Uncertainty Quantification and Inverse Problems for Fusion Energy Sciences

Adrian Sandu[1] and Alireza Haghighat[2]

Virginia Tech ([1]sandu@cs.vt.edu, [2]haghigha@vt.edu)

Introduction

Simulation and modeling of fusion system require an integrated multiphysics capability that includes neutronics for radiation effects evaluation, determination of isotopics transmutation and tritium breeding in the blanket module and its heating, electro-magnetics, plasma–material interaction, computational fluid dynamics (CFD) analysis for estimation of first-wall surface and structural temperatures, evaluation of cooling system and energy recovery, structural stress/deformation analysis, and mass transport modeling for tritium permeation estimation. This white paper focuses on the neutronics component of a fusion system, and discusses methodologies for simulation and modeling, benchmarking, sensitivity analysis, and uncertainty quantification.

Uncertainty Quantification

Neutronics simulations are affected by uncertainties from different sources such as the input data, and model representation. Haghigat et al. (1996, 1997) provide studies performed for evaluation of uncertainty of estimated neutron fluence in the pressure vessel of a fission reactor.

To obtain an accurate value for the uncertainty in a fusion system in a reasonable time, various analysis techniques have to be employed. To determine the uncertainty due to nuclear data, perturbation methods based on forward and adjoint fluxes have been used within software tools such as SUSD3D (Kodelli, 2011) or TSUNAMI (Rearden, 2005). To determine uncertainty in the isotope generation and breeding ratio, and heating of a fusion system blanket, forward and adjoint neutron and gamma calculations could be performed using deterministic code systems such as MCNP Monte Carlo (X-5, 2005), PENTRAN (Kucukboyaci, Haghigat, et al., 2011), and TITAN (Yi and Haghighat, 2010). To be able to perform a thorough study allowing for uncertainties in material composition and changes in properties due to temperature changes, response surface methods have to be employed (Haghigat et al, 2014).

New developments in the field of Uncertainty Quantification can greatly benefit Fusion Energy Sciences. For example, Adjoint-based methods offer an elegant framework to accelerate sampling. For example, recent work has shown that adjoint-based hybrid Monte Carlo sampling can be very effective in large state space dimensions (Attia et al., 2014). Second order adjoint models have proved to be a useful tool to quantify the posterior error in a Bayesian inversion framework (Cioaca and Sandu, 2012-2014; Sandu and Zhang, 2008).

Inverse Problems

A consistent integration of information from measurements and models through the solution of inverse problems is essential for a more detailed scientific understanding of the fusion processes. The solution of inverse problems produces improved estimates of the state of the system by combining (in a Bayesian framework) information from three different sources: the physical laws of evolution (encapsulated in the model), the reality (as captured by the measurements), and the current best estimate of the state (encapsulated in the prior) – all with associated errors (Carmichael et al., 2008). For example, neutron and gamma detection systems can be designed for monitoring the system behavior (Walters et al., 2014). In addition to determination of detector response, by employing either an array of detectors or a scanning system, an image of the system internals such as the blanket has been developed by comparing computed image with measurements and by employing the Maximum Likelihood Estimation (MLE) in an iterative manner (Royston and Haghighat, 2014).

Important challenges are raised by the very large dimension of inverse problems in fusion application. Two families of methods are popular to solve inverse problems at large scales. The variational approach (Carmichael et al., 2008), rooted in control theory, formulates inversion as a numerical optimization problem and searches for the maximum likelihood estimate. The ensemble filter approach (Constantinescu et al., 2007) (including the ensemble Kalman and particle filters), rooted in statistical estimation theory, deals with large dimensions by sampling.

New advances in the solution methodology of inverse problems can greatly benefit fusion applications. Nuclear sciences have pioneered the use of adjoint methodology, and many nuclear simulation codes have adjoint capabilities. This makes the application of variational techniques, where adjoints provide gradients for solving PDE-constrained optimization problems, especially appealing. Improvements for large scale optimization problems include distributed and adaptive multi-level checkpointing Sandu et al. (2005) and the use of approximate but inexpensive adjoint models Singh and Sandu (2012). Reduced-order models (ROMs) are computationally inexpensive mathematical representations of complex dynamical systems. ROMs have recently been to speed up variational inverse solutions (Stefanescu et al., 2014). Accounting for model uncertainty should become an integral part of the inverse problem formulation, leading to weak-constraint variational formulations. Second (or higher) order adjoint models are very useful to speed up the optimization process and to solve the optimization of the sensor network problems (Cioaca and Sandu, 2014; Cioaca et al., 2012; Sandu and Zhang, 2008). Aposteriori error estimates that quantify the impact of different errors on the accuracy of optimal solutions have recently become available (Rao and Sandu, 2015) and can find excellent applications in fusion sciences. Ensemble-based filters represent uncertainty (probability densities) in high-dimensional spaces by ensembles. Newly developed algorithms are able to estimate covariance matrices from very low numbers of samples (Nino and Sandu, 2015a) and lead to considerable better performance for large systems. For non-Gaussian inverse problems ensemble-based filters able to sample directly from the posterior distribution have recently been proposed (Attia and Sandu, 2014; Attia et al., 2014). Hybrid inversion methods seek to combine the advantages of both variational and ensemble-based estimation methods. New developments include hybrid estimation of posterior covariances (Cheng et al., 2010), error subspace decomposition approaches (Sandu and Cheng, 2014), and derivative-free optimization approaches that find the maximum likelihood solution in an ensemble space (Nino and Sandu, 2015b)

A problem closely related to variational inverse problems is the optimization of reactor design according to a given (quantifiable) criterion leads to PDE-constrained optimization problems, similar to the ones discussed in the context of variational inverse problems. Important developments that allow to accurately solve optimal design problems are the understanding of properties of discrete adjoints for temporal and spatial discretization schemes (Alexe and Sandu, 2007-, 2009b, 2011c), and space and time adaptivity to enhance the accuracy of the optimal design (Alexe and Sandu, 2011a-, 2011c).

Summary

The complexity of plasma physics models as well as the latest algorithmic developments in uncertainty quantification and the solution of large inverse problems, make the close collaboration between the fusion and the computational science research communities essential to enabling significant advances in the simulation and design of fusion devices. To design and operate a nuclear system such as fusion system, it is necessary account for variations of different parameters and their impacts on various physical phenomenon in a multiphysics system. For example, in a particle transport problem, there are various sources of uncertainties such as particle source distribution and its spectrum, nuclear cross sections, material composition, geometric model, and temperature effects. To be able to estimate the combined uncertainty of particle transport and its impact on other phenomenon of the fusion multiphysics system, it is necessary to utilize fast and accurate methodologies by employing forward and adjoint transport methods and take advantage of perturbation methods.

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