Role and Requirements for Whole Device Modeling

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The development of a strategic approach to whole device modeling needs to take into consideration the diverse needs of the fusion community and that opportunities exist for significantly improving research in this area. Whole device modeling is needed by large segments of the fusion community to do a wide set of tasks ranging from: interpretive modeling of experiments with sophisticated heating and current drive packages; design of current experiments including simulation of control algorithms; design of future facilities ranging from ITER to FNSF and power plants; validation of appropriate operating conditions prior to executing ITER discharges including simulation of the coupling of plasma/edge/divertor to predict heat loads on divertor and core performance; to verification and validation of the most sophisticated exascale simulations of diverse plasma physics parameters.

We are recommending developing a Whole Device Modeling capability, central to which is a transport-timescale code optimized for production runs to support on-going experimental and design activities. This code will be capable of running "stand alone", but must also be a component within a flexible workflow manager that enables the integration of many other physics modules, including first principle codes for purposes of verification and validation and the development of reduced physics modules. Common requirements for both the workflow manager and the framework within the production code are the ability to (a) easily incorporate both legacy and new physics modules, (b) use conceptually similar codes interchangeably, (c) incorporate components written in different languages, and (d) leverage the technology being developed by the ASCR-funded scientists in the context of exascale computing.

The present capabilities of whole device modeling are most thoroughly developed for core transport and axisymmetric MHD equilibria. These rely on state-of-the-art source terms including auxiliary heating and current drive system, and fueling. Currently time-dependent simulations predict the confinement and stability properties of a tokamak discharges for existing and future machines. However, significant gaps remain in the fidelity of these simulations as briefly discussed below and should be the focus of the community's effort by incorporating improved reduced models some of which may be the product of verification and validation of exascale computing models.

Core-Pedestal-Edge Integration is recognized as being of critical importance for a comprehensive model of tokamak performance. The transition from L to H-mode, height and width of the pedestal, the magnitude of frequency of ELMs affects both the pedestal and core confinement. Furthermore the edge is tightly coupled to the divertor and the plasma parameters along with the design of the facility affects the heat load to the divertor and fueling and pumping of particles and impurities.

Core confinement and MHD Stability: Plasma pressure and current profiles along with plasma shaping has a major effect on MHD stability. Similarly the occurrence of MHD modes including NTMs, ELMs, and sawteeth affect the plasma profiles including impurity confinement and influxes. Furthermore, to predict disruption-free operating regimes for ITER, it will be necessary to predict the occurrence of locked modes and RWMs in order to program the discharge to avoid them and in a real-time feedback system take preventive action.

Core confinement and Fast Ion Physics: In ITER, alpha particle heating will have a major role on plasma pressure and stability. While some aspects of fast ion physics can be predicted by classical processes, the alpha particles, as well as beam ions and RF heated ions, can couple to MHD instabilities, which in turn depend on the details of the distributions function. While progress in modeling the core transport has been made, there is on-going need to improve the transport models including comprehensive models for both bulk and energetic-particle and impurity transport.

The scientific opportunities for enhanced integrated modeling are well known and the above is meant merely to highlight some key issues. Strong emphasis must be placed on the validation of physics modules, and therefore any successful modeling using the production code as well as the workflow manager will have experimental data integration *ab initio* with the ability to perform predictive simulations with some parameters from experiment, and some parameters from a physics model (i.e. a plasma shape or temperature profile).

One example of how this framework could be developed is based on the TRANSP code. Currently, TRANSP has a large international user base, which uses it for both interpretive and predictive modeling. A more modern production code can be developed by evolving TRANSP to a plug-in architecture. The code kernel would maintain time step and logic control, and would call parallel modules (MPI, OpenMP, GPU) that compute for example sources from neutral beams and RF, transport prediction and equilibrium evolution. Data would be prepared and input into the kernel by the workflow manager. During execution of this evolved TRANSP code, intermediate results could be stored or passed to large-scale, first principles codes (e.g., for MHD stability, core turbulence, energetic particle transport, edge and SOL transport). The results of these advanced calculations could be readily compared with the interpretive or predictive data from TRANSP for physics model validation, or could be passed back into TRANSP. This structure will leverage computational frameworks to enable dynamic coupling of external modules, and will facilitate the development of interfaces that will allow straightforward coupling of external codes to TRANSP by the greater fusion community. This evolution of TRANSP could be done incrementally without affecting the existing user experience and while maintaining backward compatibility.

The United States' goal should be to provide world-leading computational models in support of ITER analysis, planning and experimental operations. The design of both the workflow manager and the computational framework should take into account the efforts underway at ITER in developing tools to support an integrated model. As a minimum, the codes developed in support of a whole device model in the United States should be able to be incorporated into the ITER architecture, and where appropriate use the tools developed at ITER and the ITER members.