Plasma Surface Interactions (PSI): XOLOTL-PSI: Code Development, Testing and Uncertainty Quantification Approaches

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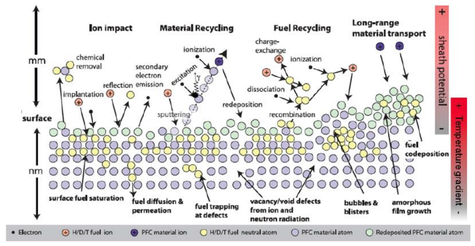
SciDAC Project Web Site: https://collab.mcs.anl.gov/display/PSIscidac/

Xolotl Web Site: https://sourceforge.net/projects/xolotl-psi/

Sponsored by: Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR)

Predicting the performance of plasma-facing components is critical to the deployment of fusion energy devices beyond ITER and DEMO!



Observed Surface Morphology in Tungsten Exposed to Low Energy Helium/Hydrogen Plasma Conditions

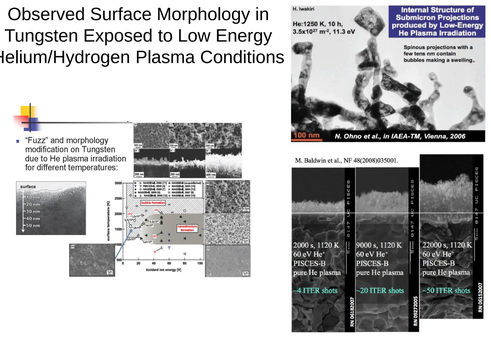


Figure of merit:
Incident plasma ion flux near divertor strikepoint: 10^{24} m^{-2} s^{-1}

Steady-state sputtering yield O (10^{-4}) on surface monolayer (10^{19} atoms/m^2) results in sputtering of every atom every 0.1 sec -> every atom sputter >10^8 times/year

* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

Cluster Dynamics Formulation

Evolution of the surface can be simulated using a cluster dynamics formulation of the time-dependent Advection-Diffusion-Reaction (ADR) equations with an incident flux source:

$$\delta_t \overline{C} = \varphi \cdot \rho + D\nabla^2 \overline{C} - \nabla \overline{v} C - \overline{Q}(\overline{C})$$

"Single-species" cluster types include helium (He), atomic vacancies (V) and interstitial defects (I). These species interact to form "mixed clusters" of helium with vacancies (HeV) and helium with interstitials (HeI). Atomic vacancies can be understood as lattice sites where the atoms of the bulk material is missing and interstitial defects are atoms occupying sites that are normally forbidden, such as those between lattice points.

Clusters interact in the following ways:

He Reaction	Description
A*He + B*He → (A+B)He	Helium clustering
A*He + B*V → (A*He)(B*V)	Helium-vacancy clustering
A*He → (A-1)*He + He	Helium dissociation

V Reaction	Description
A*V + B*V → (A+B)V	Vacancy clustering
A*He + B*V → (A*He)(B*V)	Helium-vacancy clustering
A*I + B*V → (A-B)*I, if A > B → (B-I)*V, if A < B → 0, if A = B	Vacancy-Interstitial annihilation
A*V → (A-1)*V + V	Vacancy dissociation

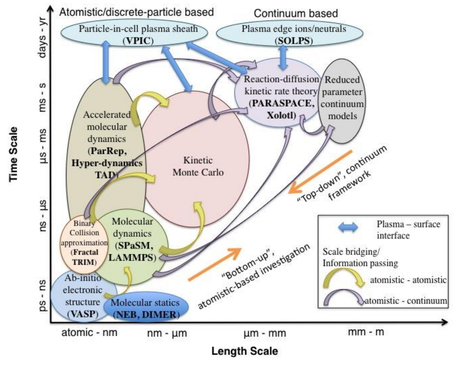
Interstitial Reaction	Description
A*I + B*I → (A+B)*I	Interstitials clustering
A*He + B*I → (A*He)(B*I)	Helium-interstitial clustering
A*I + B*V → (A-B)*I, if A > B → (B-I)*V, if A < B → 0, if A = B	Vacancy-Interstitial annihilation
A*I → (A-1)*I + I	Interstitial dissociation

Mixed-Species Reaction	Description
(A*He)(B*V) + C*He → [(A+C)He](B*V)	Helium absorption by HeV clusters
(A*He)(B*V) + V → (A*He)[(B+1)V]	Single vacancy absorption by HeV clusters
(A*He)(B*V) + (C*I) → (A*He)[(B-C)*V]	Vacancy reduction by interstitial absorption in HeV clusters
(A*He)(B*V) → [(A-1)*He](B*V) + He	Helium dissociation from HeV clusters
(A*He)(B*V) → (A*He)[(B-1)*V] + V	Vacancy dissociation in HeV clusters
(A*He)(B*V) → (A*He)[(B+1)*V] + I	Interstitial production from HeV clusters (trap mutation)
(A*He)(B*I) + I → (A*He)[(B+1)I]	Single interstitial absorption by HeI clusters
(A*He)(B*I) + (C*V) → (A*He)[(B-C)*I]	Interstitial reduction by vacancy absorption in HeI clusters

Coupling to Other Physics Codes and Lower-Length Scale Calculations (Our Other Poster!)

Many of the parameters used in Xolotl are taken from lower-length scale simulations. The atomistic computations (molecular statics, molecular dynamics, and their analysis) provide key input of two kinds. They provide the values of diffusion factors, drift velocities and all the rate constants for the various ingredients of the reaction term. They also identify all the classes of reactions that occur and provide greatly needed information on two of the most important; trap mutation and cluster dissociation near W(100) surfaces for 2He and 3He clusters.

Incoming helium and interstitial fluxes are taken from SRIM and, later, SOLPS.



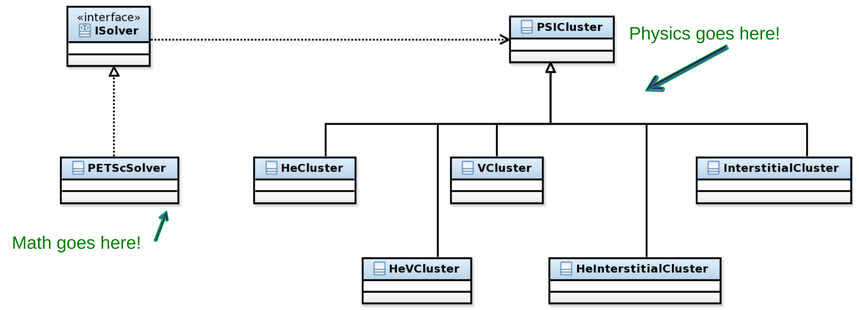
Xolotl – A Continuum Reaction-Diffusion Kinetic Rate Theory Plasma-Surface Interaction Code

- Xolotl is the Aztec god of lightning and death, pronounced SHO-lottle
- Developed "from scratch" for this project
- Designed for HPC – current and emerging architectures
  - –Multicore, multicore+accelerator
- Integrate performance measurement, in situ analysis and visualization at design time
  - –Design in resilience features: checkpoint/research and more
- Leveraging PETSc, MOAB and other Institute software
- Current version is 1D finite difference, but with 1D FEM and 2D R-z FEM to follow.
- Developed in C++ with MPI
  - –Later OpenMP, CUDA, OpenCL, OpenACC

Physics & Math Focused Design

Xolotl has a simple, physics-based design that focuses on the interactions between the cluster types. The "big" math of solving the ADR equations is handled separately from the physics, which allows the applied math challenges to be addressed without affecting the physics. PETSc is used to solve the ADR equations in Xolotl and MOAB will be used for managing the mesh in the upcoming finite element version.

I/O and communications are handled in their own "architectural layer" that is also separate from the physics and mathematics.



Part of the class hierarchy of Xolotl illustrating the relationships between clusters, their base class and solvers.

Testing and Benchmarks

Xolotl is tested with a set of unit and integration tests to check insure that the its classes behave and interact as expected. We have also developed two benchmark cases that will be run with Xolotl and the results compared to existing "prior art," including both experimental results and previous simulations on workstations.

Tungsten Benchmark

Due to its high melting temperature and low sputtering, Tungsten is a leading candidate materials for the divertor. However, it was observed experimentally that the materials surface is strongly modified (blistering of helium bubbles at low temperatures and "nanofuzz" formation for T > 1000 K) by helium irradiation which could drastically reduce the lifetime of the fusion device.

Iron Benchmark

Pure single crystal iron is implanted with 10 keV He ions at a flux of 10^{11} $cm^{-2}s^{-1}$ to a fluence of 10^{15} cm^{-2} at room temperature and then annealed with a thermal ramp at a constant rate of 1 K s^{-1} up to 1173 K. The problem is to calculate the varying concentrations of the He-V and I-clusters at different times and different depths during implantation and subsequent annealing.

Uncertainty Quantification Strategy

Method	Description
Polynomial Chaos	Expand quantities of interest in terms of orthogonal polynomials with random variables
Global Sensitivity Analysis	Index the sensitivity of the output variables to uncertainty in input variables
Sparse Adaptive Quadrature	Dynamic refinement of multiple deterministic evaluations on sparse grids
Bayesian Inference	Extract parameters using simplified likelihood functions in conjunction with simulation
Data-Free Inference	Generate a posterior probability density function given uncertain or missing data using Bayesian techniques

UQ techniques that will be used with DAKOTA and QUESO (non-intrusively)

We have worked closely with the SciDAC institute for the Quantification of Uncertainty in Extreme-Scale Computations (QUEST) to develop a strategy for quantifying the uncertainty in Xolotl. We initially worked to develop a fully intrusive uncertainty quantification (UQ) scheme for Xolotl, but discovered that the parabolic ADR equations and the existence of canard phenomenon in the rate equations made such a solution insurmountable.

We currently plan to use the non-intrusive techniques in the table at the left with DAKOTA and QUESO to quantify the uncertainty and analyze parameter sensitivity with Xolotl. We are continuing to work closely with the QUEST team to refine this strategy.

Special Thanks to the SciDAC Institutes!

Members of the SciDAC Institutes have addressed many very specific concerns that we have had about applied mathematics, performance, visualization and other topics. For that, we are extremely grateful!