Goals and Challenges Associated with Whole Device Modeling

Arnold Kritz[1] (kritz@lehigh.edu)**, Tariq Rafiq**[1] **and Alexei Pankin**[2]

[1]Lehigh University, Bethlehem, PA [2]Tech-X Corporation, Boulder, CO

The goals for Whole Device Modeling (WDM) are to provide a comprehensive predictive simulation capability for magnetically-confined plasmas that integrates the knowledge from key multi-scale physical processes to continually improve fidelity. This capability is needed to maximize exploitation of fusion experiments, especially ITER, and to establish the scientific basis for an economically and environmentally attractive source of energy. In particular, WDM software must be designed to meet the following needs:

- Model scenarios to plan new experimental campaigns in existing tokamaks or to extrapolate to planned future devices. Scenario modeling is used to optimize discharge parameters, such as maximizing fusion power production in burning plasmas, and to maximize the effectiveness of planning new experiments.
- Advances needed in the computation of core and edge turbulence and transport; large-scale instabilities; the sources and sinks of heat, momentum, plasma current and particles; and the plasma equilibrium.
- Develop code components that are well documented and that satisfy community based standards.
- Allow for verification in order to eliminate sources of error and to access the degree to which the code correctly implements the physical models used.
- Validation and/or calibration of theoretical models using experimental data and synthetic diagnostics. WDM provides a platform where the validation of individual physics models can be performed in an environment that involves the interaction of the various physics components.
- Real-time modeling of tokamak experiments that utilize the predictive capabilities and feedback control techniques. The real time modeling can be used to optimize the discharge performance and to avoid disruptive events. The real time modeling of tokamak can utilize the advances in the uncertainty quantification techniques to include the uncertainties in the experimental data measurements.
- Production of self-consistent simulation results that are passed on to other more specialized computer codes.
- Mitigate disruption effects; predict pedestal formation and transient heat loads on the divertor, and compute tritium migration and impurity transport.
- Whole Device Modeling Simulations will result in cost-effective harvesting of physics from national and international facilities and will accelerate progress to fusion power by stimulating innovations that will lead to better fusion device designs.

Within the past few years, advanced scientific computing has achieved a level where it is on par with laboratory experiment and mathematical theory enabling WDM to become as a major tool for scientific discovery. The kinds of physics problems that will be addressed with WDM codes might include:

- Predict the plasma confinement and details of transport in tokamak discharges. Currently, there are a variety of transport models that yield different predictions for confinement and fusion power production in burning plasma tokamaks such as ITER. In the future, there must be a convergence in the transport predictions based on high-fidelity turbulence and particle orbit computations. Various physics effects need to be considered including effects associated with the behavior of non-local transport.
- Predict the onset, frequency and consequences of macroscopic instabilities. Comparisons can be made with experimental data for the frequency of sawtooth oscillations, the effect that a sawtooth crash has on the plasma profiles, the onset of neoclassical tearing modes and the resulting

magnetic island widths. There is also a critical need to predict the onset edge localized modes, their frequency and width as well as the onset of disruptive instabilities and their nonlinear evolution.

- Determine the plasma boundary conditions from plasma-wall interactions through the scrape-off-layer and the H-mode pedestal. All of the plasma profiles are strongly influenced by the evolution of the plasma boundary. Some WDM codes are also used to compute interactions between magnetic coil currents and plasma currents.
- Compute the sources and sinks that drive all of the profiles in plasma discharges. Sources such as neutral beam injection, fusion reaction products, and radio frequency heating and current drive all involve the computation of fast particle distributions and their interaction with the thermal plasma profiles. Predictions are needed for the effect of fast ions on macroscopic instabilities such as sawtooth oscillations.

Whole Device Modeling simulations face the following challenges:

1. Coupling between different regions of the plasma — such as the coupling between core and edge plasma regions— using component based architecture.
2. Coupling between different physical phenomena — such as the coupling between micro-scale and macro-scale instabilities.
3. Bridging the gap between short and long time scales, or between microscopic and macroscopic space scales. An example of this last kind of integration would be the simulation of turbulence, which grows on microsecond time scales and sub-millimeter space scales, resulting in transport across the plasma and the evolution of plasma profiles over tens of seconds in a tokamak with dimensions of several meters.
4. Providing an environment and producing output that facilitates the use of the WDM code by experimentalists, theoreticians and modelers.

The required whole device modeling capabilities involve self-consistent simulations of the entire plasma discharge that include all of the relevant physical phenomena. Depending upon the requirements of each simulation, the user should be able to choose from a spectrum of models for each physical process including high physics fidelity models based on first-principles computations or reduced models for more rapid computations and validation or empirical models. Full-featured WDM simulations should be capable of simulating the entire time-span of the discharge, from start-up to shut down, and the entire spatial scale from the magnetic axis to the interaction between the plasma and the first wall and magnetic coils. There should be seamless access to experimental data or the results of previously-run simulations.

Most of the existing WDM codes are limited to axisymmetric plasmas with simply nested closed magnetic surfaces. There is a need to couple the closed magnetic surface regions of the plasma with the open magnetic surface regions at the plasma edge, including plasma-wall interactions. There is also the need to include the three-dimensional effects that result from the formation of magnetic islands, magnetic ripple, resonant magnetic perturbations and macroscopic instabilities in tokamak discharges. Future WDM codes must include more kinetic modeling — as opposed to fluid approximations — and there must be a closer coupling between fast particle distribution and the more thermal part of the distribution function. WDM codes must be developed to bridge the gap between high-fidelity turbulence simulations on microsecond time scales and the resulting transport on multiple-second time scales. WDM code must also be able to incorporate high-fidelity simulations of macroscopic instabilities such as sawtooth oscillations, neoclassical tearing modes, resistive wall modes, edge localized modes and, ultimately, disruptive instabilities. There must be integration between fine-scaled kinetic and large-scale macroscopic physical phenomena in order to produce a fully self-consistent simulation capability. The development of a widely community used WDM code requires full-time focused leadership and will not be accomplished with part-time non-focused leadership. WDM capability will embody the theoretical and experimental understanding of confined thermonuclear plasmas. The ultimate success of ITER will rely heavily on the development and use of whole device modeling.