relatively easy to motivate the use of uncertainty quantification (UQ) in computational models of fusion systems, there are numerous challenges facing the attainment of this goal. These challenges are omnipresent in both forward UQ, propagating uncertainties from model inputs to outputs, and inverse UQ, estimating uncertain inputs given data on model outputs. Further, these challenges are, in fact, fairly ubiquitous for UQ in detailed computational models of complex physical systems in general. They include:

- **Characterization of the uncertain input space:** While nominal values of model parameters and other inputs are typically known, associated uncertainties are not typically well characterized. In particular, available information usually involves error bars on *some* parameters, with no information on correlations. Aside from this, other sources of uncertainty such as model and discretization errors are not well characterized, and are, moreover, much harder to estimate or represent.
- **Large dimensionality of input space:** The number of uncertain inputs is typically quite large, necessitating significant attention to dimensionality reduction strategies to retain only those input uncertainties that have a significant impact on uncertainty in QoIs.
- **Computational cost and complexity of fusion system simulations:** Physically reliable computations of fusion devices require excessive computational resources. As a result, it is not feasible to contemplate reliance on large numbers of computational samples to propagate uncertainty in these models or to estimate their parameters given data on their output observables. At the same time, intrusive UQ strategies that might avoid sampling are faced similarly with serious challenges given the complexity of models and codes.
- **Data handling:** UQ typically further exacerbates the severe data-challenge already faced by large-scale computational modeling. The computational data volume required for estimating uncertainty in predictions, or for statistical inversion, is typically significantly larger than that for a single evaluation of the forward model.

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2 Approach

Potential approaches to meeting the UQ challenge in fusion computations, include the following.

- **Characterization of uncertain model inputs:** Probabilistic methods, including both Bayesian inference and maximum entropy methods, can be used to analyze available data or other information on model inputs, and to construct a meaningful joint density that captures the correlated uncertainty picture on the input space [5–7]. Similarly statistical methods can be used to characterize embedded model error representations [8], and to pursue probabilistic models for mesh discretization errors. Both of these goals require, however, significant innovation and targeted UQ studies in the context of fusion models.
- **Identification of important uncertain inputs:** Dimensionality reduction can be pursued using global sensitivity analysis [9, 10], (Bayesian) compressed sensing methods [11–13], and low-rank tensor analysis methods [14] that pursue and identify sparse low-rank behavior in the dependence of model QoIs on uncertain model inputs. The key challenge here of course is the need for computational samples to arrive at reliable results. Domain knowledge is crucial to augment the analysis by injecting suitable information based on expert knowledge regarding important parameters/sub-models, to address the paucity of computational samples.
- **Multifidelity and Multiscale UQ methods:** Given the high cost of computational samples, there is a strong argument for multifidelity UQ methods, relying on large numbers of low-fidelity/low-resolution computational samples, along with a few high-fidelity/high-resolution samples, to arrive at forward UQ methods that are feasible in fusion system simulations [15]. Resulting model surrogates would also enable inverse UQ. Model error representations are useful in this context to provide meaningful calibrations/parameter-estimation for low-fidelity models. A similar situation arises when physical information needs to be propagated across lengthscales and when multiscale approaches are used that couple different physical representations. The development of suitable surrogates would also be beneficial in this context, particularly for propagating uncertainty across scales, and also for inference and calibration.
- **Data:** From the data perspective, UQ is a double-edged sword. While UQ adds to the data-burden of fusion computations, it also provides paths for efficient probabilistic learning from data and associated reduced representations, thereby providing potential relief of the data-burden. Compressed sensing methods are naturally fitting for efficient/reduced reprentations of large data sets [11, 16]. Means for data-coarsening with quantified error/uncertainty are also feasible with UQ methods. Similarly, stochastic processes or random fields, be they noisy experimental measurements, or uncertain/random/noisy computational outputs, can be optimally represented using a small number of degrees of freedom with Karhunen-Loève expansions [17–21].

3 Impact

The accounting for uncertainy in fusion system computations has potential impact along various angles. To begin with, the ability to capture the dependence of models on uncertain parameters over their range of probable values will enhance understanding of models and their utility over ranges of conditions. Further, UQ will enable reliable estimates of confidence bounds in fusion system model predictions thereby facilitating model validation studies, and providing means for decision support. Finally, the proper accounting for uncertainties and their consequences on system operation will enable robust designs that exhibit more reliable attainment of system performance objectives.

4 References

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