SciDAC Project – Prospectus

Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing

Lead PI: Brian D. Wirth, Oak Ridge National Laboratory and University of Tennessee, Knoxville
bdwirth@utk.edu, Telephone: (865) 974-2554, Fax: (865) 974-0668

Tim Tautges (PI), Emil Constantinescu, Jungho Lee and Barry Smith, Argonne National Laboratory
{tautges, emconsta, julee, bsmith}@mcs.anl.gov

Vincent Chan (PI), General Atomics
chanv@fusion.gat.com

Sergei Krasheninnikov (PI), University of California, San Diego
skrash@mae.ucsd.edu

Brian Wirth (PI), David Bernholdt, Jay Jay Billings, John Canik, Jeremy Meredith, Philip Roth, Roger Stoller, Stanislav Golubov, Oak Ridge National Laboratory
bdwirth@utk.edu, {bernholdtde, billingsjj, canikjm, jsmeredith, rothpc, stollerre, golubovsi}@ornl.gov

Rick Kurtz (PI) and Kenny Roche, Pacific Northwest National Laboratory
{rj.kurtz, Kenneth.Roche}@pnnl.gov

David Ruzic (PI), University of Illinois, Urbana-Champaign
druzic@uiuc.edu

Dimitrios Maroudas, University of Massachusetts
maroudas@ecs.umass.edu

Xianzhu Tang (PI), Jim Ahrens, David Higdon, Danny Perez, Arthur Voter and Blas Uberuaga, Los Alamos National Laboratory
{xtang, Ahrens, dhigdon, danny_perez, afv, blas}@lanl.gov

The performance demands on plasma-facing components (PFCs) in future fusion power plants are beyond the capability of current materials. In defining the plasma-surface interaction (PSI), it is evident that three coupled spatial regions influence PFC materials evolution and performance. These regions consist of (1) the edge and scrape-off layer region of the plasma, (2) the near surface material response to extreme thermal and particle fluxes under the influence of, and feedback to, the plasma sheath, and (3) the structural material's response to an intense, 14 MeV peaked neutron spectrum which produces very high concentrations of transmuted elements through (n,p) and (n,α) reactions and structural material property degradation.The objective of this project is to develop and deploy validated, high-performance simulation tools capable of predicting the performance of tungsten-based plasma-facing components (PFCs) in a burning fusion plasma environment, which includes modeling surface morphology evolution in either erosion or re-deposition regimes, and the recycling of hydrogenic species. This requires the development of a leadership-scale computational code to predict PFC behavior, that is well integrated to a suite of multiscale modeling techniques to bridge the scales needed to address complex physical and computational issues at the plasma surface interface and the transition region below the surface where neutron damage processes in the bulk dominate material behavior. Successful completion of this project will provide PFC simulation tools to evaluate steady-state performance of tungsten-based PFC and divertor components in burning plasma environments. This will enable the identification of critical experiments to

confirm whether practical PFC solutions exist for magnetic fusion energy beyond ITER.
More specifically, the research activities within this project will focus on two broadly defined research thrusts:

Developing a new simulation code, XOLOTL-PSI to predict PFC operating lifetime and performance, that is specifically designed to take advantage of leadership class computing facilities; and

Integrating and applying discrete particle-based, as well as continuum-based, multiscale modeling techniques to provide scientific discovery of the mechanisms controlling PFC and bulk materials evolution under fusion plasma and 14-MeV neutron exposure; in which the challenge of scale-bridging between atomistic/microstructural modeling and the continuum-scale of PFC device performance is achieved through multiscale modeling techniques.

This project involves a number of computational challenges from the computer science (CS) and applied math (AM) viewpoints. On the atomistic/discrete particle side, simulations will be numerous, as well as potentially large, in order to explore material behavior, mechanisms and pathways. Pursuing such calculations on a “production” scale in order to provide needed inputs to the continuum approaches will involve the orchestration of multiple codes, passing information across the scales. On the continuum side, 3D simulations of the evolution of sizable volumes of materials over time scales commensurate with experiments, and ultimately with tokamak operation, will be extremely demanding in computational resources, and will require a code, or codes, capable of scaling to the largest available systems. Turning simulation results into knowledge and understanding will be an additional challenge, due to the complexity of the materials systems and the multiple phenomena occurring simultaneously.

On the continuum side, the focus is on the development and application of the XOLOTL-PSI simulation code. This offers significant opportunities to apply past CS and AM experience to a challenging computational problem, and also motivates new research and development to address as-yet unanswered questions in the CS/AM arena. From this viewpoint, the primary challenges of the XOLOTL-PSI code development are less in specific details and more in how those details are integrated into an efficient, high-performance, highly-scalable computational capability for the simulation of materials in the fusion environment. For example, the equations are well understood, but combine stiff diffusion terms with expensive reaction terms, as well as constraints. Meshes must adapt dynamically in response to changing morphologies, especially near the surface, while also adapting to depth beneath the surface to reduce computational costs. The code that accounts for all of the above factors must also provide performance and scalability across multiple leadership-class hardware architectures. Uncertainties must be understood both for the atomistic simulations that provide key parameters for the continuum reaction-diffusion code, as well as being propagated through. Understanding the results requires not just visualizing the material surface, but its 3D structure with multiple impurity species.