Integrated, Multi-Scale Plasma-Material Interface Simulation[1]

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Motivation Concerns about erosion, tritium retention, and dust generation in ITER and power producing reactors to follow led the ReNeW report [1] authors to devote three thrusts (9, 10, and 11) to the plasma-material interface problem, reinforcing a similarly strong emphasis by previous panels [2]. Most recently the 2014 FESAC "Report on Strategic Planning" [3] identified "Taming the plasma-material interface" as a high priority, tier 1 initiative. Whitepapers submitted by us [4] supported that conclusion; this document summarizes their contents.

Improvements in our ability to mitigate plasma-material interactions and to minimize their effect on the core plasma have been responsible for much of the progress in magnetic fusion research. 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 in recent years 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 experiments and from simulations calibrated on those experiments. The predictive capability of this approach is limited since it is not based upon a first principles theory. We propose a more well founded approach that will allow extrapolation beyond the existing database with confidence.

The science of plasma-material interactions differs from that of the plasma itself or that of the bulk material. The interface at which they meet is a dynamic entity, a mix of material and plasma that is governed by the history of their interactions. The spatial scale of the surface is mainly determined by the penetration depth of incident ions; typically a few nm, up to microns with diffusion. Time scales are governed by the thermalization cascade, subsequent chemistry, possible ejection and other rapid processes (tens of picoseconds, depending on the impact energy); diffusion and thermal processes take longer, nano- to micro-seconds. On the plasma side, one needs to account for in a self-consistent manner the plasma, neutral species, radiation and electromagnetic fields, as well as the kinetic physics of the Debye sheath; these phenomena encompass time scales from microseconds to seconds and sub-millimeter to meter length scales. Thus, in the interface problem, both the plasma and material systems are inherently multi-scale, requiring descriptions of phenomena over several decades of time and length scales.

The primary emphasis on integrating the simulation of a fusion plasma with the material boundary falls inherently on the plasma-material interface because the phenomenology of the interface evolves much faster than plasma time scales and because the interface traverses a wider range of scales, which overlap with the scales of the plasma. The interface must be understood and parameterized at the nanoscale, evolved to the micro-scale, and then integrated self-consistently with the plasma. Within the tokamak plasma, attempts at decoupling the problem at the apparent interfaces at the separatrix or H-mode pedestal top have not fared well. Hence, the only path to a realistic solution is to solve the entire system from wall to core in a self-consistent manner [5].

Simulations of such scope will have to make optimal use of existing and future computing facilities and exploit partnerships with the ASCR SciDAC centers in the areas of data management, data analysis, and uncertainty quantification. The relative localization in space of plasma-material interactions lends itself to a natural parallelization. However, parallelization in time is much more difficult due to the causal time ordering during the energy accumulation (e.g., preparation of amorphous graphite surface in [6]). How to realistically treat the system beyond the most fundamental time scales, when the events are not known in advance, is a real computational challenge. Mature

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computational tools exist for simulating plasma-material interaction processes over the full range of time and length scales [4]. Developing the means by which these tools can be effectively coupled (via source and sink terms) is one of the key computational problems to be addressed.

Approach At the core of this initiative is an integrated system based on first principles models, eventually providing a consistent solution of the whole device from the material surfaces to the plasma core. The XGC family of codes, developed within the CPES and EPSI SciDAC projects, simulates turbulence and transport in the scrape-off layer and divertor plasmas, as well as in the core plasma [5]. Separately, the ability of quantum and classical molecular dynamics methods to provide insight into plasma-material interactions in fusion devices has been demonstrated (LAMMPS [7] and SCC-DFTB [8, 9, 10]). The existing tools for describing plasma-material interactions at the mesoscale (e.g., micro- to millisecond) level include kinetic Monte Carlo, particle-in-cell, Lattice-Boltzmann, and continuum Navier-Stokes.

The multi-scale interface problem can be tackled by systematically studying it 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 XGC plasma models that will be compared with tokamak plasma diagnostics. An iterative approach will be developed in which information is passed from one length (and time) scale to the other to ensure that critical information is not lost.

Such a system addresses multiple shortcomings of the current “state-of-the-art” boundary plasma and plasma-material interface simulations. First, plasma turbulence and transport are simulated kinetically with first principles based models, and 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 also be based on first principles, atomistic models. Coupling of this treatment to the plasma-neutral model will yield the required consistent, integrated plasma-material simulation capability.

A key, early phase of this initiative will be validation of plasma-material interface simulations against dedicated and carefully controlled laboratory experiments. New diagnostics in operating tokamaks [11] are now also providing more precise and time resolved information on plasma-material processes. The back-and-forth information exchange associated with such detailed validation speeds progress and ensures accurate treatment of the most relevant aspects of the problem, allowing irrelevant ones to be ignored.

Accomplishments of the CPES and EPSi SciDAC edge plasma simulation projects were described in a whitepaper presented to the FESAC panel [5]. The success of the atomistic approach to simulating the plasma-material interface was vividly demonstrated in the understanding of the lithium-oxygen-carbon-deuterium system described in [10]. Again, data from laboratory experiments [11] were crucial in guiding and confirming the simulations. Work along these lines will continue on NSTX-U in collaboration with researchers from PPPL, Princeton University, U. Tennessee and the University of Illinois Urbana-Champaign.

Impact The overarching goal of this initiative 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 the plasma response to these processes, under conditions of high heat and particle fluxes. The resulting knowledge will be used to develop practical divertor solutions for future devices, including burning plasma experiments. This detailed insight may even lead in completely new “game changing” directions.

The negative impact of not pursuing an initiative along these lines is potentially discovering the limitations of the extrapolation of existing knowledge base to ITER conditions at a time too late to preclude an extended down time or failure for ITER. Either would significantly diminish enthusiasm for fusion energy development within the international community.

References

[1] R. Hazeltine, D. Hill, et al., Report of the Research Needs Workshop (ReNeW) (link) (2009).

[2] *Priorities, Gaps and Opportunities: Towards a Long-Range Strategic Plan for Magnetic Fusion Energy*, FESAC Report, DOE/SC-0102 (2007).

[3] *Report on Strategic Planning: Priorities Assessment and Budget Scenarios* FESAC Report (2014).

[4] P. S. Krstić et al., "Integrated Multi-Scale Divertor Simulation Project", presented to 2014 FESAC Strategic Planning Panel (priorities; initiatives) (2014).

[5] C. S. Chang, "First-Principles Simulation of the Whole Fusion Physics on Leadership Class Computers, in collaboration with ASCR scientists", presented to 2014 FESAC Strategic Planning Panel (link). (2014).

[6] P. S. Krstic, C. O. Reinhold and S. J. Stuart, *New J. Phys.* **9**, 209 (2007).

[7] S. Plimpton, *J. Comp. Phys.* **117**, 1-19 (1995).

[8] D. Porezag, T. Frauenheim, T. Kohler, G. Seifert, and R. Kaschner, *Phys. Rev. B* **51**, 12947 (1995).

[9] N. Goldman and L. E. Fried, *J. Phys. Chem. C* **116**, 2198 (2012).

[10] P. S. Krstić J. P. Allain, C. N. Taylor, J. Dadras, S. Maeda, K. Morokuma, J. Jakowski, A. Allouche, and C.H. Skinner, *Phys. Rev. Lett.* **110**, 105001 (2013).

[11] C. N. Taylor et al., *Rev. Sci. Instrum.* **83**, 10D703 (2012).