Integrated Multi-Scale Divertor Simulation Project

Predrag Krstić\textsuperscript{1}, Igor Kaganovich\textsuperscript{2}, Daren Stotler\textsuperscript{2}, Bruce Koel\textsuperscript{2,3}

\textsuperscript{1}Institute for Advanced Computational Science, Stony Brook University, NY
\textsuperscript{2}Princeton Plasma Physics Laboratory, NJ
\textsuperscript{3}Princeton University, NJ

ABSTRACT
The effectiveness of the divertor in magnetic fusion devices depends on the interplay between the edge plasma and the plasma-facing material interface. Science of this interface is very different from the science of a bulk material. The interface is a separate entity, mix of material and plasma, which follows its own laws of the surface physics. Spatial and time scales of the surface is mainly determined by the penetration depth of the impact plasma particles (typically a few nm) and times for the impact thermalization cascade, followed by chemistry and possible ejection and other processes, usually tens of picoseconds, depending on the impact energy. Through cumulative effects of the plasma bombardment the surface is dynamical in nature, perpetually changing its structure and chemical content, resulting in ever changing target for the impact plasma particles. The edge plasma governs particle and energy exhaust, and impurities eroded from the surfaces may reduce the fusion gain if they are transported back to the confined plasma. The other critical effects of these interactions are reduced lifetime of plasma facing surfaces due to erosion by transients, and restrictions on duty cycle due to retention of tritium in re-deposited material and in dust created by plasma surface interactions. These latter processes are evolving on much longer time scale, micro to mili seconds, the time scale of the plasma dynamics, although their fundamental phenomenology evolves at ps scale. Thus, in these interactions, both the plasma and material systems are inherently multiscale, requiring descriptions of phenomena over several decades of time and length scales. Even within the divertor plasma, especially in the detached regime, one needs to couple self consistently the partially ionized plasma, high density neutral, Debye sheath physics, and radiation fields. That complexity has prevented the assembly of a comprehensive description of the two systems and their interactions. At best, simulations to date have focused either on describing the plasma or material in detail, but not both. The most successful plasma simulation codes are even less sophisticated and utilize approximate, not first principles, descriptions of plasma transport and plasma material interactions; the inadequacy of this treatment is widely acknowledged, defining clearly a scientific priority in the long term strategy for the fusion research.

The XGC family of codes, developed within the CPES and EPSI SciDAC projects, is working towards a first principles treatment of plasma turbulence and transport in the scrape-off layer and divertor, as well as in the core plasma. Separately, the ability of quantum and classical molecular dynamics methods to provide insight into plasma-material interactions in fusion devices has been demonstrated (LAMMPS and SCC-DFTB). Both methodologies, as well as DOE High Performance Computer capabilities (HPC) are now sufficiently mature that we can successfully combine them to address the critical problems outlined above. One can incorporate radiation transport into the DEGAS 2 Monte Carlo neutral transport code, and couple it into the framework. Where needed, a fully kinetic 6-D code could be used to simulate the Debye sheath. On-HPC coupling between codes will be facilitated by utilizing EFFIS (End-to-end Framework for Fusion Integrated Simulation) that was developed in the Proto-FPS CPES project and the modern Adios technology. Since the XGC-DEGAS2 system is well-known for its ability to utilize extreme scale parallelism, the coupled divertor simulation code system will run on extreme scale HPCs.
The long term objective of the project will be to better understand the divertor plasma and the associated plasma-material interactions and then use the resulting knowledge find practical divertor solutions for future devices, including burning plasma experiments. That understanding will come from application of the developed tools to existing tokamaks, both for the purpose of model validation and to assist in experimental planning.

SIGNIFICANCE AND PRIORITIES

The plasma-material interface is a critical bottleneck in fusion power conversion. Decades of empirical experience with successively larger fusion confinement devices have evolved in a mixed strategy for the design of plasma-facing components: use of tiles of low-Z materials (carbon, beryllium) which lower radiation losses from the plasma; thin coatings of boron or beryllium; and judicious use of refractory metals (W, Mo) in high-heat load regions. This mixed strategy is the scheme envisioned currently for ITER. The heavy use of carbon tiles operating near room temperature introduces significant complications for D-T operation because of tritium retention.

For the 10-tuple higher power fluxes at the PMI expected in a DEMOnstration Power Plant (DEMO), erosion due to chemical and physical sputtering becomes much more serious, and more robust or renewable components which operate at higher temperatures will be needed. New schemes that are now being explored in toroidal experiments include: (1) all tungsten walls operating at temperatures > 1000° K, which suppress erosion and retention, but risk poisoning the fusion reaction with strongly radiating high-Z impurities; (2) liquid metal coated high-Z metal substrate or carbon substrate, which have the advantages of low-Z materials and are continuously renewed, but whose behavior is still poorly understood. Another, so far untested, scheme is to use in-situ, nano-scale surface reprocessing to maintain a low-Z coating on a metal wall.

The traditional trial-and-error approach to developing first-wall material and component solutions for future fusion devices by successively refitting the walls of toroidal plasma devices with different materials and component designs is becoming prohibitively costly because of the increasing device size, curved toroidal geometry, access restrictions, and complex programmatic priorities. For this reason, in this, as in other areas of fusion research (e.g., plasma heating/fueling, transport, and stability, coil design, etc.), the importance of developing experimentally-validated computational models to extrapolate and optimize designs is increasingly being recognized [1].

The 2007 Greenwald fusion energy panel [FESAC 2007] found research on the plasma-material interface to be of such prime importance to achieving fusion energy that it allocated to it one of the five principal fusion research themes, Taming the Plasma-Material Interface. This panel also found that of the top 5 critical knowledge gaps for fusion 4 involve the Plasma-Materials Interface (PMI). The US fusion community in its final report on a series of RENEW workshops in 2009 addressed the Greenwald knowledge gaps and is leading to calls for new research activities and facilities to be funded by the Office of Fusion Energy Science (OFES) in the next few years. [RENEW 2009] The key RENEW recommendations for new activities focusing specifically on the plasma-material interface were:

1. Decode and advance the science and technology of plasma-surface interactions. Measurement of complex interaction of plasma with material surfaces under precisely controlled and well diagnosed conditions to develop comprehensive models to uncover the basic physics. These measurements would be made on both upgraded
present facilities and new boundary plasma simulators capable of testing irradiated and toxic materials.

2. Develop improved power handling through engineering innovation. Heat removal capability would be advanced by innovative refractory power-exhaust components, in parallel with assessment of alternative liquid-metal schemes. Materials research would provide ductile, reduced-activation refractory alloys, which would be developed into prototypes for qualification in high-heat flux test devices. Practical components would be deployed on existing or new fusion facilities.

The performance demands on plasma facing components (PFCs), first wall and blanket systems of future fusion power reactors are beyond the capability of current materials, which is one of the reasons that the United States Academy of Engineering has ranked the quest for fusion as one of the top grand challenges for engineering in the 21st century.

These statements are echoed at pages 5, 9, 10, 11, and 12 of presentation of Ed Synakowski The charge for advice on strategic planning of April 9, 2014 [Synakowski 2014, ].

EXISTING AND MISSING CAPABILITIES
The high heat and particle fluxes associated with confining a multi-million degree plasma within room temperature material surfaces can damage those surfaces. Progress in magnetic fusion research has in large measure been made possible by improvements in our ability to mitigate those interactions and minimize their effect on the core plasma. Many of these improvements were discovered empirically by accident or trial and error. The significantly greater costs to operate and repair ITER and subsequent devices preclude this same approach, motivating a concerted effort to predict the plasma fluxes and the consequences of the resulting material interaction for the material lifetime and the impact of interaction products on the plasma. To date, those predictions have been made via a combination of extrapolation of data from existing experiments and from simulations calibrated on those experiments. The predictive capability of both approaches is limited since neither is based upon a first principles theory that would provide the required degree of confidence in extrapolation beyond the existing database. Furthermore, the simulations utilize simplified models for the behavior of both the plasma and materials. We propose here an integrated modeling system that will be based on first principles models and will eventually provide a consistent solution of the whole device from the material surfaces to the plasma core. We will use this system to acquire a fundamental understanding of two outstanding divertor and edge plasma phenomena: the radiative, detached plasma and the erosion, transport, and redeposition of impurities.

Obtaining a consistent solution is essential in developing predictive capability since the plasma facing materials effectively establish the boundary conditions for the plasma and at the same time represent a particle reservoir vastly exceeding that of the plasma. The importance of these interactions is evidenced by the potential for dramatic effects of wall conditioning on core plasma confinement [Strachan1987, Mansfield1996]. Over time the plasma substantially alters the first micron of the material that directly interacts with the plasma so that the two must be considered interdependent [Krstic2008, Krasheninnikov2006]. Consequently, predicting the behavior of the plasma requires accounting for the behavior of the material and interaction of the two in an integrated consistent manner.

The radiative, detached divertor [Stangeby2001] was developed as a means of spreading plasma heat and particles over a larger area. Although the tokamak divertor represents a pivotal improvement in mitigating plasma-material interactions by moving the site of those interactions
away from closed flux surfaces, doing so actually concentrates the plasma heat and particle fluxes [Pitcher1997, Eich2013, Goldston2012]. The detached divertor mitigates this effect by using neutrals or photons, neither tied to the field lines, to spread the incoming momentum and energy over a larger area. A predictive model of a detached divertor thus requires consistently describing not only the plasma and facing materials, but also neutral species and the generated radiations field [Lisgo2005]. Moreover, each of these systems is inherently multi-scale with phenomena spanning several decades of time and length scales.

Erosion of plasma facing surfaces occurs through the processes of physical and chemical sputtering. The rates at which these occur establish one limit on the lifetime of the material surface [Stangeby2011]; the products of erosion represent impurities that can reduce core plasma performance via radiation and fuel dilution. Redeposition of that material can trap hydrogenic species; in a reactor environment, this trapping of tritium sets another bound on the material lifetime [Loarer2013, Tanabe2013]. Dust particles can also be formed, the accumulation of which is also limited by safety considerations [Rosanvallon2009]. Predictions of erosion and its consequences again require an integrated consistent solution of the plasma-material system, including the evolution of the material state and transport of impurities through the plasma.

The present state of the art of divertor simulations is represented by the SOLPS [Schneider 1992] (aka B2-EIRENE [Reiter 2005]) codes used to design the ITER divertor [Kukushkin 2009, Pitts 2009]. Considerable effort has been invested in incorporating the relevant physics into EIRENE [Reiter 2005], including radiation transport via a detailed Monte Carlo photon transport calculation [Kotov 2006 and references therein]. In particular, this treatment incorporates photo-excitation into the collisional radiative model that provides the effective ionization and recombination rates used in simulating the transport of neutral hydrogen. The EIRENE model accounts for Lyman-alpha and beta lines, natural and Doppler broadening as well as Zeeman splitting [Kotov 2007].

These improvements to EIRENE (and SOLPS) were motivated by attempts to validate it against existing machines. One of the persistent, acknowledged shortcomings is its inability to reproduce the experimental observation that the inner divertor detaches at a much lower core plasma density than the outer; the nominal result in simulations is that the two detach at the same density (Fig. 1) [Wischmeier 2009]; the EDGE2D-EIRENE code, used at JET, yields similar results [Guillemaut 2013]. Multiple papers [Coster 2011, Wischmeier 2011, Guillemaut 2013] have proposed that kinetic effects missing from the fluid plasma transport code, B2, in SOLPS are responsible.

A second shortcoming is the inability to reproduce the Mach speed parallel ion flows in the scrape-off layer [Erents2004]. Since these flows in large part determine the migration paths for impurities, understanding their origin is key in making predictions for future devices. A series of papers by Chankin et al. [Chankin2007, Chankin2009] connect the problems with the magnetic field dependent contribution to the simulated ion flows to discrepancies in the simulated divertor temperatures and then to the radial electric field across the outer SOL; note that the field-independent contributions are attributed to the ballooning character of transport into the SOL [Asakura2006]. Kinetic effects are again proposed as an explanation [Chankin2009] for the too low electric fields, although ion neoclassical transport from inside the separatrix undoubtedly plays a larger role [Chang2004].

Classical drifts contribute to scrape-off layer transport and have been implemented in SOLPS, EDGE2D, and UEDGE [Rognlien 1994], although they are rarely used in practice due to numerical difficulties [Rozhansky 2009]. The role of plasma-material interactions (PMI) in these
simulations is also rarely considered beyond choosing a value for a local recycling coefficient since only rudimentary models are employed.

We are here addressing some of these shortcomings. First, plasma turbulence and transport are simulated kinetically with first principles based models. The behavior and transport of neutral species are described via a directly coupled model. Second, a multi-scale description of the plasma facing materials and plasma-material interactions will be developed starting from first principles, atomistic models. Coupling of this to the plasma-neutral model would provide the required consistent, integrated plasma-material simulation capability. Radiation transport, needed to describe the detached divertor, could be incorporated into the neutral transport code. The integrated model could be validated against data from existing experiments. Subsequently, simulations analogous to those used in the ITER divertor design could be performed; any significant differences would be examined and documented.

We aim to understand and improve integration of the HPC computing of the divertor plasma coupled to the plasma-material interface (PMI). We would develop and deliver a new generation of theories, algorithms, and codes for both the computationally intense forward atomistic simulation methods and the challenging material and plasma optimization design, building upon our team's expertise that spans molecular and solid state electronic structure and response theory, classical/semi-classical/quantum molecular and coarse-grained dynamics, in particular classical molecular dynamics (MD) and first-principles quantum-classical MD (QCMD) with input from density functional theory (DFT) and mesoscale with kinetic Monte Carlo, chemistry kinetic, Particle-in-Cell, lattice Boltzmann, and continuum Navier-Stokes approaches. These simulations could be applied self-consistently to the dynamics and chemistry of the solid-liquid-plasma interface, exposed to high energy influx of plasma particles, in the presence of mixed materials and various contaminants. The overarching goal of the new initiative - simulation effort is to enhance our abilities to efficiently and accurately predict the processes of erosion of the plasma-facing materials, hydrogen retention and recycling, as well as plasma pollution at plasma-liquid – solid material interfaces far from equilibrium, under conditions of high heat and particle fluxes and to ultimately tailor the plasma and the interfaces to the desired specifications of stable plasma burning.

To integrate time scales of the plasma calculations in XGC-codes (time step of µs, time elapses to tens of ms) and the PMI, the mesoscopic scales need to be directly coupled to the plasma.

Our approach to develop a multiscale methodology in which we will systematically study the problem at different length scales using the more fine grained models (atomistic) to provide parameters and inputs to coarse grained models (mesoscopic) and finally to the particle in cell models that will provide a link between theory and experiments. In performing these calculations we intend to develop an iterative approach which will be performed as we pass information from one length scale (and time scale) to the other in order to ensure that we do not loose the critical information needed to connect the length and time scales. The overarching goal of our approach is to provide design criteria that will allow the whole device level modeling capability. To achieve this goal we need to develop mesoscopic models that can bridge the more detailed models that describe the PMI to the time scales of the plasma calculations in XGC-codes (time step of µs, time elapses to tens of ms).
References

[Synakowski 2014] E. Synakowski’s 9 April 2014 presentation "The charge for advice on strategic planning"


