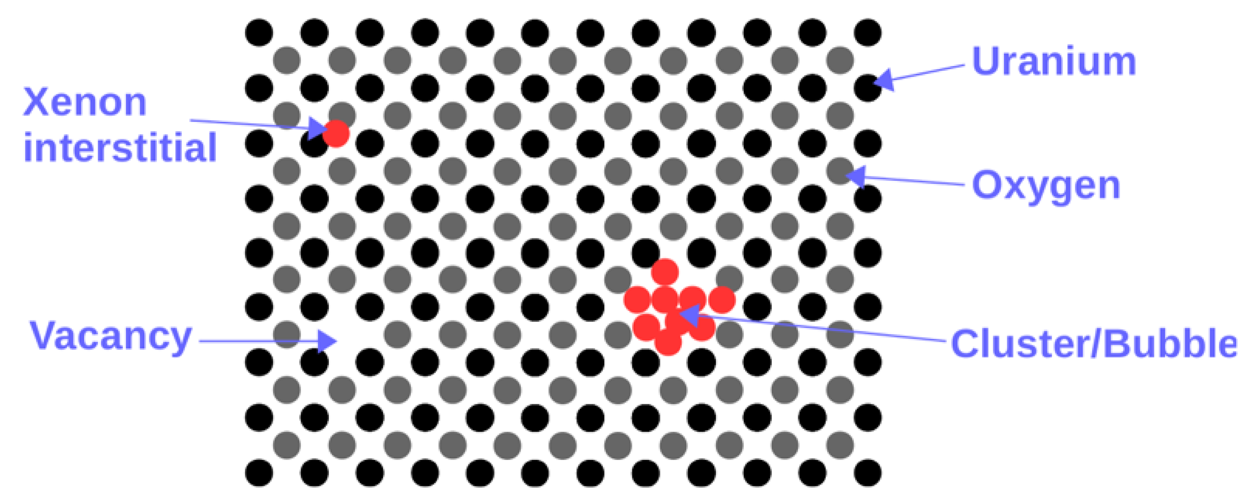
# Xolotl: a cluster dynamics code to predict gas bubble evolution in solids

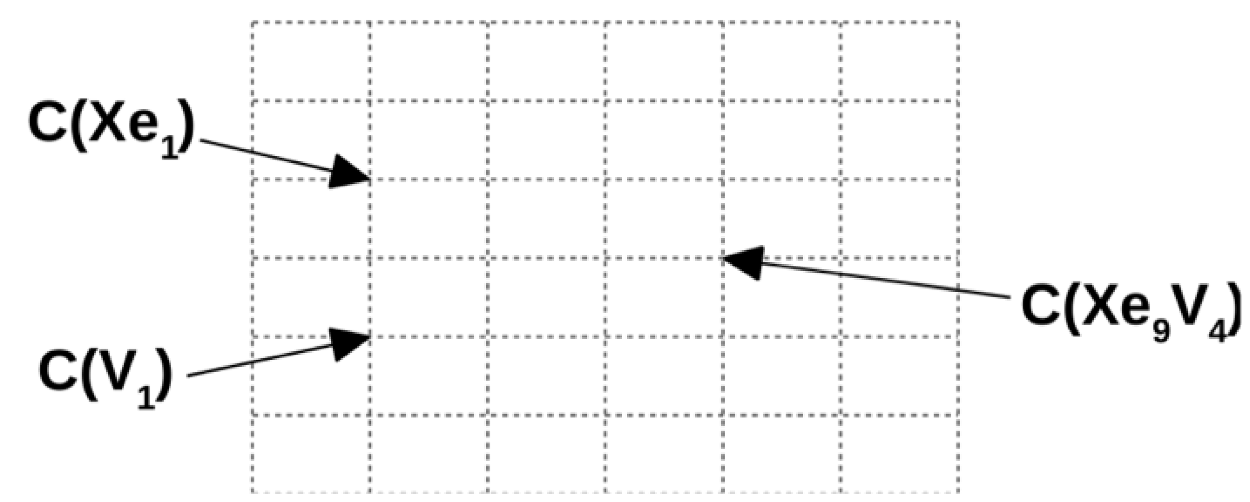
Sophie Blondel[1], Philip C. Roth[2], David E. Bernoldt[2], David Andersson[3], Brian D. Wirth[1,2]
[1]University of Tennessee, Knoxville, TN
[2]Oak Ridge National Laboratory, Oak Ridge, TN
[3]Los Alamos National Laboratory, Los Alamos, NM

## Introduction to Xolotl (`https://github.com/ORNL-Fusion/xolotl`)

**Xolotl**, named after the Aztec god of death and lightning, predicts the evolution of gas in a solid by solving the cluster dynamics formulated Advection-Diffusion-Reaction (ADR) equations with a volumetric source term, and is being used by both the NE (fission gas) and FES (Plasma Surface Interactions) SciDAC projects

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




- A network of clusters represents the material (interstitial and vacancy) and the gas atoms and clusters.
- The solver (PETSc) is in charge of the time evolution of the concentrations.

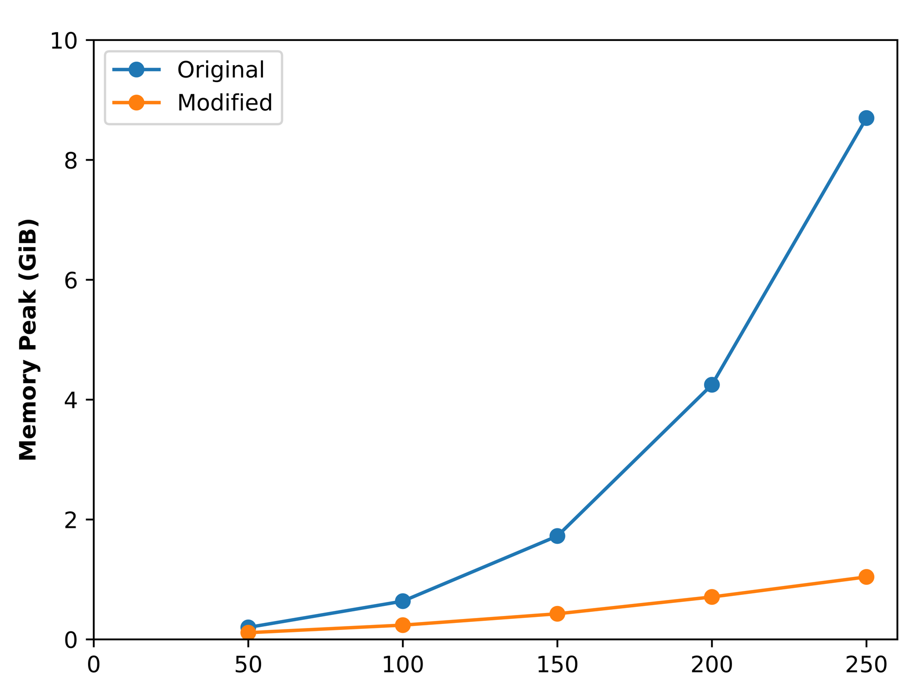
## Specificities

Past collaborations with SUPER, SDAV institutes, and current collaborations with FASTMath and RAPIDS.

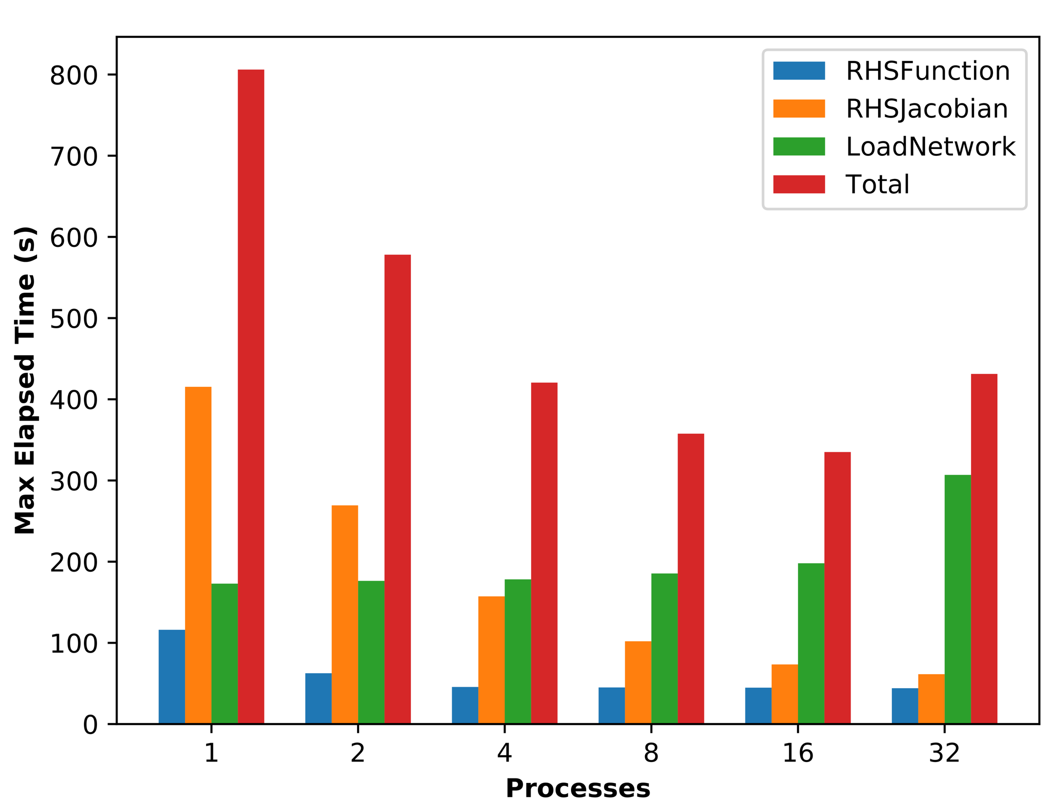
- Developed from from "scratch" using C++ and MPI
- 0D/1D/2D/3D implemented
- Typical problem size: O($10^4$) clusters, O($10^2$) grid points ⇒ O($10^6$) equations in 1D.
- Close collaboration with the PETSc team to select the adequate methods and improve them when needed.
- Performance data collection (time, event, and hardware counters) based on PAPI if available or XPerf (developed by Phil C. Roth).
- Visualization of Xolotl data at each time step using EAVL in the past was converted to using VTK-m.
- Parameter file to easily change simulation conditions.

## Recent Optimizations

Large amounts of memory were needed during the PETSc solver setup causing out-of-memory errors. We determined that the use of two large non-sparse matrices caused the problem, and developed an alternative PETSc interface function that takes sparse matrices to address the problem. **The peak memory usage of the modified version was 88% smaller than the original version, and the modified version ran approximately $1.2\times$ faster.**




We studied the performance impact of trading off processes for OpenMP threads when running Xolotl:

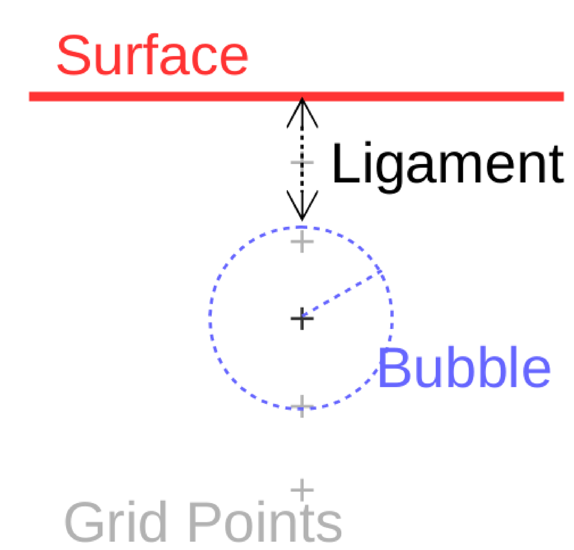



Time required to run the three most expensive activities of a Xolotl simulation run when trading off processes for threads. Timings shown for 1D problem on 32 total threads in 1 OLCF Eos compute node. **Threading gave best performance for program initialization, but a process-only configuration gave best performance during time steps.**

## Bubble Bursting

**Description:** under fusion conditions, a cluster of helium atoms is trapped in tungsten vacancies, grows close to the surface and ruptures by freeing the helium atoms.

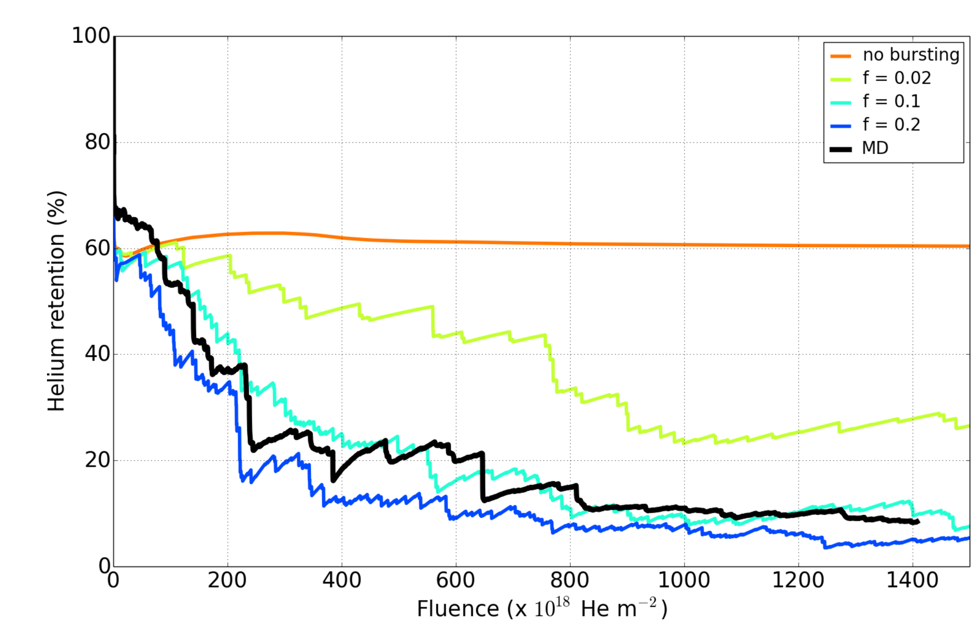
**Simplified Model:**




Burst if the ligament thickness is $\leq 0$; otherwise, with a probability proportional to the ligament thickness and decreasing with depth,

$$P_{\text{burst}} \propto (1 - L/d) \times f \times \min(1, e^{-(d-\tau_d)/2\tau_d})$$

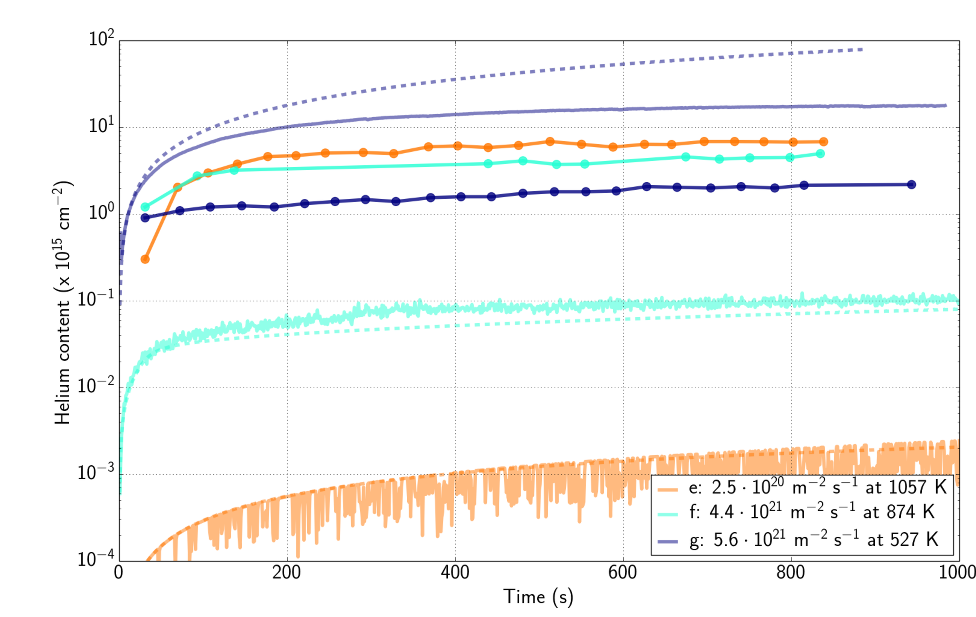
**Comparison of helium retention to MD results:** (at 933 K, $5 \cdot 10^{27}$ m$^{-2}$ s$^{-1}$)




⇒ Xolotl shows the same behavior as MD simulation with the bubble bursting model. The best agreement is for $f = 0.1$.

Sefta *et al.*, J. Appl. Phys. 114, 243518 (2013)
Zhang *et al.*, J. Nucl. Mater. 438, 178 (2013)

**Comparison of helium content to DIONISOS results:**

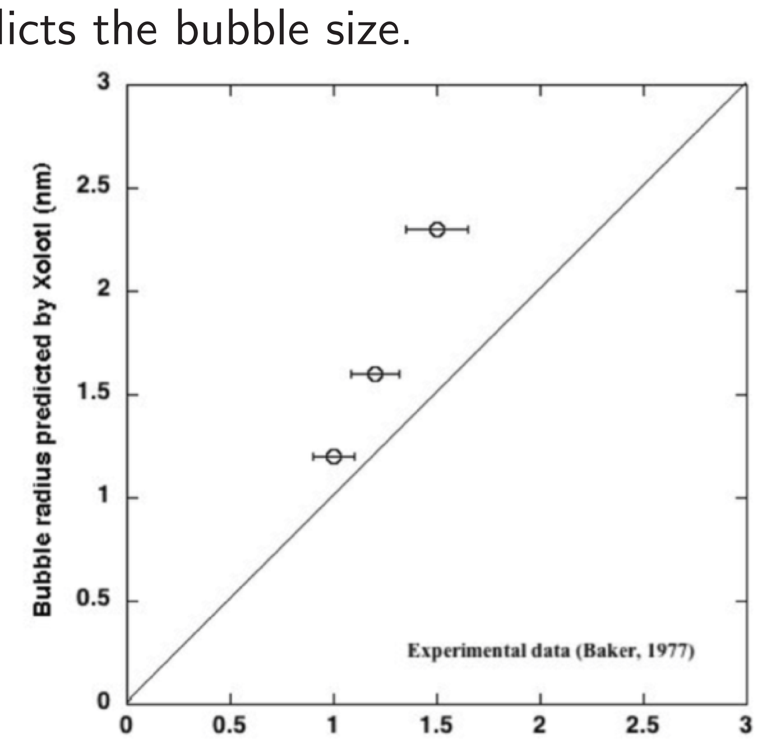



⇒ similar helium content evolution as recent experimental results although disagreement about the T dependence which are currently under inverstigation.

Ito *et al.*, Phys. Scr. T159, 014062 (2014)
Woller *et al.*, J. Nucl. Mater., 463, 289-293 (2015)

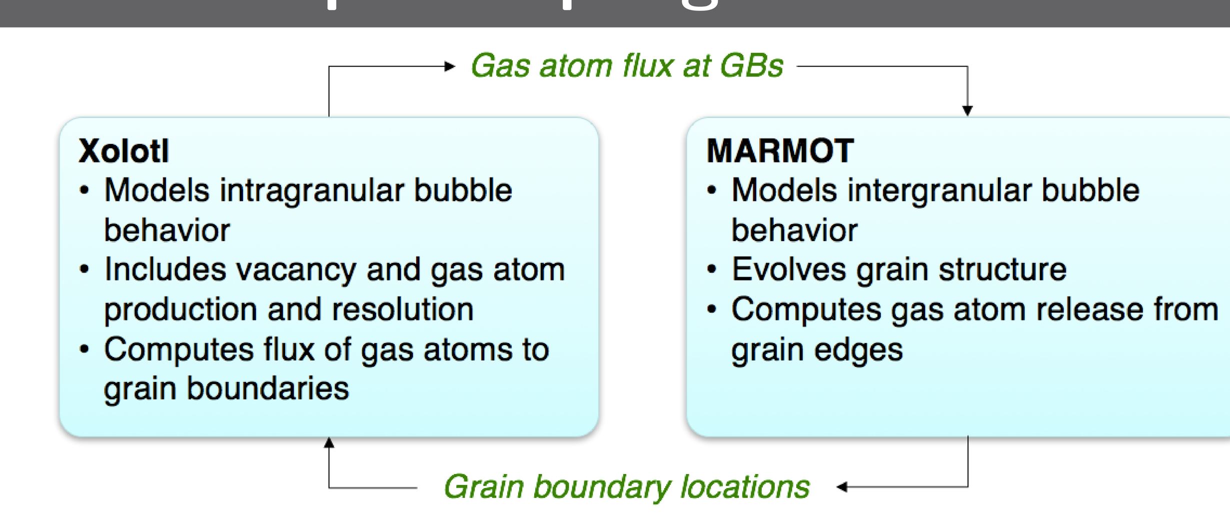
## Fission Gas Results

Preliminary comparison to experimental results: good predicted agreement of bubble radius without adjustable parameters, although Xolotl slightly over-predicts the bubble size.




⇒ Fission fragment induced bubble re-solution model soon to be implemented.

## Next Step: Coupling with MARMOT




Improved predictions of fission gas release in nuclear fuel are anticipated by coupling Xolotl model of fission gas bubbles in grain interiors with MARMOT model of grain boundary gas evolution.

## Acknowledgments

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