Applications of Uncertainty Quantification to Models of Magnetically Confined Plasmas

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When computational models are used to make predictions, it is important that the uncertainty in the predictions be quantified so that their reliability is understood [6]. Further quantification of uncertainties in model outputs is necessary for meaningful validation of models against experimental observations (see below).

There are numerous sources of uncertainty in the analysis and simulation of complex systems such as in magnetically confined fusion. These can interact non-linearly to affect simulation results in unexpected ways, leading in the worst case to misleading results, incorrect conclusions and poor decisions regarding the system. As increasing computational power has enabled computational models of increasing complexity, the characterization of uncertainty in such simulations has become increasingly important. A wide variety of algorithmic and computational tools to treat uncertainty in such simulations have been and are being developed. This is a very active area of research in computational and applied mathematics, as for example in the QUEST SciDAC center. Deploying the tools of uncertainty quantification (UQ) for magnetic fusion presents a number of algorithmic challenges, which will be discussed at the end of this note. Perhaps more important, however, is the formulation of meaningful uncertainty representations and applications that can help advance the state of the art in magnetically confined fusion. Discussed below are several representative examples of UQ formulations and applications that are informed by the authors' experience in the EPSi SciDAC partnership.

Experimental Data Analysis Experimental measurements are commonly used to provide a variety of inputs to computational models, such as initial and boundary conditions, and to provide data for calibration and validation of models. Usually, however, measurements made in a complex system are indirect; that is, instruments generally sense some other directly accessible quantity and the quantity that is of real interest is inferred through a computational model, a "data reduction model." For example, spectroscopy is used to infer a wide range of quantities. It is of course routine to characterize measurement uncertainties, but it is less common to account for uncertainties introduced by data reduction models. Data reduction models often need to be calibrated, and since the measurements used to do so are themselves uncertain, the resulting calibration parameters are uncertain and contribute to the uncertainty in the inferred quantity. Further, in many cases, the quantity being measured is inferred through an inverse problem, that is the measured quantity appears as an input to the data reduction model and it is determined by matching the output of the model to the sensed outputs. In the presence of uncertainty, this becomes a statistical inverse problem, as is the calibration discussed above. A complete treatment of measurement uncertainties then requires application of UQ tools to data reduction models, including inverse problems, e.g. via Bayesian inference, and forward propagation of uncertainties in parameters and sensed quantities. UQ applications of this sort are being pursued by M. Greenwald and team at MIT [1].

Sampling Uncertainties In gyrokinetic models such as those implemented in XGC1 [3], the model solution is chaotic, and the underlying model is stochastic. Generally then, simulation outputs are averaged, and the finite averaging that is done introduces an uncertainty which should be acknowledged in analysis of the simulation results [4]. More interesting, however, is that the stochastic nature of the gyrokinetic model arises due to the evolution of a random sample of computational particles that represent the dynamics of charged particles. There is therefore a sampling uncertainty in the dynamics of the system as a whole, due to the finite number of particles employed. A UQ analysis of the consequences of this sampling uncertainty would allow, for example, the number of particles to be adapted to ensure a target accuracy in simulation outputs, or to inform multi-fidelity approaches (see below). Further, advanced UQ algorithms might lead to more sophisticated sampling of particle dynamics.

Validation Under Uncertainty Validation of magnetic fusion models is necessary to ensure reliable simulations [2]. Validation of a model of a complex system requires determining whether the model's outputs are consistent with experimental observations. In the presence of uncertainty, this is a question of whether observed discrepancies are explained by uncertainties in measurements and model outputs. Uncertainty in measurements is discussed above, as is model uncertainty due to sampling. A potentially larger source of model uncertainty is from inputs. These could include uncertain parameters in constitutive models (e.g. recycling models), but also uncertainties in the experimental conditions. Conditions such as the imposed magnetic field, the heating power and distribution and the initial density are important inputs which are determined through uncertain measurements. These input uncertainties should be considered as part of validation testing. Finally, given measurements with uncertainties and model outputs with uncertainties, determining whether they are consistent is potentially difficult, especially if there are many observed quantities with correlations among the uncertainties (e.g. points on a profile). Probabilistic validation criteria devised to be appropriate for tests of magnetically confined fusion models are needed.

Multi-fidelity Modeling High fidelity models designed to represent the edge plasma, such as the turbulence resolving, full-f gyrokinetic model embodied in XGC1, are computationally very expensive. For example, a large-scale simulation can take tens of millions of core hours or more. Clearly one would prefer to use a less expensive model, but it would presumably be lower fidelity. This is especially important if simulation of many cases is required, as for example when exploring a large input parameter space, performing an optimization (e.g. for design), or conducting an uncertainty analysis. There are of course many models of various fidelities that have been developed in the fusion problem domain, and presumably others could be developed for different purposes. Of course, models make various approximations, simplifications and/or omissions. It would be extremely useful to have an uncertainty analysis that quantifies the uncertainty in simulation outputs of interest that are introduced by these approximations. This would allow one to switch to higher fidelity models when the uncertainties become too large for the purpose of the simulation. This would help to enable an integrated multi-fidelity simulation approach. One of the challenges to UQ of this type is developing meaningful representations of uncertainty due to modeling errors. Development of such representations is fundamentally a problem in physical modeling in addition to the mathematics of uncertainty. This sort of uncertainty modeling is being pursued in the modeling of hydrodynamic turbulence [5].

Algorithmic Challenges Models for magnetically confined plasmas present several challenges for uncertainty quantification analysis. Two in particular are worth noting here. First, turbulence-resolving models are expected to have chaotic solutions. This means that several advanced methods for uncertainty analysis, such as those relying on adjoint solutions or stochastic galerkin approximations, cannot be applied using current algorithms. The problem is fundamental and has to do with the exponential growth of perturbations in chaotic systems. This limits the available algorithmic tools. This problem occurs in a variety of other physical systems, and improved algorithmic approaches are needed. Second, high-fidelity models, such as full-f gyrokinetic models, are extremely expensive to evaluate. This makes more than a few evaluations as part of an uncertainty analysis impractical. Advanced algorithms minimize the required number of evaluations through the development of surrogates and other techniques, but a large number of model evaluations are fundamentally required to explore the input space of the model, especially if it is high-dimensional. For this reason, application of UQ analysis in inexpensive low-fidelity models as discussed above is obviously useful and practical. However, there are uncertainties in even the highest fidelity fusion models, and these also need to be quantified. One approach is to use less expensive models, perhaps with reduced resolution, fewer particles or reduced toroidal domain sizes, as a surrogate for the purpose of estimating uncertainties. The validity of these approaches for specific model outputs will need to be checked.

In simulations of magnetic fusion, there is great value in the treatment of uncertainty as discussed above. But, there are significant challenges to a comprehensive treatment of uncertainty in fusion simulations. Many of the algorithmic challenges are the subject of research in a variety of projects, including the QUEST SciDAC 3 center. Just as important are the challenges of formulating meaningful characterizations of uncertainty that respect known physical constraints of the system. Addressing this challenge will require deep collaboration between fusion physicists and computational mathematicians working in uncertainty. It should be a priority in fusion simulation development.

References

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