Emphasis on Reduced Models for Integrated Modeling

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Primary panel: **C**   Secondary panel: **D**

Overview

In this note we suggest that the most effective strategy to achieve **improved realism** in integrated and whole-device modeling is through additional emphasis on **reduced model** development. This is in contrast to a Fusion Simulation Program (FSP)-style philosophy for which increased reliance on massively-parallel simulation is asserted as the obvious key to improved realism. Millions of core-hours spent running very expensive direct numerical simulations (DNS) dynamically (in a modeling loop) would be traded, for example, for millions of core-hours spent populating a database of results that can be systematically synthesized into an advanced reduced model. In terms of development flow, we suggest

Large-scale simulation → Advanced Reduced Models → Whole Device Model

Fidelity in a specific topical domain

Improving upon realism (i.e., fidelity) in tokamak modeling is a continuous challenge and is an important measure of the progress in fusion energy research. In specific topical domains, the challenge of improved realism is normally met by developing more comprehensive analytic formalisms, writing advanced simulation algorithms/codes, and running more expensive computer simulations. Progress this way is consistent with the SciDAC model of using large computer simulations to inform scientific discovery. In this model, researchers carry out 10s to 100s of “large” simulations. Typical strategies include examining different plasma scenarios, or performing systematic parameter scans. The results are then analyzed and distilled. Conclusions can be based on inferred trends, comparisons with theory, with other codes (verification) or with experiments (validation). The end result is a very large number of runs carried out over time (often months) to establish a physics story. This type of fundamental research is critical and enables a very narrow, precise physics focus. It is also a proven approach for effective utilization of ASCR resources.

Fidelity in integrated modeling

In both interpretive and predictive modeling, the approach is different: here one attempts to couple numerous domain-specific phenomena to more completely simulate tokamak operation and performance. These include equilibrium, collisional transport, turbulent transport, current drive and diffusion, beam heating, RF heating, alpha heating, particle fueling, impurity accumulation, evolution of profiles (temperature, density, electric field), and so on. Models for less-well-understood nonlinear phenomena can also be included (3D viscosity, kink/sawtooth evolution, island formation, etc). Here, the validity of the individual components is tacitly assumed, such that predictions are generally seen to have a level of credibility that is in line with the average credibility of the individual components.

Current approach to integrated modeling

In the context of integrated modeling, researchers would generally agree that productivity is maximized by using very fast, reduced models for separate plasma phenomena. Conversely, productivity will quickly grind to a halt if one component is significantly slower than the others. This is precisely why modelers use reduced models almost exclusively. When direct solvers are used (say, for EFIT equilibria) the expectation is that execution takes on the order of seconds. Further, the robustness of the overall simulation effort is also directly linked to the robustness of the individual components. If one component is time-dependent and produces noisy or resolution-sensitive results, then this adversely affects the entire modeling loop. Because reduced models are generally smooth functions of input parameters, the complete integrated model will often inherit this robustness. This is in contrast to DNS, which may compute fluxes/sources using time-averaging, particle averaging or some other ensemble mean used to reduce statistical uncertainty. This explains why, for example, TGLF is a mission-critical tool for integrated modeling. Whereas the capability for profile prediction using GYRO (via TGYRO) has been available for more than 6 years, nobody uses this approach to improve modeling fidelity. Instead, the demand for TGLF continues to grow in the US and abroad. This also clarifies the path forward: as improvements to GYRO are made (for example, in the case of multiscale simulations and electron transport), these improvements can be distilled into an improved version of TGLF, and the improved version of TGLF used to enhance the fidelity of whole-device modeling.

Whereas the FSP popularized a 2-step notion of doing predictive modeling with advanced simulation codes engaging exascale resources, we advocate an alternative approach that focuses on the 3-step approach suggested in the outline. By this we mean utilization of large-scale simulation using ASCR resources (step 1) to support the development of advanced reduced models (step 2) which are integrated to produce a fast, robust whole device modeling capability (step 3). Further, users would strongly prefer that fidelity of predictive modeling increase without significant added cost of expensive or non-robust component modules.

A suggestion for future development practices

Increased effort on reduced-model development would keep intact the traditional SciDACs separated by discipline (turbulence, heating, energetic particles, MHD, edge). It would maintain the aggressive use of leaderships-scale simulations for *scientific development*, but would simultaneously add a new focus on *distillation* of these results and physics insights into ever-improving reduced models. For example, given a large database of (verified and validated) simulation results, a neural network could be constructed to provide fast lookup of model outputs. If a new region of parameter space is encountered on a modeling application, this could generate a request to add specific new elements to the database using first-principles simulations. The new physics contributed by these simulations would then be use to further improve reduced models. This approach provides a very clear connection to ASCR expertise and resources.

In summary, we argue for formal, intensive development of more sophisticated, higher-fidelity reduced models as the key to advancing predictive modeling on a 5-10 year timescale.