Xolotl: A Plasma Surface Interactions Simulator

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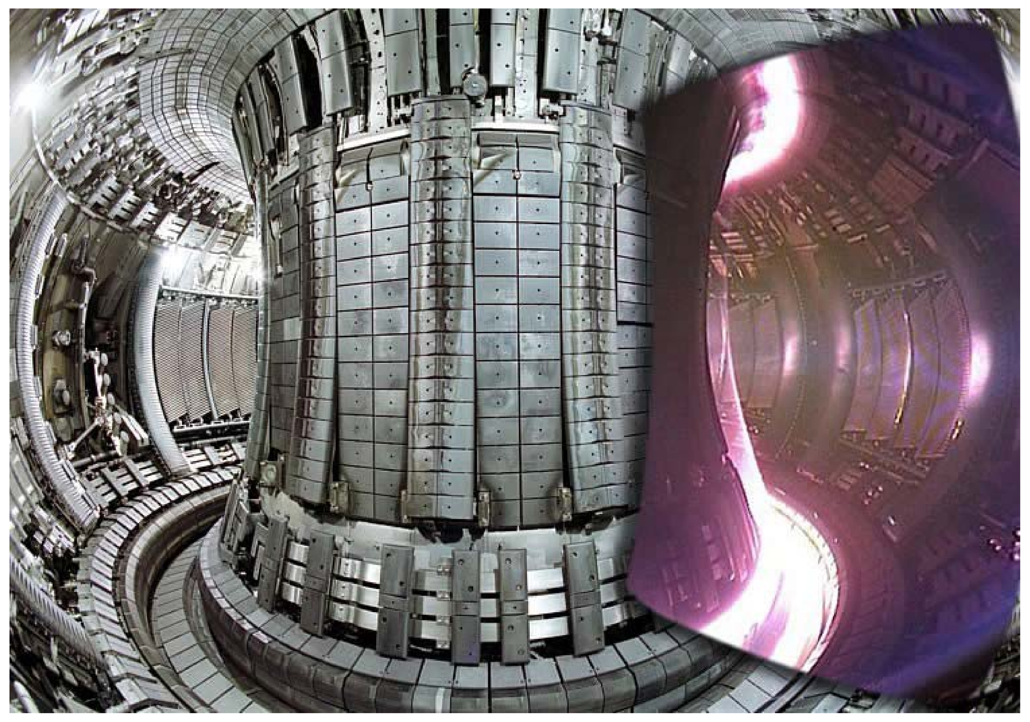
SciDAC Project Web Site: `https://collab.mcs.anl.gov/display/PSIscidac/`

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

Oak Ridge National Laboratory

Plasma-Surface Interaction



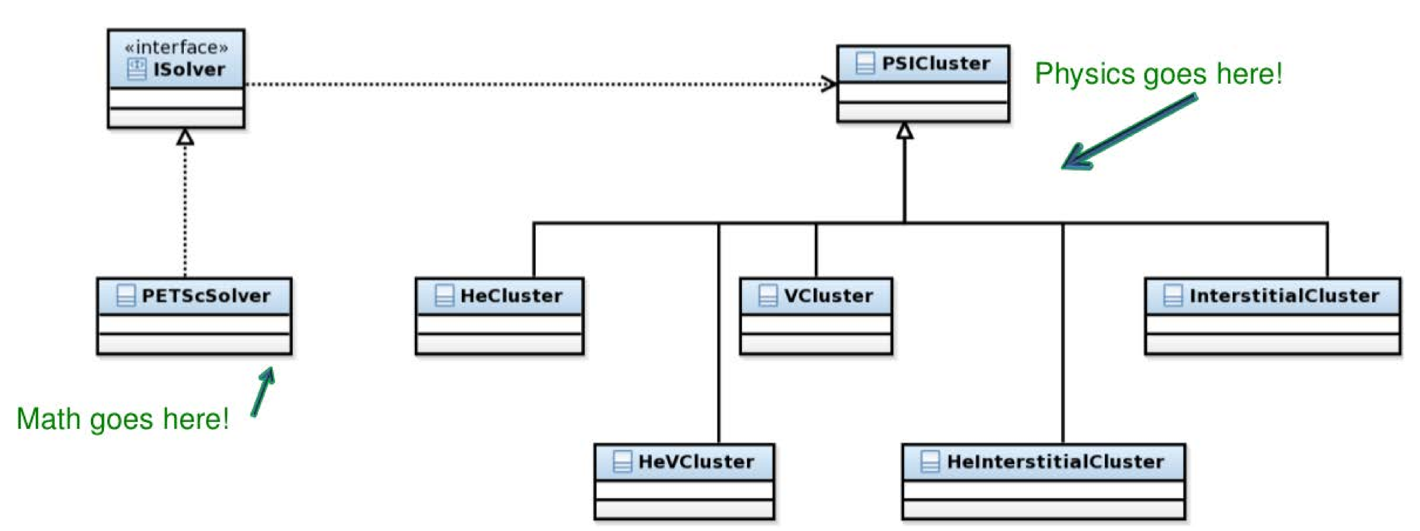
The Plasma-Surface-Interactions (PSI) SciDAC project is focused on predictive modeling of material damage in the tungsten wall material of the plasma divertor in a Tokamak fusion reactor system. The effort includes multiscale modeling techniques involving particle in cell (PIC) methods, molecular dynamics (MD), and continuum modeling, for which a high performance simulator named Xolotl is being developed.

Xolotl (`http://sourceforge.net/projects/xolotl-psi/`) predicts the evolution of the surface of the material by solving the cluster dynamics formulated Advection-Diffusion-Reaction (ADR) equations with an incident flux

$$\delta_t \bar{C} = \phi \cdot \rho + D\nabla^2 \bar{C} - \nabla \bar{\nu} C - \bar{Q}(\bar{C})$$

Framework

- Started from scratch using C++ and MPI.
- The solver part is independent of the physics part.



- Other tools: Eclipse as an IDE, CMake, HDF5 to store the results, Java for the preprocessor.
- Unit and integration tests with BOOST to insure the correct behavior of the code.

Future Improvements

- Comparison of the results with the results from other software.
- Use of OpenMP for multithreading.
- Add support for GPUs.
- Implementation of the 2D problem.

Acknowledgements

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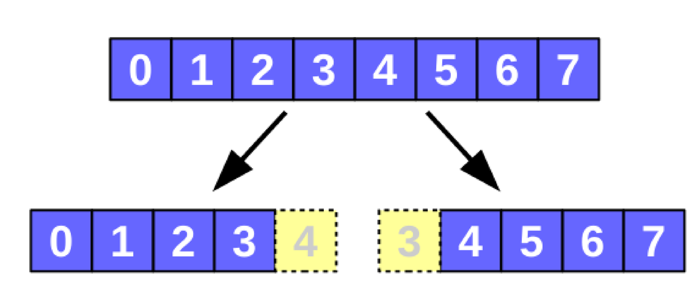
The Solver

- PETSc (`http://www.mcs.anl.gov/petsc/`) "is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations".
- 1D implementation of the ADR equations using finite difference.
- Use PETSc's Adaptive Runge-Kutta Implicit Time-Stepper: the size of the time step is adaptive and changes at each time step.
- This size depends on the stiffness of the problem.

High-Performance Computing

- Discretization of the problem over a grid: possibility of spreading the grid over many processes and solving the ADR equations at each grid point almost independently.
- PETSc takes care of: splitting the grid between the processes, communication between the processes, *etc.*

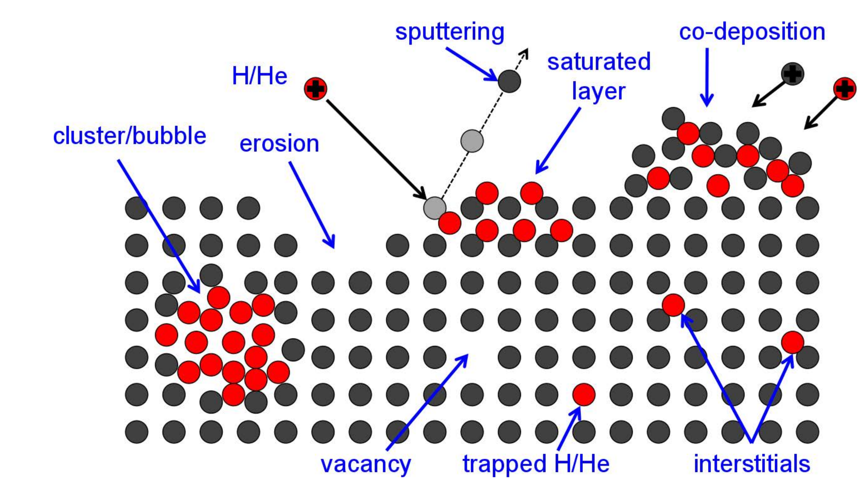


Preprocessor

- In order to falicitate the use of Xolotl for a new user a Java preprocessor was created.
- Generates all the files and options needed by Xolotl to run: network file, performance and visualization handlers, PETSc options, . . .
- Ability to modify these option simply through the command line when the preprocessor is executed.

Some Physics

- A network of clusters represents the material (interstitial (I) and vacancy (V)) that is irradiated by a helium flux (helium (He) and mixed clusters).
- The population of each cluster is given by its concentration at all spatial positions.
- The solver is in charge of the time evolution of these concentrations.



Reactions:

Single species clustering

$$X_A + X_B \rightarrow X_{A+B}$$

Helium-vacancy clustering

$$He_A + V_B \rightarrow He_A V_B$$

Helium absorption by HeV cluster

$$He_A V_B + He_C \rightarrow He_{A+C} V_B$$

Single vacancy absorption by HeV cluster

$$He_A V_B + V \rightarrow He_A V_{B+1}$$

Vacancy reduction by interstitial absorption in HeV cluster

$$He_A V_B + I_C \rightarrow He_A V_{B-C}$$

Vacancy-interstitial annihilation

$$\begin{aligned} V_A + I_B &\rightarrow V_{A-B} \; if \; A > B \\ &\rightarrow I_{B-A} \; if \; A < B \\ &\rightarrow 0 \; if \; A = B \end{aligned}$$

Single species dissociation

$$X_A \rightarrow X_{A-1} + X$$

Single helium dissociation from HeV cluster

$$He_A V_B \rightarrow He_{A-1} V_B + He$$

Single vacancy dissociation from HeV cluster

$$He_A V_B \rightarrow He_A V_{B-1} + V$$

Trap mutation

$$He_A V_B \rightarrow He_A V_{B+1} + I$$

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