Kinetic Simulation of Scrape-off and Edge-Core Plasmas Using PIC Method for High Fidelity PMI Research

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The study of tokamak scrape-off and edge-core physics is a scientific grand challenge due to the several inter-related physical complexities including: a) the non-equilibrium state of edge 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 plasma through atomic cross-sections, d) the complex geometry including the magnetic separatrix and material wall, and e) the strong non-local interaction among core-edge plasma, scrape-off plasma, and PMI. In order to obtain the necessary kinetic information input to the high fidelity PMI simulation, such as the local angular and energy distribution of the bombarding ions on the material surface, we need to model the scrape-off plasma correctly that is part of these complex physics system. An added complexity is that the PMI, in return, affects these complex physics system nonlinearly, thus affecting the property of the scrape-off, the pedestal and the core plasma strongly. First-principles kinetic simulation, which includes all these complex physics phenomena and PMI data self-consistently, is needed for a predictive understanding of the PMI science.

a) **Non-equilibrium state of the edge/SOL plasma**: Strong source and sink drive the edge/SOL plasma into a non-equilibrium state. There is no heat-reservoir for edge plasma as assumed in the non-equilibrium statistical theory. The environment --core plasma and the wall-- is strongly coupled non-locally and nonlinearly to the behavior of the edge/SOL plasma. PMI provides most of the particle source and sink. Impurity PMI is also connected to the radiative loss. There are also internal non-equilibrium drivers. The pedestal gradient scale-length is roughly the same as the neoclassical orbit excursion width. Size of the nonlinear holes and blobs are also on the same scale. 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 edge plasma into large scale edge localized mode (ELM) instabilities. Even in a quiescent state, the edge/SOL plasma contains large-amplitude blobby turbulence. These physics cannot be described by equilibrium thermodynamics. It will be very 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 edge/SOL physics phenomena – turbulence, neoclassical particle dynamics, macroscopic edge localized instabilities (ELMs), and neutral transport – have significantly overlapping space-time scales. The pedestal profile may evolve more slowly than others without ELMs, but its radial gradient scale length is similar to others. PMI influences all these multi-physics. These multi-physics, including PMI, interact nonlinearly with each other to form the edge/SOL plasma. The conventional modular theoretical and computational approach that assumes scale separation among the multi-physics phenomena has very limited validity applied to the edge, 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**: Since the neutral particles are intrinsically in a non-thermal state as well, they needs to be studied kinetically for a higher fidelity simulation. Thus, the plasma-neutral model must be kinetic-kinetic for reliable PMI physics. For a more accurate evaluation of the sputtered impurity re-circulation at the material wall, a six-dimensional Debye sheath calculation is 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.

d) **Complicated geometry**: The geometry effects –including the flux surface, separatrix and wall shapes— are important on the plasmas in all spatial regions including the edge pedestal, the scrape-
off and the divertor; hence on PMI. The numerical method that is used to study edge/SOL and PMI needs to be robust to difficulty caused by the complicated magnetic topology and wall geometry.

After carefully analyzing available models and numerical methods for solving the gyrokinetic equations in the scrape-off and edge-core region under the constraints given above, we have chosen to use the particle method. An ODE particle code is much less susceptible to the show-stopping CFL stability condition in both configuration and velocity space than PDE codes are. 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 strong collaboration between the OFES and the ASCR scientists is fully utilized to solve the difficult 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 edge simulation, containing neoclassical physics, neutral particle recycling and transport, atomic cross-sections, blobby electrostatic turbulence, and edge-core interaction. XGC1 has been revealing for the first time the physics of edge pedestal, blobby turbulence, edge momentum source, and divertor heat-load width at first-principles level.

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.

Besides the electromagnetic turbulence, there are other important physics features to be added to XGC1 in order to complete the edge-core, SOL and PMI-data physics capabilities 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. The non-Maxwellian plasma bombardment information from the large and small ELMs will be of great asset to a higher fidelity PMI.

Control of ELMs by external RMP coils or molecular injection is another outstanding edge research 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.

In return for easier and complete edge physics capability, 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 parallel 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 edge-core and SOL physics, and PMI data, 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.