Xolotl: A Plasma Surface Interactions Simulator


SciDAC Project Web Site: https://collab.mcs.anl.gov/display/PSIscidac/
Xolotl Web Site: https://sourceforge.net/projects/xolotl-psi/

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

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

Framework

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

This work has been supported by the U. S. Department of Energy, Offices of Fusion Energy Sciences and Advanced Scientific Computing Research through the SciDAC-3 program, and by the ORNL Postgraduate Research Participation Program which is sponsored by ORNL and administered jointly by ORNL and by the Oak Ridge Institute for Science and Education (ORISE).

The Solver

- PETSc takes care of: splitting the grid between the processes, communication between the processes, etc.
- 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.
- The solver is in charge of the time evolution of these concentrations.

High-Performance Computing

- PETSc goes here!
- Math goes here!
- Preprocessor
- Preprocessor
- Preprocessor

Preprocessor

- In order to facilitate 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 options simply through the command line when the preprocessor is executed.

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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

$$He_A + V \rightarrow He_AV_B$$

Helium absorption by HeV cluster

$$He_AV_B + HeC \rightarrow He_AV_B + HeC$$

Single vacancy absorption by HeV cluster

$$HeAV_B + V \rightarrow HeAV_{B+1}$$

Vacancy reduction by interstitial absorption in HeV cluster

$$HeAV_B + I_C \rightarrow HeAV_{B+C}$$

Vacancy-interstitial annihilation

$$V_A + I_B \rightarrow V_{A-B} \text{ if } A > B$$
$$I_{B-A} \text{ if } A < B$$
$$0 \text{ if } A = B$$

Single species dissociation

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

Single helium dissociation from HeV cluster

$$HeAV_B \rightarrow HeAV_{B-1}V + HeC$$

Single vacancy dissociation from HeV cluster

$$HeAV_B \rightarrow HeAV_{B-1} + V$$

Trap mutation

$$HeAV_B \rightarrow HeAV_{B+1} + I$$