First Principles Integrated Simulation of Boundary Multi Physics Using PIC Method

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The study of tokamak boundary physics is a scientific grand challenge due to several inter-related physical complexities including: a) the non-equilibrium state of boundary plasma, b) the highly nonlinear scale-inseparable multi-physics that interacts both in velocity and configuration spaces, c) the wall-born neutral particles that interact with the plasma through atomic cross-sections, d) the complex geometry including the magnetic separatrix and material wall.

a) Non-local non-equilibrium state of the boundary plasma: Strong plasma source and sink drive the boundary plasma into non-equilibrium state. There is no heat-reservoir for boundary plasma as often assumed in the non-equilibrium statistical mechanics. The environment --core plasma and wall-- is strongly coupled non-locally to the boundary plasma. Core temperature responds in a stiff manner to the boundary plasma. There are also internal non-equilibrium drivers. Wall interacts with boundary plasma through PMI. The pedestal gradient scale length is roughly the same as the neoclassical orbit excursion width and the blobby turbulence size. The kinetic physics information is continuously mixed between different pressure regions at the time scale of particle orbital motion, which is inseparable from the turbulence, edge instability and neutral transport time scales. When the pedestal gradient becomes too steep, the strong free energy drives the boundary plasma into large scale edge localized mode (ELM) instabilities. Even in a quiescent state, the bolundary plasma contains large-scale blobby turbulence, which may not be described by equilibrium thermodynamics. It will be highly difficult, if not impossible, to close properly the fluid equations under these situations. *A fully kinetic approach is needed.*

b) Scale-inseparable nonlinear multi-physics: All the important boundary physics phenomena – turbulence, neoclassical particle dynamics, edge localized instabilities (ELMs), and neutral particle transport – have significantly overlapping space-time scales. The pedestal profile may evolve more slowly than others in the absence of ELMs, but its radial scale length is similar to others. These physics components interact nonlinearly with each other to form the boundary plasma. The conventional modular theoretical and computational approach that assumes scale separation among the multi-physics phenomena has very limited validity applied to the boundary, and will face very difficult mathematical constraints at best. A common first-principles set of equations needs to be solved, containing the multi-physics without scale-separation.

c) Neutral particles: Plasma interaction with the material wall produces neutral particles that are an important particle, momentum and energy source/sink to the whole plasma. Since the neutral particles are intrinsically in a non-thermal state as well, their transport needs to be studied kinetically. Thus, the plasma-neutral model must be kinetic-kinetic for reliable predictions.

d) Complicated geometry: The plasma boundary crosses the magnetic separatrix surface, which divides the closed and open (SOL) magnetic regions. The SOL plasma is in contact with arbitrary-shaped material wall. The geometry effects on the boundary plasma are known to be important for all spatial regions including the edge pedestal region, the scrape-off layer and the divertor region leading. The numerical method that is used to study boundary plasma needs to be robust to difficulty caused by the complicated topology and geometry.

After carefully analyzing available models and numerical methods for solving the gyrokinetic equations in the boundary region, we have chosen to use the particle method as the primary tool. An ODE particle code is much less susceptible to the show-stopping CFL stability condition in both configuration and velocity space under large amplitude fluctuations. For a particle code, the field part is separated to grid, and only accuracy of particle dynamics is required leading to an indirect CFL-like accuracy-condition in configuration space. Particle methods are amenable to modeling arbitrary-shaped recycling boundary conditions and neutral particle transport from first principles. This endeavor has already been selected as a joint OFES and OASCR project, currently the Center for Edge Physics Simulation (EPSI) in the SciDAC-3 program. A very strong collaboration between the OFES and the ASCR scientists is fully utilized to solve the difficult boundary plasma problem. As a result, the edge gyrokinetic particle code XGC1 has emerged, fully utilizing the largest open-science computing platforms. XGC1 is the leading international code in the field of kinetic boundary simulation, containing neoclassical physics, neutral particle recycling and transport, atomic cross-sections, blobby electrostatic turbulence, and edge-core interaction. XGC1 has been revealing the physics of pedestal, blobby turbulence, edge momentum solurce, and divertor heat-load footprint at first-principles level for the first time. There are continuum edge gyrokinetic codes under development in US: the ESL code at Livermore, and the Gkeyll code at PPPL that employs a new technique: discontinuous Glerkin method.

XGC1 has successfully acquired the electromagnetic turbulence capability using the gyrokinetic ions and fluid electrons. Various verification exercises have been performed including the tearing modes. The linear and nonlinear onset of kinetic ballooning modes is presently being studied in the edge pedestal plasma. Work is underway to develop fully kinetic electron extensions to the electromagnetic model in XGC1.

Besides the electromagnetic turbulence, there are a few other challenging physics features to be added to XGC1 in order to complete the boundary physics capability at first-principles level. ELMs are not really scale-separable from turbulence, and their mutual interactions could be strong. In XGC1, in the future, ELMs will be simulated together with neoclassical and turbulence physics from the same set of gyrokinetic equations. The fluid or MHD codes are capable of studying only the large-scale Type-I ELMs. However, ITER may have to rely upon small scale ELMs, which have not been seen from the fluid/MHD codes nor been understood. XGC1 will investigate the small ELM physics, too.

Control of ELMs by external RMP coils or molecular injection is another outstanding issue. XGC1 needs to include these capabilities in the future. With the XGC1's capability in combining MHD/fluid modes, electromagnetic turbulence, neoclassical physics, and neutral-atomic physics, a comprehensive study of ELM control could be possible at first-principles level. A reduced version XGC0 already possesses the kinetic RMP penetration and plasma transport response capabilities.

Having a realistic PMI model is important for the fidelity of the boundary plasma simulation. XGC1 can evaluate the ion bombardment data that are necessary for accurate PMI modeling, which include the ion flux PDF in the incident angle and the incidence kinetic energy at each wall position. For a more accurate evaluation of the sputtered impurity re-circulation at the material wall, a six-dimensional Debye sheath calculation could be desirable, instead of the "logical" sheath that XGC1 is presently calculating. XGC1 can use an embedded 6D simulation technique in front of the material wall for this purpose.

In return to the easy and physics capabilities, computation in XGC1 is expensive due to the large number of particles required for Monte Carlo noise reduction, hence requiring an extreme-scale HPC with good code scalability. Throughout the development of the XGC1 particle code, a hand-in-hand partnership with the ASCR scientists in all four SciDAC Institute areas (Data Management, Applied Mathematics, Performance Engineering, and Uncertainty Quantification) has been required to overcome the challenges. As a result, XGC1 scales efficiently to the maximal hardware capability, with a high degree of portability, on the major leadership class computers; including the heterogeneous Titan, and the homogeneous Mira and Edison. Production runs utilize the maximal available capability of these HPCs. The more powerful the computers are, the more physics XGC1 can include.

With the new hardware and software architectures employed by the future leadership class computers, and with further development of XGC1 to include more complete boundary physics, the collaboration with ASCR scientists will continue to be highly important. The technical merit of XGC1 development into exascale has been proven by the recent selection into the main pre-exascale programs at OLCF CAAR and NERSC NESAP.