

Reducing the Memory Footprint of a PETSc-based Cluster Dynamics Simulation

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A RAPIDS-FASTMath collaboration reduced the memory footprint of the Xolotl cluster dynamics simulator by up to 88% per compute node

Xolotl

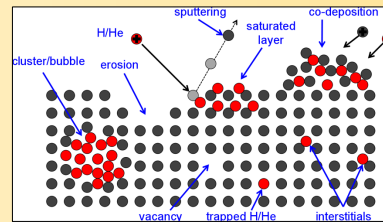
Cluster dynamics simulator used to predict gas bubble evolution in solids

- Solves advection-diffusion-reaction equations with incident flux

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

- Used in two SciDAC applications projects

- Plasma Surface Interactions (PSI2, PI: Wirth): simulate He/H bubble formation near surface of divertor in fusion reactor
- Fission Gas Simulation (FGS, PI: Andersson): simulate Xe bubble formation in nuclear fuel of fission reactor



A New PETSc API to Reduce Memory Usage

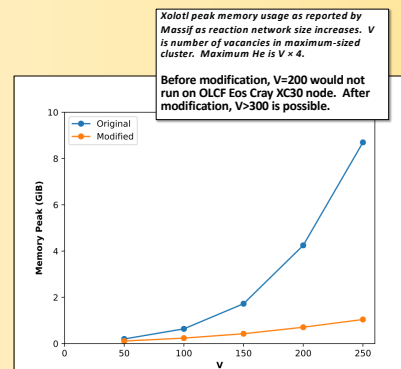
Problem: Xolotl exhibited out-of-memory errors with smaller-than-expected problem sizes

- Used Valgrind Massif memory profiler to determine peak memory usage occurred when describing item coupling to PETSc during initialization
- Required constructing two large 2D matrices (>10K items per dimension) of Boolean data (dense representation with integer item data type)
 - Large numbers of degrees of freedom in PSI2 problems, few non-zeros
 - Traditional PETSc implementation converts dense form to sparse before use

Collaborated on new PETSc API to reduce memory requirement

- RAPIDS prototyped alternative API to take sparse matrix form directly
- PETSc maintainers validated prototype implementation and accepted into PETSc distribution as of release 3.10

New API resulted in significant reduction in Xolotl peak memory usage (up to 88% per node for test problem on OLCF Eos)



Future Plans

Collaboration on GPU acceleration of Xolotl functions called by PETSc (e.g., compute right hand side function, compute Jacobian matrix, monitor functions)