

First-Principles Simulation of Whole Fusion Device on Leadership Class HPCs in Collaboration with ASCR Scientists

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The traditional approach to magnetic fusion science has been piecemeal; i.e., solving each physics element and each configuration-space problem separately assuming scale-separation and linear superposition. The absence of nonlocal behavior is typically assumed. The conventional integrated simulations, either attempted or suggested, are also based upon this traditional picture. However, there exists ample experimental and theoretical evidence that fusion plasmas are governed by fully nonlinear and nonlocal self-organization. Most of the important physics phenomena are not scale-separable in space or time. One must solve the important fusion physics together using the most fundamental kinetic equations, including micro-turbulence, wall-interaction and atomic physics data, MHD/fluid instabilities, energetic particles and plasma heating. The geometry must be realistic and it should be the whole volume including the divertor as the tokamak experiments unanimously shows that the core confinement is nonlocally influenced by edge condition in a sensitive manner. The fully global, nonlinear and kinetic approach will not only remove the unjustified scale-separations or local-physics approximations, but also remove the insurmountable mathematical issues in the coupling of many different codes in higher dimensions and in the loss of necessary kinetic information. The unified kinetic multiscale/multiphysics method, if successfully applied, will advance the fundamental scientific understanding. Such a model will provide improved reduced models appropriate for the conventional integrated model approach.

The issue in this approach has been in the necessity for an extreme scale computing and the big data handling. With the exa-scale computing expected to be realized in several years and the present US HPC computing power already being well over 10 peta flops, the time is ripe for an initiation of first-principles simulation of the whole device physics without scale-separation, as a long-term joint OFES-OASCR endeavor. The OASCR scientists can play critical role by providing technologies for data management, scalable solvers and meshes, extreme scale scalability and optimization, uncertainty quantification (UQ), algorithm verification, etc. Strong participation by OFES experimentalists, in collaboration with UQ scientists for the challenging sensitivity studies at extreme scale, will be necessary for the laboratory validation.

Recent progress made by the XGC1 5D gyrokinetic code in SciDAC-3 Center for Edge Physics Simulation (EPSi) has shown promises in this approach. XGC1 has simulated together the background plasma dynamics, electrostatic turbulence, neutral particle recycling with atomic physics data, and simplified plasma heating in the whole tokamak volume including realistic diverted tokamak geometry. Electromagnetic turbulence is presently being added into XGC1. However, addition of the MHD/fluid activities, energetic particles with fusion reactivity, and realistically detailed heating physics, which can simulate even the disruption physics and edge localized mode activities, is far beyond its present scope. The 5D gyrokinetic simulation may need to be upgraded to the full 6D kinetic simulation in some specific situations, such as the Debye sheath physics in front of the material wall or the high frequency plasma-wave interactions. A larger scale, longer-range effort needs to be initiated in the fusion community to achieve this longer term goal. Total of \$4M/year funding, with \$2M/year spent by ASCR scientists, is expected to be an adequate funding level.