Large-Scale Integrated Modeling of Plasma Boundary and Plasma-Material Interactions

D. Curreli, J.P. Allain, D. Andruczyk, and D.N. Ruzic

Center for Plasma Material Interaction, Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana Champaign, Urbana USA, 61801

Corresponding author: dcurreli@illinois.edu

White Paper for Oral Presentation to Panel Topic B - Integrated Simulations Workshop:
Plasma boundary, including the pedestal, scrape off layer, and plasma-materials interactions

Motivation

Can we reliably extrapolate conditions at the wall of today's pulsed confinement machines to future steady-state reactors? Is it possible to predict the impact of surface evolution on an equilibrium plasma state and on plasma facing component lifetime during steady-state operation? These questions appear as key issues in ReNeW's [1] Thrust 10 ("Decode and advance the science and technology of plasma-surface interactions"), highlighting that a strong theoretical basis is required to further the understanding and prediction of the PSI (Plasma Surface Interaction) processes in magnetically confined fusion plasmas. The need for reliable models of PMI is however not limited to Thrust 10, but is necessarily linked to multiple other thrusts across the ReNeW, comprising *Thrust 6* ("Develop predictive models for fusion plasmas, supported by theory and challenged with experimental measurement"), *Thrust 9* ("Unfold the physics of boundary layer plasmas"), *Thrust 12* ("Demonstrate an integrated solution for plasma-material interfaces compatible with an optimized core plasma") and, at system level, *Thrust 15* ("Create integrated designs and models for attractive fusion power systems"). Taming the plasma-material interface by gaining fundamental understanding and predictive capability is a key scientific issue that need to be addressed for the realization of nuclear fusion power. Here we discuss how large-scale computing, together with integrated modeling and model validation, represent an essential tool to tackle the problem.

Approach: key efforts and recommendations

(1) Deciphering the plasma-material dynamic coupling via integrated modeling. Past PMI models have mainly focused on describing either the plasma phase (eg. fluid SOL models, PIC, etc.) or the solid wall (eg. MD, TRIM, TRIDYN, MC, etc.), always avoiding an actual dynamically-coupled description of the plasma-material interface. However, the near-surface plasma-material interface is place of a multitude of inter-linked phenomena, which cannot be precluded to being *either* plasma- *or* material-only. The plasma-material interface has to be seen as a single dynamically-coupled environment, where mutual interactions must properly be taken into account to reach a reliable description with predictive capability. For example, the magnetized plasma sheath modifies the ion energy-angle distribution functions at the wall [2], which in turns trigger a non-linear dynamic response including, but not limited to, sputtering, implantation, modification of the material composition, changes in thermo-mechanical properties, and morphology evolution; all these processes in turn affect the sheath structure, the particles and current balances at the wall, etc. Fully dynamically-coupled models, including validated extensions of the descriptions currently available, can be obtained integrating together a full spectrum of powerful, robust, well-verified computer codes. Furthermore, by dynamically coupling multiple codes together, a key interpretative tool can be obtained for next generation of data that will become available from *in-situ* diagnostics. Multi-scale integration of plasma and material models will

have to proceed in tight connection with validation activities, as described in detail in a dedicated white paper [3].

(2) Develop new HPC s/w platforms specifically targeted to PMI. New software platforms dedicated to plasma-material interactions will be needed in order to fully exploit the computational resources currently available. Resolving the plasma-material interface at scales from nano- to milli-meters and from picoseconds to minutes means computing at the petascale and beyond. In order to tackle the multiple spatial and temporal scales involved in the PMI problem, new PMI simulation tools able to run efficiently on high-performance computing facilities are highly needed. Full leverage of heterogeneous CPU/GPU architectures with hybrid shared/distributed-memory paradigms will serve as an enabler for new discovery science on PMI. Unfortunately, most of the software infrastructure currently used for PMI simulations is based on outdated software technology, incapable of exploiting efficiently the supercomputing resources available. Dealing with old software means in many cases dealing with low degree of maintainability and extensibility. A remarkable, recent exception is the Xolotl code, an open-source, high performance plasma-surface interactions simulator that is under development within the DOE's PSI-SciDAC program [4]. Linking codes like Xolotl to an opportune kinetic description of the plasma sheath and plasma boundary will offer a first near-surface dynamic model including plasma kinetics and wall response.

(3) Need of new mesoscale models of the plasma-material interface. Probably the largest key gap in the plasma-material interaction science is the almost-total absence of opportune mesoscale models of the plasma-material interface. Here by "mesoscale" we mean spatial scales from tens/hundreds of nanometers to tens of micrometers, and time scales from microseconds to tens of seconds. This range is too large to be treated even with large-scale Molecular Dynamics simulations, and too small to be treated properly with standard continuum models. However, it is on these scales that the most interesting and relevant PSI phenomena occur, like changes in thermo-mechanical properties, material degradation induced by plasma irradiation, surface morphology modification, etc. New mesoscale models of the plasma-material interface will have to be developed, verified, and validated, so that they can act as a necessary link between 'micro' and 'macro'.

References

[1] "*Research Needs for magnetic Fusion Energy Sciences*", Report of the Research Needs Workshop (ReNeW), Bethesda, Maryland – June 8-12, 2009.

[2] R. Khaziev, D. Curreli, Phys. Plasmas 22, 043503 (2015)

[3] J.P. Allain, D. Curreli, B. Wirth, and P. Krstic, *Challenges and strategies to experimental validation of multi-scale nuclear fusion PMI computational modeling*, PMI Workshop, PPPL, 2015

[4] https://sourceforge.net/projects/xolotl-psi