Improving computational efficiency of Xolotl for modeling gas bubble evolution in nuclear materials

**Problem**
- Xolotl reaction-diffusion cluster dynamics code developed within Plasma Surface Interactions (PSI) SciDAC project and adapted for nuclear fuel simulation in NE-SciDAC-Pilot project with collaboration from SciDAC Institute for Sustained Performance, Energy, and Resilience (SUPER)
- Xolotl reaction network initialization did not scale well with respect to problem size
  - Adequate performance for smaller PSI reaction networks
  - Desired NE test problem scales were intractable due to poor reaction network initialization performance

**Approach**
- Diagnosed performance bottlenecks using Xolotl’s built-in performance infrastructure
- Modified reaction network lookup maps to use key strings instead of composition maps – cheaper to compare and enables reuse
- Made supercluster reactant grouping more efficient by removing many reactants at once and eliminating redundant examination of known reactants

**Impact**
- Optimizations reduced Xolotl reaction network initialization time for nuclear fuel applications from 23+ hours to under 7 seconds (improvement of 10⁴ times)

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Performance improvements benefit both NE-SciDAC-Pilot and the OFES-PSI versions of Xolotl, enabling initial comparisons of bubble radii predicted by Xolotl with experimental results.

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**Reaction network initialization time (blue) and total run time (orange) for NE test problem, performed on Oak Ridge Leadership Computing Facility’s Eos system. Left-to-right, bars indicate performance of initial, baseline version to optimized version. Note elapsed times are plotted on a log scale.**

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