A National Validation Initiative for Guiding Predictive Model Development

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Request Oral Presentation: No
Primary Panel: Whole-Device Modeling (C) **Secondary Panels:** all others

Motivation

A top strategic goal of the current US magnetic fusion energy (MFE) research program, as stated on the Offices of Fusion Energy Science (OFES) homepage, is to "*Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source*". This goal was recently articulated more specifically as:

> "*[M]assively parallel computing with the goal of validated whole-fusion-device modeling will enable a transformation in predictive power, which is required to minimize risk in future fusion energy development steps.*"

In addition to the significant computing challenges achieving this research goal faces, a viable plan for meeting the *validation* requirement is needed. We propose that one approach to addressing this issue is through a new national validation initiative, detailed below. The key aim of this initiative will be to develop and maintain a dynamically evolving database of experimental datasets corresponding to various predictive modeling use cases. These datasets will be used to quantify the performance of existing models (with results made publicly available), assess the progress of in-development models, and eventually serve as one (of many) inputs into funding decisions on both model and diagnostic development efforts.

Approach

A fundamental concept in the broader validation literature, particularly for whole-systems modeling, is the idea of a validation hierarchy [1]. Such a hierarchy can be envisioned as a pyramid consisting of four levels or tiers. For the case of MFE systems, going from bottom to top, one might classify: predictions of local turbulent fluxes as a *unit problem*, prediction of equilibrium kinetic profiles as a *benchmark case*, prediction of the full discharge evolution of a plasma as a *subsystem case*, and prediction of the overall fusion reactor plant behavior, including both the plasma dynamics as well as (for instance) heating, loading, and erosion of vessel walls and tritium generation, as a *complete system*. Construction of such a hierarchy has been identified as a key element for effective management of large validation projects, and is needed for "best practices" approaches to validation such as "Phenomena Identification and Ranking" (PIRT) tables used in fission power plant and defense model validation work.

In order to implement this approach for a MFE predictive modeling capability, we propose that a new initiative be undertaken, which begins by constructing a validation hierarchy of whole-device modeling (WDM)-relevant predictive modeling use cases. One possible approach to constructing this hierarchy would be to mirror the "component"-based approach current WDM tools use, and to rank the various use cases into different tiers based upon the number of components used. Thus the unit test level would correspond to testing of a single component, the benchmark case to perhaps the integration of 2-3 components, and so on.

Once this hierarchy has been constructed, the next task will be to define use case-specific validation metrics (including definitions of methodologies to be used for error analysis and uncertainty quantification). Once these metrics have been agreed upon, one or more experimental datasets for each use case element of the validation hierarchy must be obtained. These datasets must be of sufficient quality to meet the requirements (including uncertainty characterizations) for the agreed-upon validation metrics. The data should be obtained from the full range of US experimental devices, including relevant validation platform devices at various universities.

Finally, a database of model validation results corresponding to the different use cases should be assembled, quantifying the performance of existing models and components (beginning with those most regularly used for predictive modeling of ITER and other reactor studies) using the defined metrics. Once these results are obtained, this initiative should enter an iterative stage, with focused validation efforts aimed at improving the fidelity of our predictive modeling capabilities using the validation outcomes as a key input for prioritization (along with readiness and impact on mission-critical WDM applications). As part of this iterative process, the dynamic nature of the database must be emphasized and supported. Existing use cases will evolve as new datasets and diagnostics become available, and new use cases will be identified as our predictive modeling capability matures. Moreover, the iterative process (particularly when paired with other validation best practices such as PIRTs) will help clarify key gaps in both model and diagnostic capabilities, and should therefore inform how resources are allocated in future development of both. As multiple iteration cycles are completed, one goal should be that models receiving significant development support exhibit quantifiable improvement in their performance for relevant use cases. We propose that a commitment to, and demonstration of, such progress be a condition of continued development funding for mature codes and models after several award cycles.

In order to successfully carry out this initiative, sustained funding will be required (for increased modeling development and execution, conduct of validation experiments, diagnostic development, and data management needs for supporting the database in a widely-accessible fashion). However, this initiative will only succeed if there is real buy-in from the modeling community and experimental facilities. In order to obtain this buy-in from as broad a fraction of the community as possible, we propose that existing organizations and meetings (such as the USBPO and Transport Task Force Workshop) be charged with leading as much of this work as is feasible.

Impact

This initiative will enable the US MFE community to better coordinate research across theory, computation, and experiment, allowing it realize the goal of a validated predictive modeling capability in a finite time and with finite resources.

References

[1] W. L. Oberkampf and C. J. Roy, “Verification and Validation in Scientific Computing,” Cambridge University Press 2012