First-Principles Whole Device Modeling of Fusion Plasma on Extreme Scale Computers, in collaboration with ASCR scientists

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This white paper describes the need and method for the whole-device fusion-physics modeling using first-principles full-function 5D gyrokinetic or 6D kinetic equations, which includes most of the important multi-physics except for those that are undoubtedly scale separable from the rest. This is the way to achieve the highest fidelity predictive simulations.

Plasma profiles and transport in a hot tokamak is dominated by nonlinear interactions and self-organization among multi-physics that are mostly scale-inseparable in the time and configuration spaces. For example, MHD type activities (such as neoclassical tearing modes, resistive wall modes, saw-tooth activities or edge localized modes), turbulence, energetic particle driven modes, penetration of the 3D magnetic fields into the plasma, and neutral particles can interact strongly with each other in wavelength, frequency, and configuration spaces. Global plasma profile establishment from hot core to cold scrape-off plasma from such a nonlinear, nonlocal, self-organization dynamics can over-ride the localized Fick’s law type transport concepts and does not warrant the accuracy of the component-physics integration approach that assumes scale separation or spatially localized physics. First-principles simulation of the whole device multi-physics as much as possible, without scale separation, is needed for a higher fidelity understanding and predictability of fusion reactor performance, and for improvement of the component-physics integration methods by identifying the gaps. The geometry effect including the kinetic X-point effect and the wall shape must also be included in the self-organization physics.

One specific example for the consequence of the global nonlinear self-organization is that the long-distance interaction between the core and edge macroscopic observables can happen within the turbulence, MHD, and plasma self-organization time scale (several ms in the present tokamak devices) even in the absence of the violent global MHD activities. Such a core-edge turbulence and plasma gradient interaction phenomenon has already been observed in major tokamak experiments (for example, see [1]). In comparison, the core-edge interaction time through the conventional Fick’s law type plasma transport mechanism would predict a much longer time scale (0.1 – 1s) than what is observed in the experiments because the change in the turbulence would happen as a result of the change in plasma gradient via the Fick’s-law type plasma transport over a long distance.

First-principles approach to the whole device physics does not come cheap. First of all, it requires at least 10X more powerful computers, approaching exa flops, than what are available today. Fortunately, DOE is installing a few such pre-exascale computers within a few years at OLCF, ALCF and NERSC. Exa scale computers are then expected to arrive in a few years after that, before ITER’s first plasma operation, giving us ~100X computing power than what we have now.

The second expense is in the necessity to join forces with the applied mathematicians, the computer scientists, the performance engineering scientists and the uncertainty quantification scientists. As we have already experienced at 10 peta flop level, taking advantage of a leadership class computing at 100 peta flops or higher rate will be a very difficult task for physicists alone. To name a few, the new hardware and software architectures will be quite different from what we are used to today and difficult to use, and most of the data management, analysis and visualization must be done on node-memory and on the fly without relying on external I/O processes, which also should include fault tolerance technologies. Code verification and uncertainty quantification at extreme scale are also daunting tasks.

For lower hanging fruits, we propose to use full-function 5D gyrokinetic equations with improved accuracy, with embedded 6D simulations where needed. In the regime where the validity of the 5D
gyrokinetic equations are in question, we can change the 5D gyrokinetic particles to the full 6D particles. Debye sheath region (see FIG. 1), description of particles in the reconnection region, and the particle dynamics in resonant with ion cyclotron waves are a few representative examples. When the particles are outside of such 6D space-time region, they can come back to be 5D gyrokinetic particles. The present form of the gyrokinetic Poisson equation may need some modification for this purpose.

FIG. 1. Schematic diagram of how the full 6D Vlasov particles can augment the 5D gyrokinetic particles where needed. Debye sheath is used here as an example.

Material science will need to be handled separately and coupled into the whole device modeling with PMI data, with the first-principles plasma providing the needed angular and energy distribution of the bombarding ions on the material surface. RF propagation simulations may also need to be handled separately for a low-hanging-fruit whole device simulation. Since many of the plasma particles are not in thermal equilibrium --especially those in the scrape-off layer, fusion produced alpha particles, rf resonant particles-- a fully nonlinear Fokker-Planck operator should be used to describe the Coulomb collisions [2].

Feasibility of the first-principles whole device modeling approach has already been demonstrated in the SciDAC-3 Center for Edge Physics Simulation (EPSI). The neoclassical and turbulence dynamics have been simulated together in the full-f 5D gyrokinetic code XGC1 with central heating, torque input, and neutral recycling at the material wall surface [3] in realistic magnetic separatrix geometry (see FIG. 2). Nonlinear self-organization among the global core-edge background plasma profile, the turbulence profile, and the neutral particle profile is a natural output from the simulation. Data table and analytic cross-sections have been used for the atomic physics interactions. The nonlinear coherent turbulence structures called “blobs” have been produced in XGC1 [4]. XGC1 can also include the MHD type modes self-consistently in the first-principles gyrokinetic simulation. Again, these whole-device simulations and physics discoveries in EPSI would not have been possible if the full-function first-principles approach has not been taken, if not supported by the leadership class HPCs, or if there were no ASCR funding to the applied mathematics and the computational scientists within the project. The ASCR scientists made the XGC1 code to produce science using full capacity leadership class computers at ORNL (Titan), ANL (Mira) and NERSC (Edison).

FIG. 2. Plasma turbulence from a limited whole-device modeling of a DIII-D plasma in the gyrokinetic code XGC1. Neoclassical, turbulence and neutral particle physics are self-consistently simulated in realistic X-point geometry.