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Scientific and Computational Challenges in Coupled Plasma Edge/Plasma-Material Interactions for Fusion Tokamaks*

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Plasma/material interactions is a critical scientific issue for fusion power, with major potential limitations on plasma core and edge operating parameters. Gaining understanding and predictive capability in this area will require simultaneously addressing complex and diverse physics occurring over a wide range of lengths (angstroms to meters) and times (femtoseconds to days). This requires further development and validation of detailed physics models and computational strategies at each of these scales. The overriding numerical need is for petascale real-time coupling between 3-D material response/evolution/trapping codes, plasma edge/SOL codes, and impurity transport codes. We discuss selected science and modeling/computational challenges in this area and our ideas for achieving these goals; this from the standpoint of our existing simulation codes.

1 Introduction

Plasma/material interactions significantly affects existing magnetic fusion devices and will critically impact the design, performance, and economic feasibility of DEMO and future commercial fusion tokamak reactors. Key issues are lifetime of plasma facing components (PFC's) due to steady state sputter erosion; erosion/damage by plasma transients; surface ultrastructure and mixed-material evolution; plasma contamination by eroded material; tritium codeposition in redeposited material; and plasma operating limits due to these factors. A REDEP/WBC code-package analysis, for example, shows that a beryllium first wall is probably acceptable for the low duty-factor ITER but would not extrapolate post-ITER, due to high sputter erosion and T/Be codeposition [1]. A HEIGHTS code-package analysis shows that the ITER outer tungsten divertor may not even survive a single full-power disruption, or tolerate so-called giant ELM's [2]. However, these and other studies have pointed the way to acceptable operation, e.g. with plasma regimes having moderate ELM activity only, high-Z wall and divertor surfaces with appropriate plasma edge parameters, and possibly liquid metal divertor surfaces. In general, solutions appear definitely possible but we need major scientific and engineering understanding and predictive capability. It is an unusual and unsatisfactory situation that such a critical issue has not been far more resolved for a major engineering project such as ITER, as well as for post-ITER devices. The need for such resolution has also been identified in several fusion community evaluations, including the US RENEW workshop [3] and Extreme-Scale Computing Workshop [4], and in the journal literature, e.g. [5].

In this paper we discuss selected scientific issues and challenges in modeling plasma/surface interactions in the context of our respective codes for plasma edge/scrape-of layer (SOL) solutions, surface material response to the steady-state and transient plasma, and resulting plasma and material evolution. For each code we briefly summarize the covered science and computational methods, modeling challenges, and possible responses. We

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then discuss some overall coupling, computation, and validation strategies. While we naturally focus on our own codes we believe that many of the issues and proposed solutions can apply to a number of simulation tools used in the world fusion community.

2 Plasma/material interaction science and prediction requirements

The general science requirements are for rigorous self-consistent modelling of the complex array of interacting processes that include plasma edge and SOL parameters with ion, atom, and molecule fluxes to/from the material surfaces, tokamak-type oblique incidence sheaths, single and mixed-material surface evolution/chemistry and sputtering in response to the normal plasma, emitted impurity transport, and finally and critically the PFC response to ELM's, disruptions, and other high-power plasma transients. Time/distance scales vary by some 10-18 orders of magnitude, from femtoseconds/angstroms to picoseconds/microns (e.g., atomic collisions, radiative transitions, sputtering) to centimetres/microseconds-meters/seconds (redeposition, tritium migration, turbulence, plasma transport, plasma transient event/response) and finally through days/meters (surface equilibration). Full time-dependent simulations, in 3-D reactor configurations, are ultimately needed.

Required information includes:

- Net erosion of plasma facing components (first wall, divertor target, etc.)
- Tritium codeposition in sputtered/redeposited material, D-T retention and recycling in irradiated material
- Plasma contamination from sputtered and plasma-transient (ELM's, disruptions, VDE's, runaway electrons) released and transported material
- Dynamic surface evolution in mixed-material environments, including microstructure changes, irradiation effects, surface chemistry, helium irradiation, bubble and dust formation
- Lifetime prediction of overall PFC materials and nearby components
- Identification of acceptable and unacceptable plasma core/edge solutions
- PFC design optimization and innovation to prolong lifetimes

3 Science areas and simulation tools

3.1 Erosion/redeposition during normal-plasma operation

REDEP/WBC Code Package

This code package, e.g. [6,7], computes sputtering and other atom/ion emission (evaporation, etc.) from plasma facing materials, near-surface impurity transport and redeposition, plasma contamination, and tritium codeposition. The level of description is 3-D, fully kinetic (3-V), sub-gyro-orbit motion of an emitted particle in a given background D-T plasma. The package contains hundreds of sub-models/data-inputs for surface geometry, magnetic and electric fields, plasma parameters, impinging D, T, He, B, O, etc. ion and neutral fluxes, sputtering coefficients and sputtered velocity distributions, atomic and molecular processes (electron and proton impact ionization, recombination, charge exchange, and misc. processes), carbon chemical sputtering and hydrocarbon transport, material and temperature-dependent tritium codeposition rates, dual-structure tokamak type sheath parameters via BPHI-3D code [8], and related phenomena. Self-sputtering from redeposited impurity particles is self-consistently modeled; this is critical for determining maximum acceptable plasma edge temperature. REDEP/WBC has been used to study plasma material interactions in all major US tokamaks (TFTR, C-MOD, DIII-D, NSTX), world tokamaks (e.g. JET), planned devices (INTOR, ITER), and misc. applications (mirror machines, lab devices, diagnostic mirrors, non-fusion plasma applications). The code package interfaces with other codes, including UEDGE, DEGAS, ITMC-DYN–these codes to be discussed–but currently on an off-line basis.

REDEP/WBC uses a wide variety of numerical techniques with a focus on Monte Carlo. Individual emitted atom/ion motion is solved via Newton's law, with Lorentz force and charge-changing and velocity-changing collisions. The latter is computed via Fokker-Plank treatment and using a rigorous extended Braginski method

for arbitrary-mass impurity ion collisions with plasma ions/electrons, and using a test particle colliding partner method for impurity atom collisions with the background plasma ions/neutrals. The collision terms depend on background plasma electron and ion temperatures and temperature gradients, ion and electron densities, and fluid velocity and velocity gradient. So-called thermal forces and viscosity terms are included. Bohm (anomalous) diffusion is also modeled. Other numerical techniques are employed as needed (e.g. PIC for sheath sub-package).

REDEP/WBC plasma/material interactions analysis of present devices has generally shown good code/data agreement. For future devices REDEP/WBC studies have been most useful in defining broad trends, however, there are present limitations in satisfying the major need for a full, precise, predictive capability. One example is a study of ITER first wall sputtering erosion with the critical plasma physics phenomenon of edge/SOL convective ("blob") transport [1]. This analysis used UEDGE and DEGAS-2 calculated plasma edge/SOL parameters, with full-kinetic sputtered impurity transport, and TRIM-SP sputter computations. Convective plasma transport is predicted to result in much higher particle fluxes to the wall and consequently ∼20-40 times higher wall sputtering than for radial diffusion-only physics. Figure 1 shows sample calculated trajectories for wall-sputtered beryllium. In spite of high sputter yields, the net erosion rate (∼0.3 nm/s), plasma contamination, and T/Be codeposition (∼2 gT/400-s shot) for the reference beryllium coated wall appear to be acceptable for ITER–with low (∼3%) duty factor–but are high enough that ongoing analysis with continuing improved models and code coupling is clearly needed. Another key prediction is a significant wall-to-divertor beryllium transport; the implications of this on Be/W divertor mixed-material formation and performance have been examined, but need much more detailed assessment.

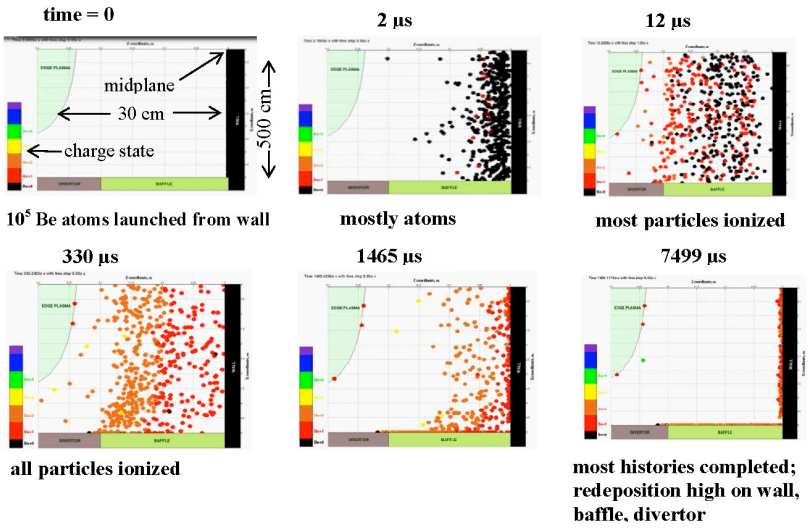

Fig. 1 REDEP/WBC code package full-kinetic transport calculations of beryllium, uniformly sputtered from ITER outer first wall. Transport shown in poloidal flux coordinates; computation region from outer midplane to core plasma, divertor, and baffle region. From Ref. [1] analysis.

While this analysis is encouraging for ITER, there are major uncertainties due to the need for auto-coupled self-consistent codes and improved material response modeling. Coupling is needed, in addition to establishing consistency between interacting systems, for better statistics for spatially-resolved charge exchange neutral flux/energy impingement on the first wall, time-dependent convection effects, and spatially-resolved first wall erosion and resulting T/Be deposition. In any event, REDEP analysis shows that low-Z material (Be, C) will not be acceptable surface materials for post-ITER devices due to high erosion and tritium codeposition. We also note uncertainties/differences in predicted erosion for a tungsten first wall, e.g. between studies [1] and [9], apparently mostly due to edge plasma solution differences including charge exchange D-T energy spectrum predictions.

An uncertainty for any first wall plasma-response modeling is the sheath potential (if any) and structure at the first wall. In contrast to the divertor, the magnetic field geometry can vary greatly at the wall including regions of being purely tangential. Although some models exist for these cases, a full 3-D wall sheath theory/model is

needed along with supporting experiments. Also needed is evaluation of multiple plasma solution dependence of PFC response, and conversely, the plasma edge dependence/iteration on/with sputtered impurity transport.

Regarding divertor erosion/redeposition, some advancements are likewise needed, for high-confidence predictive capability, particularly for high-Z materials and high edge density plasmas. Here, the net erosion rate is of order 1% of the gross rate (i.e. ∼99% redeposition), thus requiring high-fidelity low variance analysis. Among the scientific challenges for ITER etc. are detailed evaluation of tungsten ultrastructure (nm-μm scale "tendrils") formation and response, due to simultaneous D, T, He impingement, and mixed-material Be/W formation/response.

Erosion/redeposition calculations were made for the National Spherical Torus (NSTX) outer liquid lithium divertor (LLD), with low D recycling, and with anticipated high heating power plasma shots [10]. The goal was to determine the basic compatibility of an LLD with NSTX (or similar device) high heating power operation, from the standpoint of Li evaporation, sputter erosion, and core plasma contamination. The results are encouraging showing significant D^+ sputtering but non-runaway self-sputtering, acceptable net erosion rate (∼5 nm/s), and acceptable edge and core plasma contamination (∼10% edge, ∼0.1-1% core Li/D). However, liquid lithium is a very complex material involving ion (∼66%) and atom (∼34%) sputtering, Li^+ ion reflection, surface chemistry/mixing/trapping with D, C and redeposited Li, and related issues. A key challenge is to predict D retention/recycling for a lithium surface that is evolving with surface impurities and "slag" during plasma operation. This will require a major increase in employed computing speed, with coupled codes, and with advanced models from both binary-collision and molecular dynamics material response codes. Likewise, a self-consistent assessment of the effect of emitted Li on the near-surface plasma is needed.

Also analyzed for NSTX was a molybdenum divertor surface, subject to D, Li, and C impingement [11]. This was done via REDEP/ITMC analysis, using a SOLPS fluid code and EIRENE Monte Carlo neutrals code plasma solution [12] with outer strike point located on the inner Mo divertor, and with high-recycling boundary condition. Figure 2 shows the computed time dependence of the sputtering yield of Mo and the deposited C and Li, at the strike point, over the 1 s discharge time. Initially, the surface is pure Mo and then continues to be enriched in C and Li. This results in a decrease in Mo sputtering yield and an increase in the sputtering yield of C and Li. A steady state surface concentration of Mo, C, and Li is not yet reached at the end of the discharge.

A next obvious but major step would be fully coupled, self-consistent, computations of material evolution from the ITMC-DYN code with REDEP/WBC calculations of sputtered impurity transport, and for the entire divertor surface. In particular, we require future computation capability for all divertor points, with full time-dependent self-consistent point-to-point coupling, and with a wide range of plasma conditions corresponding to anticipated operational windows. A desirable simulation would typically involve ∼100 spatial points @ 10,000 sputtered particle histories per point, totaling $\sim 10^6$ histories for one plasma time interval. For order of 1000 time intervals and 10 plasma conditions (e.g. with variable D recycling coefficient, plasma heating power, and magnetic field topology) an NSTX (or like device) material assessment would involve some 10^{10} particle histories. Also, improved numerical treatment of sputtered particle distributions is required, using on line coupling with ITMC and CMD-DFTB or similar codes. The need is thus for fully coupled codes, using $\sim 10^5$ cores.

3.2 Composite/mixed-material response and surface evolution

3.2.1 ITMC-DYN kinetic Monte Carlo code

This code [13, 14] computes surface atom sputtering and interaction within evolving textured surfaces, hydrogen isotope retention and release, diffusion and effect on bubble formation, chemical erosion in the presence of impurities, and atom segregation to near-surface layers. Dynamic tracking of surface evolution in nano/micro layers, with modeling of relevant duration times (several hours) and time-dependent update of target composition is performed. The code is Monte Carlo, using the binary collision cascade approximation (BCC) for the selection of the struck atom from a compound and for modeling of the atomic collision processes. The capability is for a target with multiple layers, materials, and thicknesses. ITMC-DYN updates the composition of target layers at each time step. Motion of ions and atoms in the target is modeled using pseudo particles with interval and particle flux weighting. The dynamic part of the ITMC-DYN code was benchmarked against recent experimental data from the deposition of low energy ions of C and Fe on Si substrate [14].

Diffusion process inclusion is very important in simulating realistic fusion reactor conditions where target materials operate at high temperatures and the diffusion of the incident particles can significantly influence the

material surface composition and hence plasma-material interactions and the overall performance of the fusion reactor. ITMC-DYN calculates the diffusion coefficients in multi-component materials depending on the target composition. Also computed is the very important issue of release of the helium and hydrogen isotope implanted gases from the target material. In particular, tritium retention and inventory in plasma facing components is modeled, and affects both safety and plasma performance, and also affects sputtering of the target material (via a dilution effect by the hydrogen isotopes). Output from ITMC-DYN has been used in REDEP/WBC, but on an off-line basis, necessitating simplifications and not permitting efficient self-consistent time-dependent material evolution calculations.

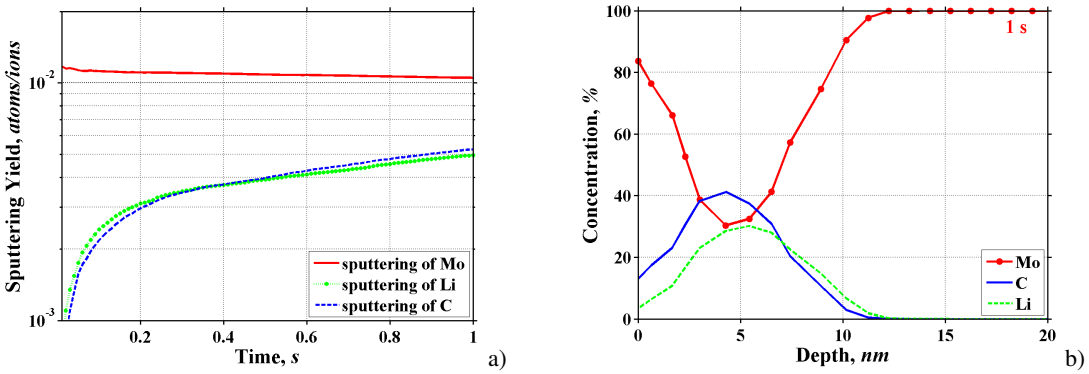

Fig. 2 NSTX molybdenum divertor analysis: a) time dependence of divertor sputtering at strike-point due to D, 1% Li, and 1% C impingement and Mo self-sputtering; b) depth distribution of the deposited C and Li in the Mo substrate, at strike point, after 1 s. Initial surface (pure Mo) is changed substantially after only one second. REDEP/ITMC-DYN analysis. From Ref. [11].

Required model improvements include detailed description of D-T interaction with materials and compounds and corresponding integrated modelling of hydrogen isotopes trapping, diffusion, agglomeration, recombination and desorption. Further benchmarking, e.g., of H-isotopes retention with experimental results in the US and Germany, is also in order.

3.2.2 CMD and QCMD advanced molecular dynamics (MD) codes

Molecular dynamics is a computationally intensive technique most applicable for collective effects modeling, low energy impingement (non-BCC regime), and/or complex chemical effects. MD simulation serves as a good complement to kinetic type codes such as ITMC. The classical (CMD) and quantum-classical (QCMD) codes [15,16] compute PFC material response, e.g. for Li using polar Li-C-O-H-Mo mixed material quantum-classical molecular dynamics, with full inclusion of the relevant chemistry, and covering the range of sub-eV to keV impact D^+ ions. It is found via these codes that the surface oxygen plays a key role in trapping hydrogen and reducing erosion, for a lithiated carbon surface [16].

For tungsten, the codes simulate radiation damage to obtain vacancies, displacements, interstitials, and other damage induced by high-fluence, high-energy particle impacts. We start from well-ordered, crystalline surfaces, then follow the surface evolution and damage produced by the cumulative plasma particle irradiation. The short time and length scales, where atomic collisions and chemical reactions take place in the PFC materials, are described using an MD formulation employing complex classical and quantum density-functional tight-binding (DFTB) many-body potentials. The latter formulation is an approximation to Density Functional Theory (DFT) and is significantly faster than first-principles methods, but still much slower than classical MD that utilizes predefined bond order potentials.

Figure 3 shows example QCMD calculations–using the self-consistent charge density functional tight binding (SCC-DFTB) theory quantum component–of the retention and sputtering yields upon bombardment with 5 eV D atoms, on pure carbon, and various C, Li, D, and O containing material matrices: Matrix A: 100% carbon; Matrix B: 80% carbon; 20% lithium; Matrix C: 60% carbon, 20% lithium, 20% oxygen; Matrix D: 52% carbon, 16% lithium, 16% oxygen, 16% deuterium; and Matrix E: 80% carbon, 20% oxygen.

Particle impact on a material surface is a stochastic process, requiring many thousands of trajectories in order to obtain reliable yields of the investigated processes and parameters in MD. For example, 30,000 CPU hour hours are needed for 5000 trajectories (cores) on the Kraken computer at the National Institute of Computational Sciences of University of Tennessee, with 500 fs long (quantum-classical) evolution of a computation cell containing a thousand mixed-material atoms bombarded by single-energy deuterium projectiles of a few eV. This approach is well suited for current super-computing capabilities. Treatment of diffusion and transport effects in this approach can rely on the kinetic Monte Carlo solution of a Liouville type master transport equation (a 6-dimensional 2nd order partial differential equation).

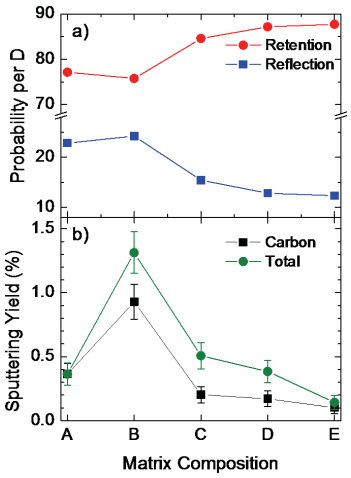

Fig. 3 QCMD MD example analysis. From Ref. [16] results.

We have developed, in collaboration with K. Morokuma and S. Moeda of Kyoto University and of S. Irle of Nagoya University, SCC-FTB parameterizations for all the plasma-facing materials of current interest, including the W-H-He-Re-O system as well as LI-C-O-H-Mo, permitting immediate calculation of the relevant processes such as T-retention and sputtering. The classical potentials for W-Be-C-H-He system are available as well, though not experimentally validated.

A large portion of molecular dynamics simulations can be performed with the SCC-DFTB theory for electrons. An important element for future progress for fusion materials analysis is the gradual orientation toward quantum mechanics for the description of electronic dynamics. Most plasma particles impinging on the tokamak surfaces are ions, generally in excited electronic states, transferring their energy and charge along the collision cascade in the solid not only to the atomic but also to the electronic degrees of freedom, causing excitations, charge transfer, ionizations, and chemical reactions. The electronic processes are not described within the current classical MD approaches and need to be addressed through appropriate quantum mechanical methods. A key challenge is to include, self-consistently, two new features in transition to the quantum dynamics: interatomic potentials and charges, in the SCC-DFTB framework.

In our previous calculations of hydrocarbons [17] we have used our classical molecular dynamics (CMD) code on up to 26,000 processors, each treating independently the evolution of one random impact event, for 5-30 ps. Such level of statistics is essential for the meaningful calculation of small yields and requires a large number of processors in a simple parallelization approach, with almost perfect scaling. Similar statistics is needed also for DFTB calculations, however the time needed per trajectory is about a factor 1,000 longer for the same size of the simulation cell, which requires reduction of the simulation cell by an order of magnitude. In addition, Self-Consistent Charge calculations, required for calculations of lithium-based mixed materials increase the processing time by about a factor of 3 in comparison to non-polarized DFTB calculations.

3.3 Fluid/kinetic edge plasma parameters

UEDGE-BOUT codes

These codes [18,19] are used for computing edge and near-surface plasma conditions and ion/energy fluxes to the surface materials, and resulting effects on the plasma from emitted impurities. UEDGE [18] is a multispecies,

2D (toroidally axisymmetric) transport code that evolves edge and scrape-off-layer main-fuel ions (D-T), helium, electrons, sputtered impurities, and neutrals. Time-dependent transport equations are solved for the density of species including neutrals from surfaces, their parallel velocity along the magnetic field, separate electron and ion temperatures, and the electrostatic potential. Velocities across the magnetic field are computed from classical drift motion, an anomalous diffusion/convection model, and charge-exchange and neutral-neutral collisions. Realistic toroidal tokamak geometry is used with a body-fitting mesh to conform to divertor material surfaces that can be extended to include adjacent surfaces. A finite-volume discretization of the equations is used to ensure accurate particle number density conservation, which is very important for high-recycling divertor surfaces where the net pumping is a very small faction of the recycling particle flux. A fully implicit Newton-Krylov algorithm is used to advance the solution in time. Particle and energy fluxes are computed to all material surfaces, including the energy released when ion and electrons recombine near the material surface. Additionally, UEDGE computes the surface energy flux from line radiation arising from impurities within the edge plasma region.

Wall/near-wall inputs to UEDGE include continuum-model material thermal profiles and transport, ionized hydrogen & Monte Carlo impurities, and dust near the plasma-surface sheath. The WBC code has provided impurity input to UEDGE–e.g. Li with order of 10% Li/D in the SOL, as discussed above for the NSTX tokamak Liquid Lithium Divertor. Such high impurity levels can significantly influence the plasma solution thus requiring plasma-code and erosion/redeposition-code iteration. Sputtered impurity species densities also have high spatial gradients; this can compromise plasma solver efficiency and robustness.

BOUT++ (with its predecessor, BOUT, developed by X.Q. Xu) is a 3D turbulence code [19] for computing intermittent edge/scrape-off-layer short wavelength instabilities leading to plasma "blob" transport and, most recently, also MHD instabilities yielding ELMs; these and associated processes determining the SOL heat-flux width and thus plasma fluxes to material surfaces. The code evolves turbulence from profiles of the main-fuel species and electrons provided by experiments or, e.g., UEDGE, and is being upgraded to include neutrals. Time-dependent equations are solved for ions and electron density, their parallel velocities along and across the magnetic field, separate electron and ion temperatures, and the electrostatic and magnetic vector potentials. A finite-different discretization of the equations is used, and a Newton-Krylov algorithm is applied to solve the system. While the equation set is similar to the transport model in UEDGE, inclusion of toroidal variations allows simulation of a number to low-frequency (well below the ion cyclotron frequency) drift instabilities. Such instabilities typically lead to nonlinearly generated 3D filaments that are believed to be a central element of localized particle and heat fluxes to material surfaces.

The need to obtain a consistent model of SOL plasma profiles to predict particle and heat flux profiles to PFCs provides an example of coupling models. Because 3D BOUT++/BOUT simulates the detailed turbulence time scale, it can be inefficient to evolve the plasma profiles over the long time required for recycling to establish a steady state SOL plasma. Consequently, an algorithm has been developed to couple the turbulence fluxes from BOUT to the 2D UEDGE transport code and in return, use the resultant modified plasma profiles within BOUT to evolve a new turbulent state. This iterative procedure has been shown to converge after about 10 iterations [20] using a procedure known as relaxed-iterative coupling. It is important to note that here it is the radial turbulent fluxes that are coupled, rather than diffusive transport coefficients that can be inferred from the turbulence. The resulting plasma fluxes to the main chamber wall are shown in Fig. 4, where inclusion of the coupled turbulent fluxes shows the potentially strong fluxes to the main chamber (though the heat fluxes in this low-power DIII-D example are still modest). More recently, a more advanced model of the impact of plot propagation on radial heat flux has been developed [21]. Increased utilization of such coupled models, or more direct 3D simulations with neutrals and profile evolution, would substantially improve the realism of plasma fluxes to materials.

There are significant numerical challenges for these and similar plasma codes. In general, the accuracy of the discretization schemes should be improved. BOUT++ is finite-difference; this can cause important long-time particle conservation issues if used for transport. There are issues regarding accurate radial derivatives in strongly sheared magnetic fields, and with fluctuation levels $\sim$100% in the far SOL. Transport codes are typically only 1st or at most 2nd order; 1st order upwinding is often used for robustness. Turbulence codes have made more progress in using higher order schemes, though they are sometimes of mixed order. The codes would benefit from consistent high-order discretization.

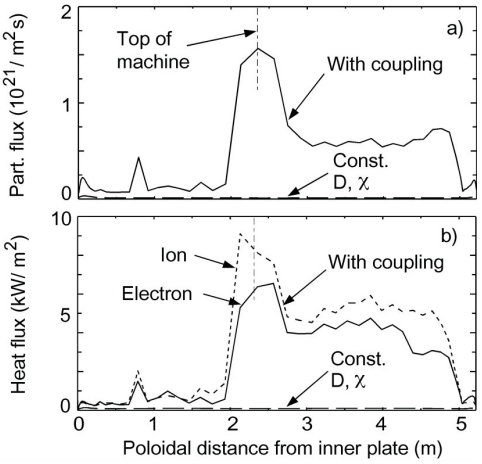

Fig. 4 Plasma fluxes to the DIII-D main-chamber wall showing comparison of simulations with ad-hoc constant radial diffusivities and those coupled to the 3D BOUT turbulence code for low-power conditions [20]. The strongly increased wall fluxes with coupling illustrate the importance of modelling self-consistent turbulent plasma transport.

3.4 Neutral transport in the plasma

DEGAS-2 code

This is a time-dependent 3-D code that uses a Monte Carlo technique to solve the Boltzmann equation for the velocity space distribution function of the neutral species [22]. Collisional processes (dissociation, ionization, charge exchange, etc.) with specified (usually Maxwellian) background plasma are treated in full kinetic detail, via a differential scattering cross section. Nonlinear neutral-neutral scattering is simulated with an approximate, BGK technique. The most important source terms are those due to plasma-material interactions, e.g. backscattering/reflection and desorption. Again, the use of the Monte Carlo algorithm allows these processes to be described kinetically and in arbitrary detail. Since the simulated neutral particle histories are independent, the Monte Carlo algorithm parallelizes naturally. Consequently, DEGAS-2 was designed from the outset to run on parallel machines, including the use of a specialized random number generator that provides reproducible results in such environments.

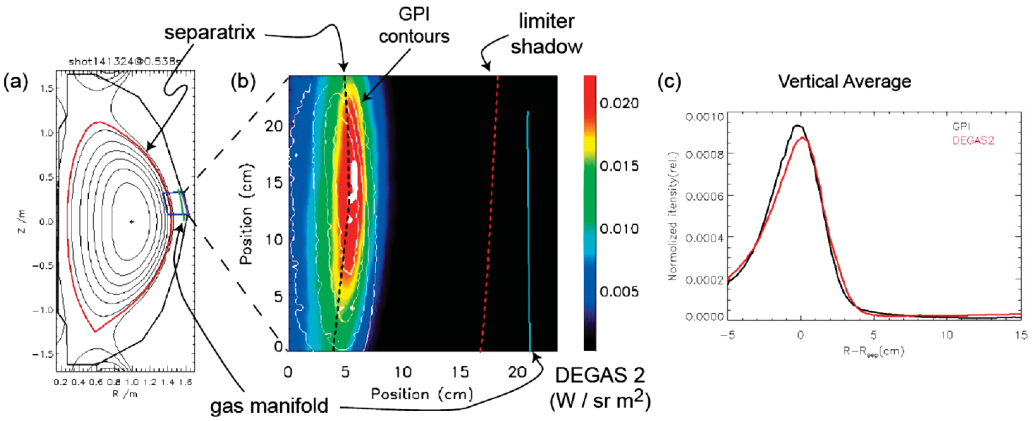

Fig. 5 3-D DEGAS-2 simulation of NSTX Gas Puff Imaging (GPI) experiment. (a) The GPI camera views along the field line the D_α light emitted by gas puffed from the manifold. (b) The equally spaced white contours are computed from the time averaged GPI images for shot #141324; the color contours represent the DEGAS 2 simulated camera image. (c) 1-D profiles are obtained by normalizing the 2-D data to the sum over all pixels and then averaging over vertical pixels. Good code/data agreement seen. Adapted from Ref. [23].

Figure 5 shows DEGAS-2 code/data comparisons for NSTX using light emission data from a gas puffing diagnostic [23]. The simulation matches the data well. One conclusion from this is that the relatively simple

atomic physics model used to describe the D2 molecules, ignoring the effects of excited states, is adequate for simulating the relatively high-temperature, low density plasmas found in the main chamber of NSTX.

DEGAS-2 has previously been coupled to UEDGE in an iterative fashion to obtain consistent plasma-neutral solutions and has also been used in conjunction with the REDEP/WBC package. Key features of DEGAS-2 are its flexibility and kinetic characterization of the neutral species. One algorithmic improvement that needs to be addressed is the inclusion of REDEP/ITMC/MD-computed sputtering as a new source term. Plans also exist to extend the code to effectively utilize hundreds of thousands of processors.

3.5 TRANSIENT RESPONSE

3.5.1 HEIGHTS Code Package

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HEIGHTS (High Energy Interaction with General Heterogeneous Target Systems), e.g. [24, 25], is considered the world's leading tool for comprehensive simulation of plasma surface interaction and bulk response during various transient events. HEIGHTS computes detailed vaporization loss, melt layer formation and splashing erosion, secondary damage to nearby plasma facing components (PFC), and eroded material transport and contamination in the SOL and bulk plasma.

It is vital to fusion development that PFC material erosion and plasma contamination during transients be very well simulated. Edge localized modes (ELM's), for example, appear to be an unavoidable part of high performance plasma operation, but there is a wide spectrum of ELM frequency, energy content, and power loading that may obtain, and the acceptable operating parameter window must be identified. Transient plasma material erosion is an extremely complex self-consistent problem where the exposed local areas are coupled through MHD and radiation transport processes. Our simulations show the potential for significant damage to PFC surfaces in ITER-like devices, during giant ELMs, disruptions, runaway electrons, and other transients, both directly from the disrupting core plasma flux, and as a result of the divertor material evolution and secondary plasma radiation flux. Figure 6 shows a typical HEIGHTS computation of a fusion reactor PFC response; the predicted energy/power flux and carbon erosion under impact of plasma particles during a disruption event in the region near a carbon divertor module in ITER.

The most significant erosion and plasma contamination problems in tokamaks are macroscopic melt splashes and MHD–related losses from metallic divertor plates and wall materials into the core plasma [26]. We implemented the volume of fluid model to predict the flow of plasma and liquid tungsten as two immiscible fluids of different densities. The plasma-liquid tungsten fluids are separated by a sharp interface under the effects of gravity and surface tension. We predicted the phenomena of continuous liquid tungsten ligaments, their elongation by the plasma flow and development of long, thin threads that eventually can break into liquid droplets [27]. The loss of molten tungsten in the form of continuous long ligaments was clearly observed during melt splashes in recent TEXTOR experiments [27], confirming this phenomenon. Further refinement of melt layer behavior models is needed in areas of viscosity effects, temperature-dependence of surface tension, melt-solid adhesion forces, heat and mass exchange, and melt crater finite size effects.

HEIGHTS analysis [28] for the ITER W divertor shows that tungsten will start to melt for giant ELMs of energy Q_{ELM} >7-8% of plasma energy Q_0, released at the midplane. The surface temperature will exceed the melting temperature and a melt layer thickness of 100 μm is developed for giant ELMs (Q_{ELM} ~10% Q_0) deposited in 1 ms-duration. A key HEIGHTS result, however, is that carbon has similar ELM and other transient concerns as tungsten. Also, radiation from the resulting vapour cloud for either material can damage nearby components. We have identified acceptable and unacceptable ELM parameter windows for ITER [28, 29]. For the unacceptable giant ELM of $\geqslant$10% deposited core plasma energy in 0.1 ms on the divertor (energy density > 3 MJ/m^2), the erosion is high for carbon (0.2 μm/ELM). For tungsten there is less vaporization erosion than carbon but significant melting. For longer deposition times (~1 ms) and/or lower ELM energy the surface response for all materials is much better.

HEIGHTS can interface with the above mentioned codes for pre-transient plasma edge/SOL parameters. The HEIGHTS simulation package itself includes five main integrated modules: Monte Carlo block of disrupting plasma particles interaction with solid and plasma facing materials; MHD block of plasma evolution taking into account magnetic field diffusion; heat conduction and vaporization block for tokamak plasma facing components; heat conduction block for vapor and plasma; and Monte Carlo radiation transport. The radiation transport block is

based on optical data calculated by the HEIGHTS atomic physics package. Current HEIGHTS high performance numerical methods and code parallelization is based on the message passing interface (MPI). Parallel algorithms of hydrodynamics, magnetic diffusion and thermal conduction blocks use approximately equal domain partition according to the number of processors available, employing utilities for optimum domain decomposition.

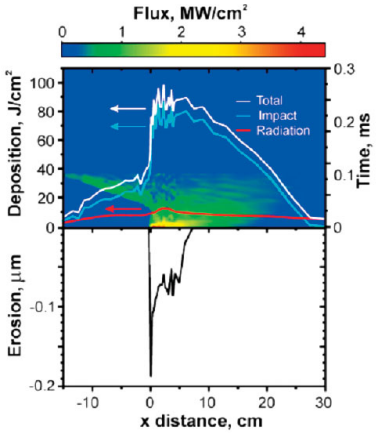

Fig. 6 Time integrated energy deposition, energy flux evolution (color background) and divertor erosion (black curve) during 0.1 ms giant ELM, for ITER carbon outer divertor, strike point at x=0. HEIGHTS code package analysis. From Ref. [2].

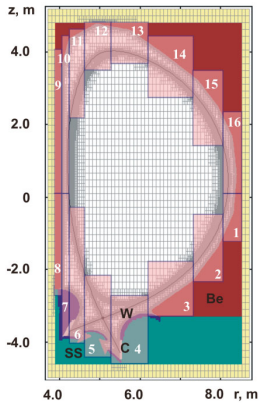

Fig. 7 ITER SOL zones for 16 processor HEIGHTS PFC transient response modeling.

We recently developed an unstructured adaptive mesh computational approach, and reconstructed all integrated physical and numerical processes of the HEIGHTS package. A scheme using five spatial scales spanning 6 orders of magnitude (m to μm) is used for accurate simulation of the entire SOL plasma transient response. Fig. 7 shows an example mesh setup. This approach aids in calculating the fully integrated material transient response in a reasonable time on multiprocessor computers. In general, HEIGHTS can simulate the plasma evolution and surface erosion dynamics in divertor and nearby areas following a plasma transient, using one week of a typical (16-32 processor) computer cluster. However, a full simulation, of the whole reactor concept, would take months, depending on the event duration. Therefore, we need a major expansion to order of 10^5 cores.

3.5.2 ALE-AMR code

This open-source code [30,31] complements the HEIGHTS package to implement critical 3D effects in plasma-wall interactions. By combining Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics with Adaptive Mesh Refinement (AMR), the code is able to accurately calculate 3-D bulk deposition effects as well as resolve small-scale structures in the solid material, e.g. void generation, and molten material/droplets formation. Calculating the response to dynamic loading requires anisotropic material strength models with material time history, and models for void generation, which are available in the code. A molten layer can be created on plasma facing components following dynamic loading, and surface tension plays a critical role in the evolution of this layer. Imbalances in vapor pressure leading to Rayleigh-Taylor instabilities can affect droplet formation. In addition, droplets behavior is affected by Marangoni stresses associated with temperature dependent surface tension. Currently, there are two models for surface tension implemented in the ALE-AMR code. The first is based on the advective Cahn-Hilliard equations, which allow for droplet breakup in divergent velocity fields without the need for imposed perturbations. The second is based on the Korteweg representation that couples the surface tension effects into the stress tensor.

The application of the ALE-AMR code, which was developed for inertial confinement experiments, to magnetic fusion devices, can leverage a large effort in material response to dynamic loading. It provides a good technique to strengthen and advance the capabilities afforded by the HEIGHTS package. Combining ALE hydrodynamics with AMR can allow us to accurately calculate critical phenomena such as volume ablation, material response including void generation, and surface droplet formation and splashing.

3.6 Other codes

We believe that many of the strategies outlined here could apply to a number of other codes, from the extensive set used in the fusion community. Such codes include those for overall plasma solutions, e.g. B2/EIRENE [32], impurity transport, e.g., ERO [33], and various codes for surface response, dust issues, and so forth, such as noted in Ref. [5].

4 Common needs and computational issues

The above codes/packages individually consider localized reactor plasma and material science areas. The full picture of the plasma/material response in the entire reactor configuration with various involved physics "talking to each other" can be achieved by integration of these (or alternative) codes into two self-consistent main code packages, for steady state and transient response respectively. Because individual codes have their own various extensive physics, and different algorithms and methods for parallel calculations, the challenge is to employ computational strategies with advanced algorithms and optimization methods to address the coupling of these codes over extremely broad physical phenomena length and time scales, viz. angstroms to meters and femtoseconds (e.g., for individual particle trapping/reflection) to hours/days (e.g. for surface micro-structure changes), and with highly disparate code execution times.

The overriding numerical goal is for petascale real-time coupling between material response/evolution/trapping codes, near-surface plasma codes, and impurity transport codes, and with specific needs such as common incorporation of PFC CAD geometry, and 3-D plasma and B field mesh generation/use. Use of $\sim 10^5$ cores is needed and would enable major increase in predictive capability. Advanced numerical tools and solution methods in an integrated parallel environment need to be used to efficiently couple these codes/packages, to ensure high accuracy and minimize execution time. This should include implementation of unstructured meshes for the entire PFC surfaces with extra surface refinements to account for details of surface evolution and erosion processes at the micro and nano scale levels.

Full implementation of this goal would likely take on the order of 5 years, obviously depending on the effort level. However, significant progress can be made in a staged program. The best initial means for coupling these codes is probably a loosely coupled model. Here, the run time environment is used to address the control and start-up of jobs in the parallel environment, and exchange of data is primarily through file communication. Later, one can consider using a more tightly coupled framework for coupling at the distributed shared memory (DSM) level. Capabilities to be exploited include end-to-end performance optimization, single-node performance, interprocessor communication, load balancing and I/O and performance portability for new systems, including heterogeneous processors and new memory hierarchies.

Most of the codes above mentioned have been in use for a decade or more, consequently certain fundamental code verifications has been completed. Nonetheless, additional verification tests of individual codes and integrated code packages would be needed, against reference solutions where available, and/or to develop test solutions as needed, to improve confidence in the codes and to provide a starting point for subsequent error analysis and uncertainty quantification (UQ).

Some codes have similar capabilities, but target disparate length and time scales. Where those scales overlap, the two codes can be compared, with one essentially serving as a "reference" solution for the other. A cross-code comparison can essentially broaden the parameter space covered by a verification effort. An example is the accelerated molecular dynamics techniques that can provide effectively first principles material response simulation capabilities at microsecond to millisecond time scales. An obvious opportunity for verifying such a code, given adequate resources, is to perform a brute-force run of the fundamental MD code to a much longer time scale than it is typically run and to compare with the result of the accelerated MD technique.

5 Conclusions

Plasma material interactions is the single most critical engineering issue for fusion tokamak development. We have described some key science/modeling issues and computational challenges for predictive simulation of the self-consistent plasma edge/SOL and plasma facing component response. For the most part, the required computer codes/packages, supercomputers, and numerical techniques already exist. There are some significant

science/model gaps, however, such as in the areas of the first wall sheath, tungsten ultrastructure, mixed-material surface properties/response, melted material properties, lithium issues, interatomic potentials for MD codes, and edge plasma turbulence. Theory/modeling advancements in these areas should of course complement a vigorous experimental program.

We suggest that petascale computing with current parallel processing techniques is a reasonable and practical approach to the predictive simulation challenge. A logical division is for a normal plasma response coupled "super-package", anchored by erosion/redeposition simulation, and incorporating surface response and detailed edge/SOL plasma solutions; and secondly, a transient response super-package with similar inputs. Such coupled codes/packages would use verification/validation and UQ efforts as roughly outlined here.

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