

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

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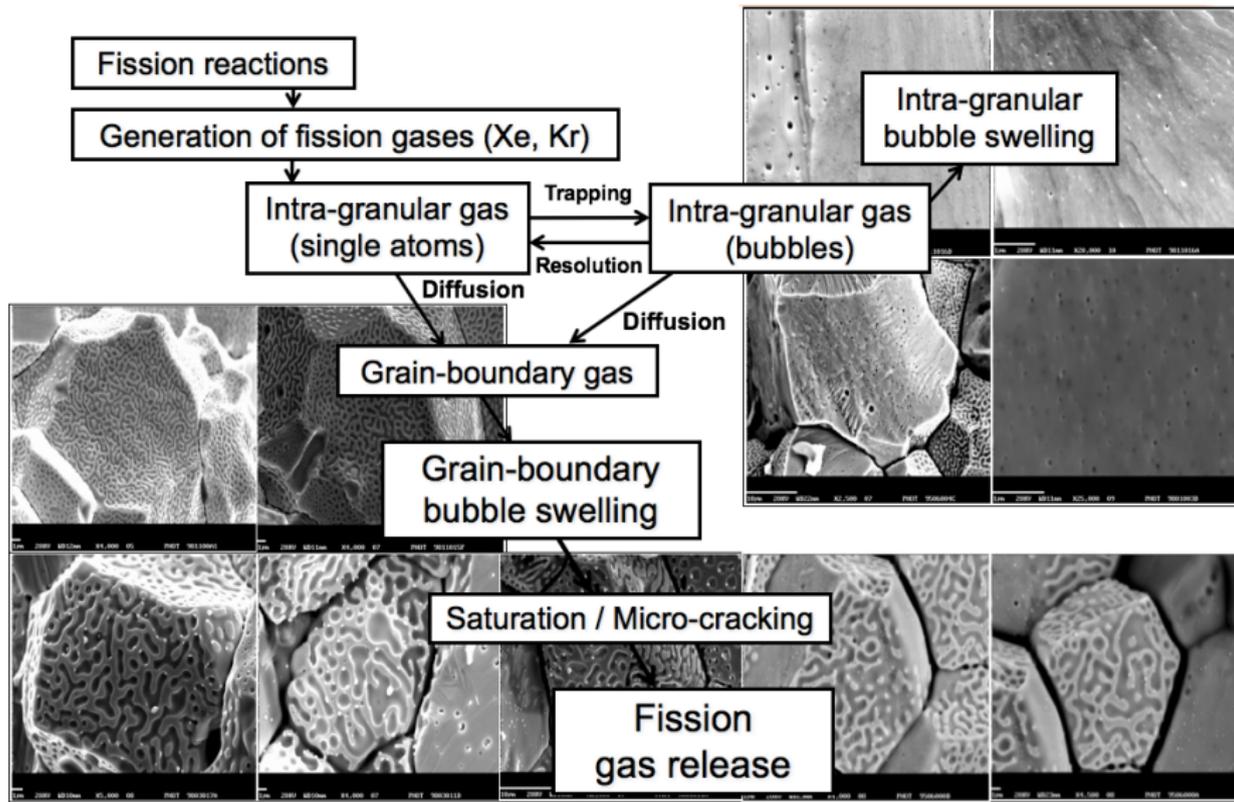
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Overview

- 1 Introduction
- 2 Material Model & Equations
- 3 Xolotl Benchmarking
- 4 Applications
- 5 Conclusion

The Long Standing Fission Gas Problem

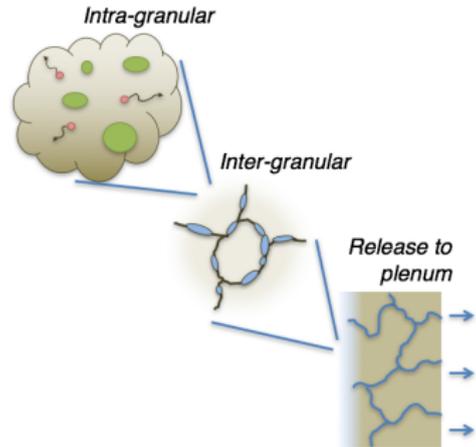


* G. Pastore (INL) – micographs from White, Corcoran and Barnes, Report R&T/NG/EXT/REP/02060/02 (2006).

The Long Standing Fission Gas Problem

Fission gas located in:

- Mobile gas atoms
- Intra-granular bubbles
- Inter-granular bubbles



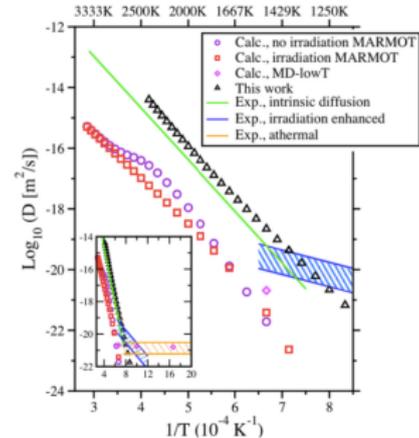
Gas release driven by inter-granular bubble interconnection:

- Creation
- Diffusion
- Absorption
- Re-resolution

Effective Diffusion Rate:

$$D' = Db' / (b' + g)$$

* D. Andersson (LANL)



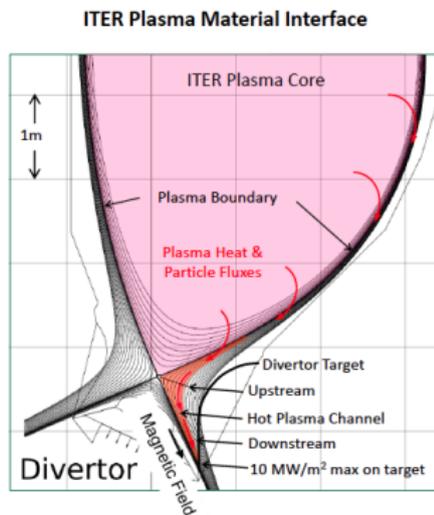
The Challenge of Plasma-Surface Interactions

Plasma facing components must remove plasma exhaust, which involves unprecedented power and particle fluxes and fluences, while limiting release of impurities to the core plasma.

Issues:

- Erosion lifetime and plasma compatibility
- Tritium inventory
- H/He blistering

Tungsten is a good material candidate due to its high resistance to heat.



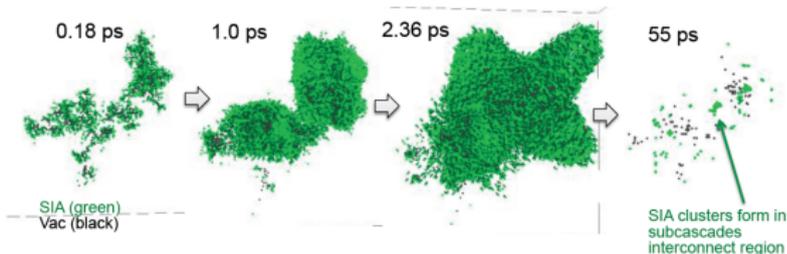
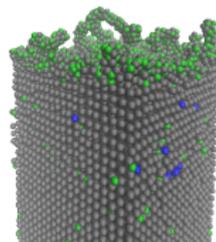
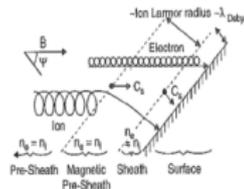
⇒ We want to be able to predict the material evolution.

* B. D. Wirth (UTK/ORNL)

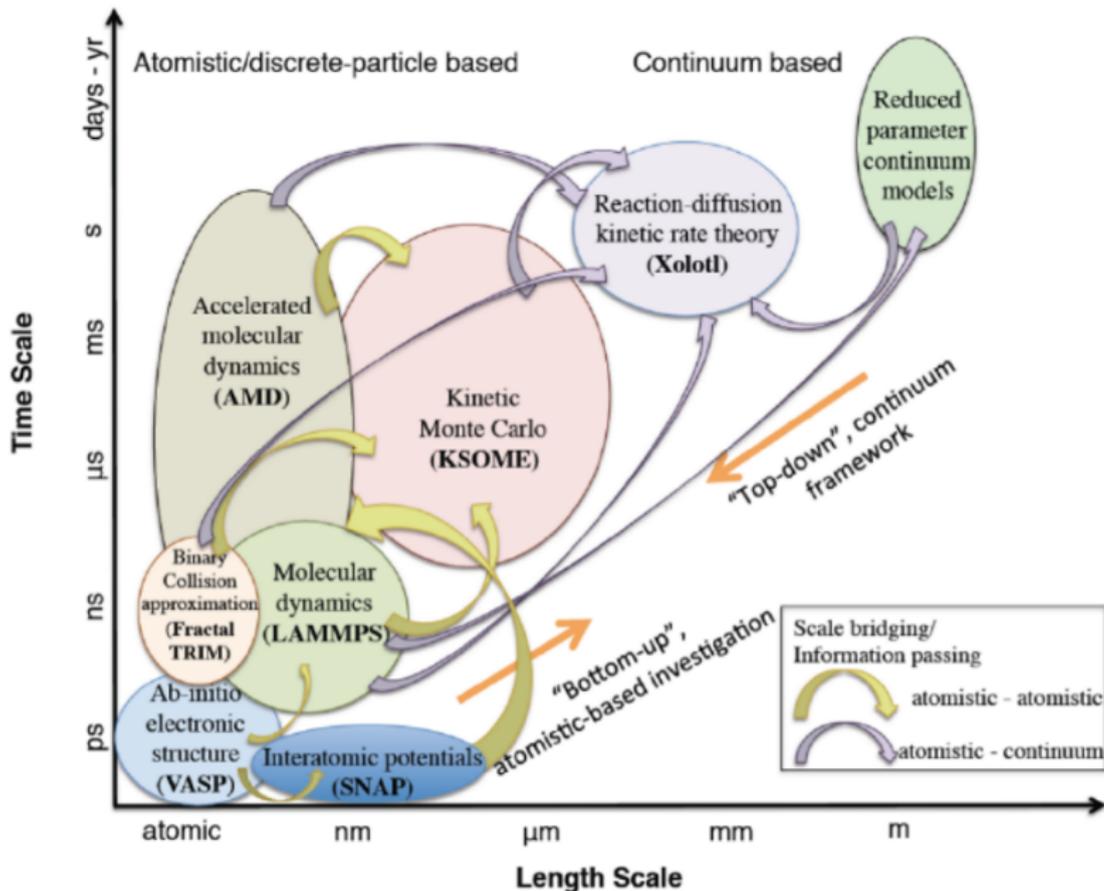
Plasma-Surface Interactions Objective

Develop PSI simulation capability across three coupled spatial regions:

- ▶ Edge/scrape-off-layer region of the plasma, with sheath effects (mm above the surface)
- ▶ Near surface material response to plasma exhaust, with neutron damage and with influence of/coupling to plasma sheath ($10^2 - 10^3$ nm under the surface)
- ▶ Structural material response to intense, 14 MeV-peaked neutron spectrum ($10^{-3} - 10^2$ mm under the surface)



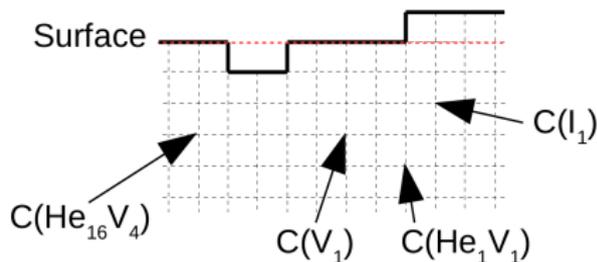
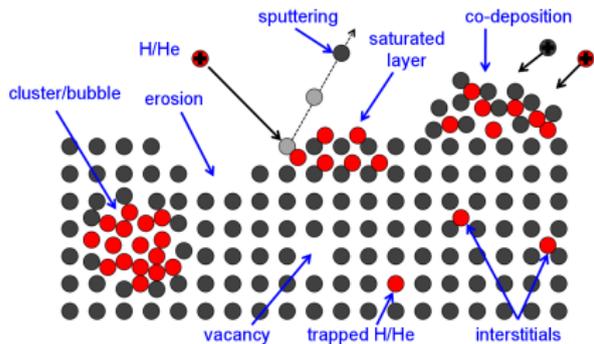
Multiscale Approach



The Material Model

The tungsten material is represented by the concentration of clusters at each spatial grid point:

- **Interstitials:** atoms of tungsten that are no longer on a lattice site
- **Vacancies:** missing atoms of tungsten on a lattice site
- **Helium:** helium atoms that are irradiated
- **Mixed:** combination of helium atoms trapped in tungsten vacancies



Reaction-Diffusion Equations

$$\delta_t \bar{C} = \phi \cdot \rho - \nabla \bar{J} - \bar{Q}(\bar{C})$$

- ▶ $\phi \cdot \rho$ is the incoming flux, the helium distribution profile is obtained from SRIM or MD simulations
- ▶ $\bar{J} = -D \nabla \bar{C} + u \bar{C}$ is the Fickian diffusive and drift fluxes, with D_i following the Arrhenius equation

$$D_i = D_{0,i} e^{-E_m/k_B T}$$

with $D_{0,i}$ and E_m obtained from MD and DFT simulations

Reaction-Diffusion Equations

- ▶ $\bar{Q}(\bar{C})$ is the reaction term:

Production:



$$\frac{dC_A}{dt} = \frac{dC_B}{dt} = -\frac{dC_E}{dt} = -k_{A,B}^+ C_A C_B$$

$$k_{A,B}^+ = 4\pi(r_A + r_B)(D_A + D_B)$$

Dissociation:



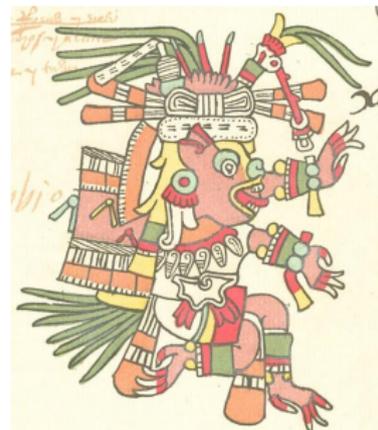
$$\frac{dC_F}{dt} = -\frac{dC_G}{dt} = -\frac{dC_H}{dt} = -k_{G,H}^- C_F$$

$$k_{G,H}^- = \frac{1}{\Omega} k_{G,H}^+ e^{\frac{-E_b}{k_B T}}$$

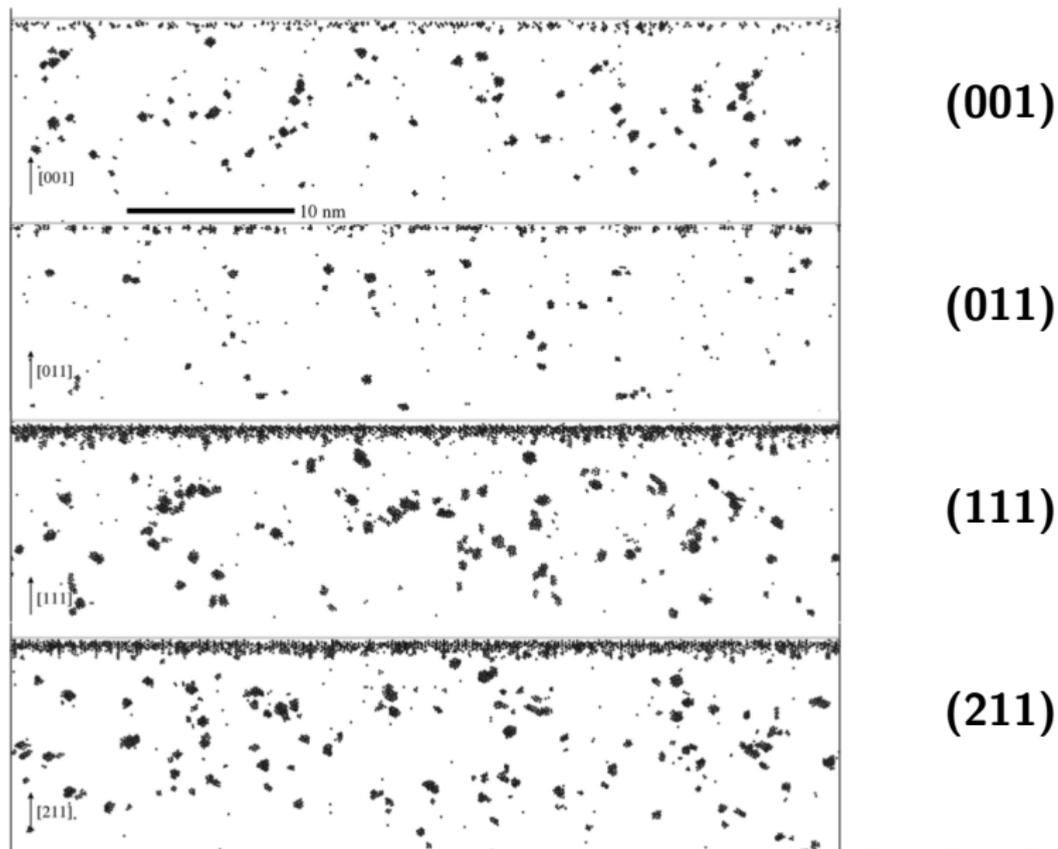
- the capture radii r_i and the atomic volume Ω are calculated from geometric considerations and lattice parameter a_0
- the binding energy E_b associated to the dissociation is computed from the formation energies E_f given by MD and DFT simulations

Xolotl

- ▶ Xolotl is the Aztec god of death and lightning
- ▶ Developed from scratch using C++ and MPI
- ▶ The solver part (using PETSc) is independent of the physics part and it uses the finite difference approach
- ▶ A preprocessor creates the default options and kinetics needed to run Xolotl
- ▶ 2D/3D has been implemented
- ▶ Open source code available at <https://github.com/ORNL-Fusion/xolotl>



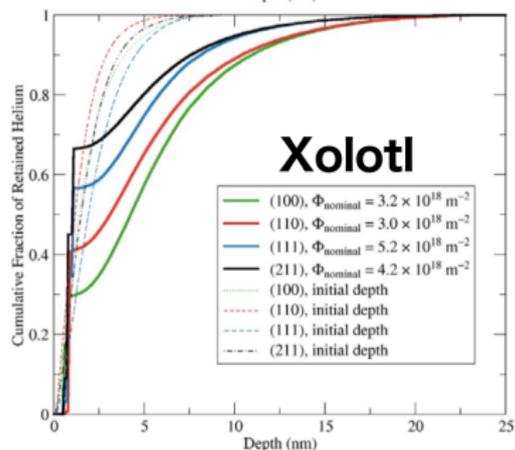
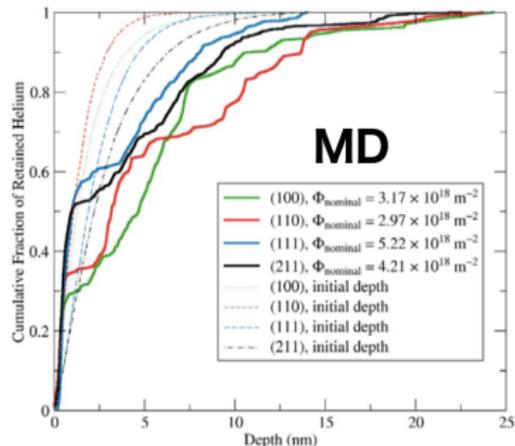
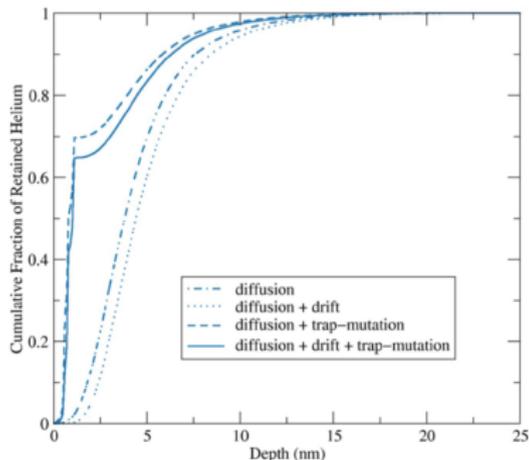
Large-Scale MD Simulations (at a fluence of $\sim 4 \cdot 10^{18}$ He m^{-2})



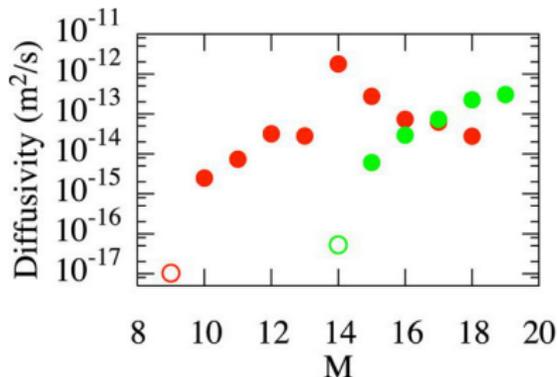
Near Surface Helium Behavior

Molecular Dynamics and Molecular Statics simulations have generated parameters of mobile helium clusters for different surface orientations:

- helium implantation
- biased drift
- modified trap mutation

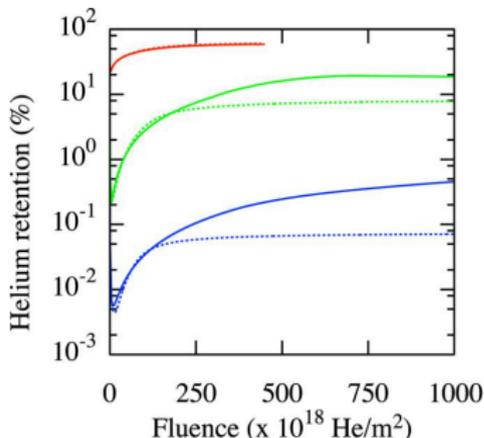


Mobility of Small HeV Complexes



Measurement of $\text{He}_M\text{V}_{1,2}$ clusters mobility through Accelerated MD simulations.

⇒ Implementation in Xolotl shows its importance at lower fluxes.

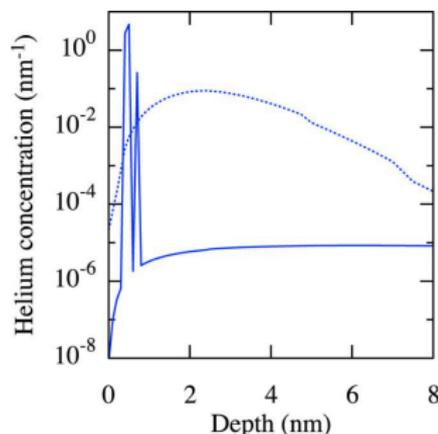


Flux ($\text{He m}^{-2} \text{ s}^{-1}$):

$4 \cdot 10^{25}$

$4 \cdot 10^{23}$

$4 \cdot 10^{22}$



D. Perez *et al.*, **The mobility of small vacancy/helium complexes in tungsten and its impact on retention in fusion-relevant conditions**, Sci. Rep. 7, 2522 (2017)

Bubble Bursting: How Does It Work?

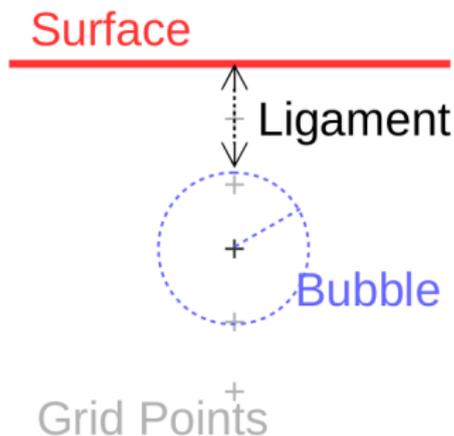
At the end of each time step loop on all the grid points:

- compute the total quantity of helium atoms (n_{He}) present at this grid point
- compute the radius of the helium bubble, using $n_V = n_{He}/4$ and

$$r_{He_x V_y} = r_V + \left(\frac{3a_0^3 y}{8\pi} \right)^{1/3} - \left(\frac{3a_0^3}{8\pi} \right)^{1/3}$$

- compute the ligament thickness ($L = d - r$)
- burst if the ligament thickness is 0, or with probability proportional to the thickness

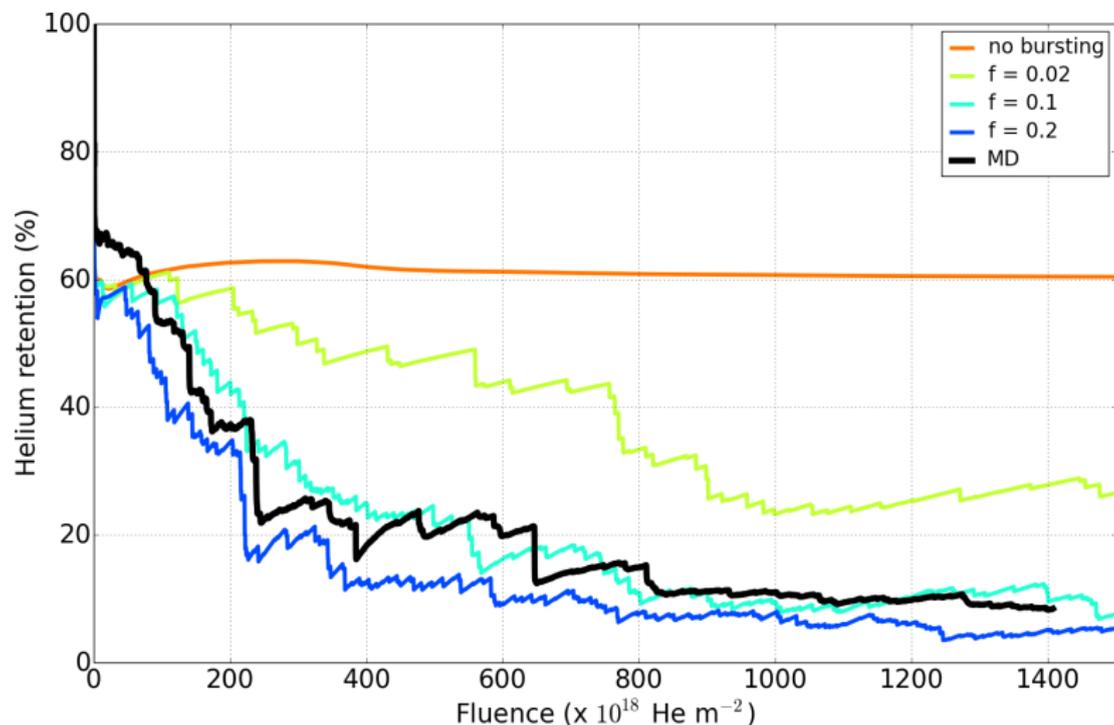
$$P_{burst} \propto (1 - L/d) \times f \times \min(1, e^{-(d-\tau_d)/2\tau_d})$$



When bursting,

- the concentration of each HeV cluster is transferred to the same size V cluster
- He clusters are just set to 0.0

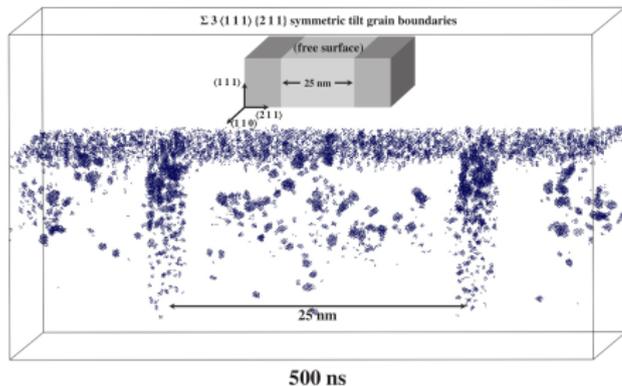
Bubble Bursting: Comparison to MD Simulation



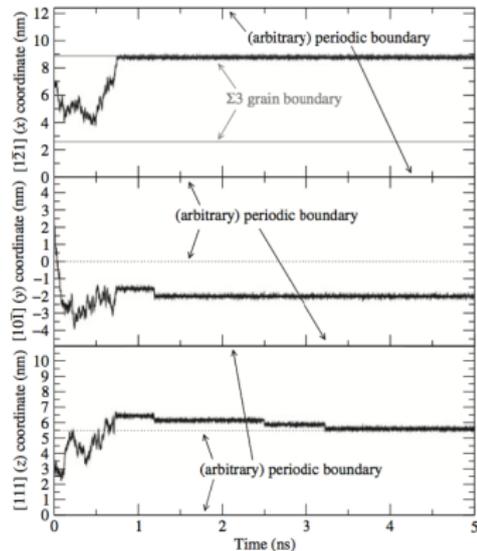
Flux: $5 \cdot 10^{27} \text{ He m}^{-2} \text{ s}^{-1}$ at 933 K.

Grain Boundaries

Grain boundaries act as sinks for mobile helium clusters like the free surface.

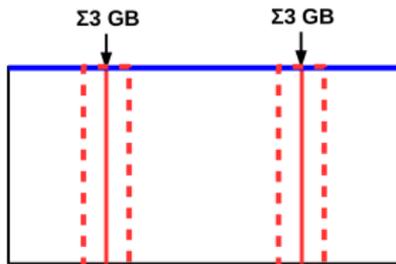


MD simulations show that once on the GB helium clusters no longer diffuse.

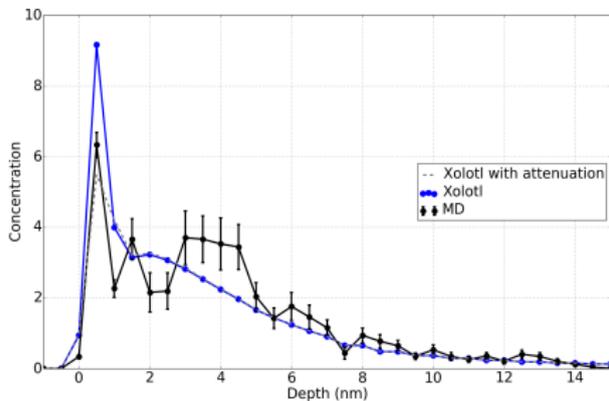


Hammond *et al.*, **Helium impurity transport on grain boundaries: Enhanced or inhibited?**, Europhysics Letter 110, 52002 (2015)

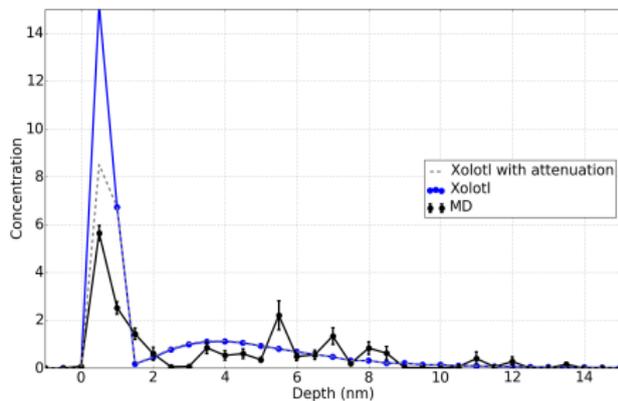
Grain Boundaries: Helium Concentration at $2 \cdot 10^{19} \text{ He m}^{-2} \text{ s}^{-1}$



On GBs

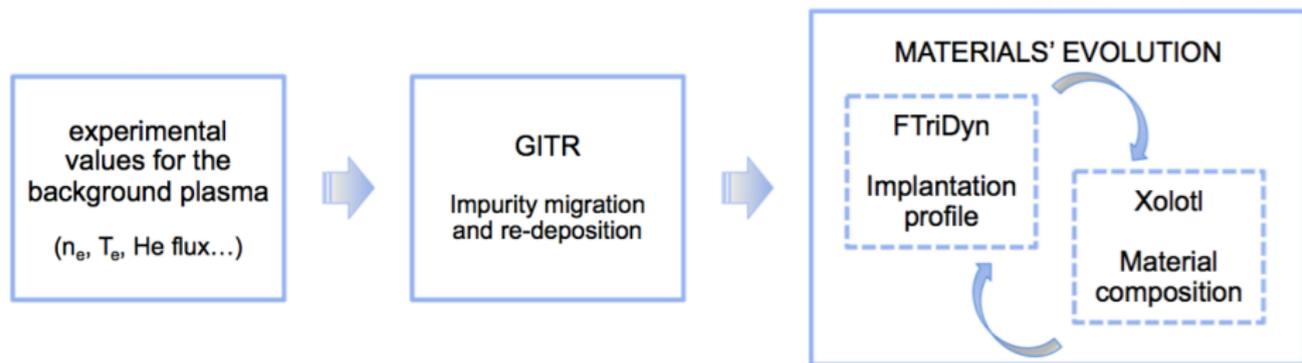


Away



Blondel *et al.*, **Benchmarks and Tests of a Multidimensional Cluster Dynamics Model of Helium Implantation in Tungsten**, Fusion Science and Technology 71, 1 84-92 (2017)

Code Integration in Fusion



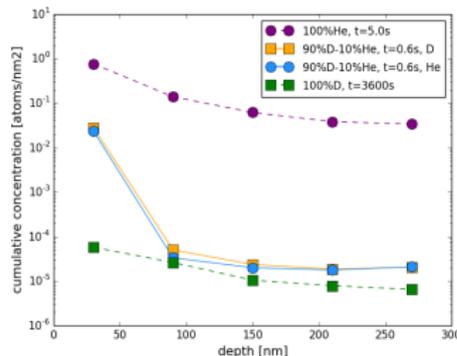
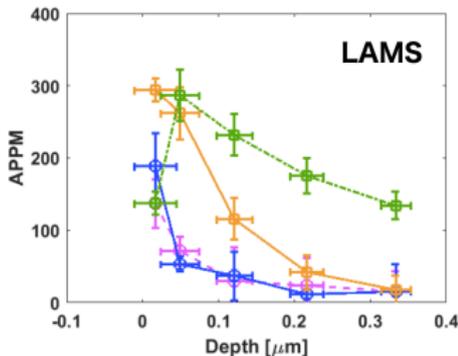
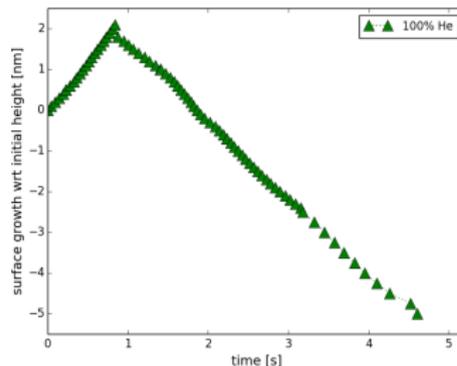
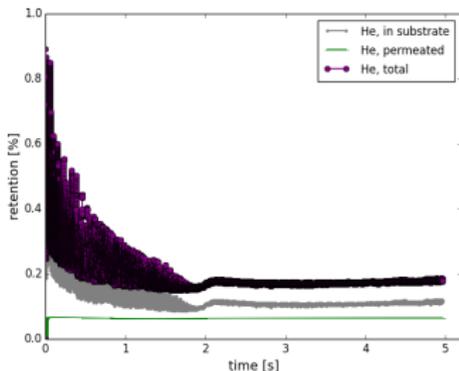
Xolotl is part of a multi-physics code integration effort using the Integrated Plasma Simulation framework.

Scripts are automatically generated to have the codes exchange data and loop together.

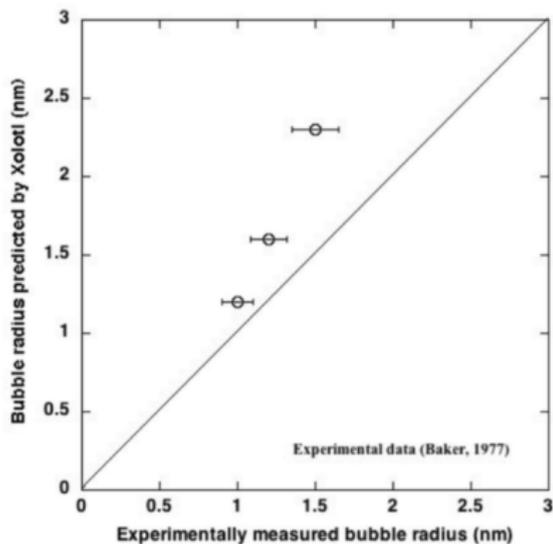
* A. Lasa (UTK)

Application to PISCES Dedicated Experiments

Linear plasma device with biased target (250 V) to enhance erosion, flux of $5.4 \cdot 10^{22} \text{ He m}^{-2} \text{ s}^{-1}$ for 100 s, surface temperature of 1093 K.



Fission Gas Application

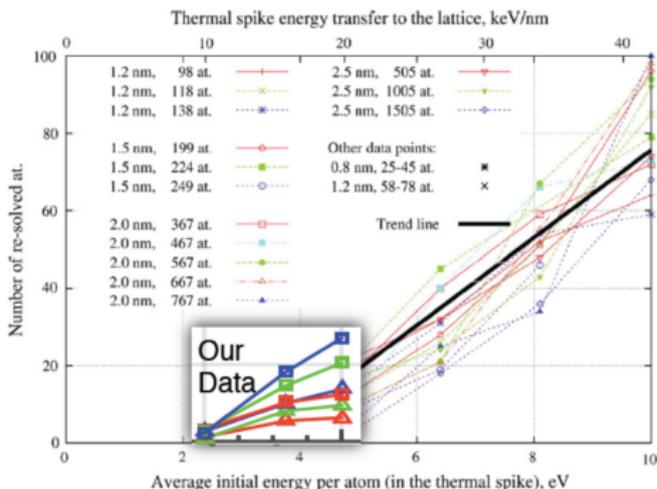


Preliminary comparison to experimental results: we overestimate the bubble radius.

⇒ Need to add a re-resolution model

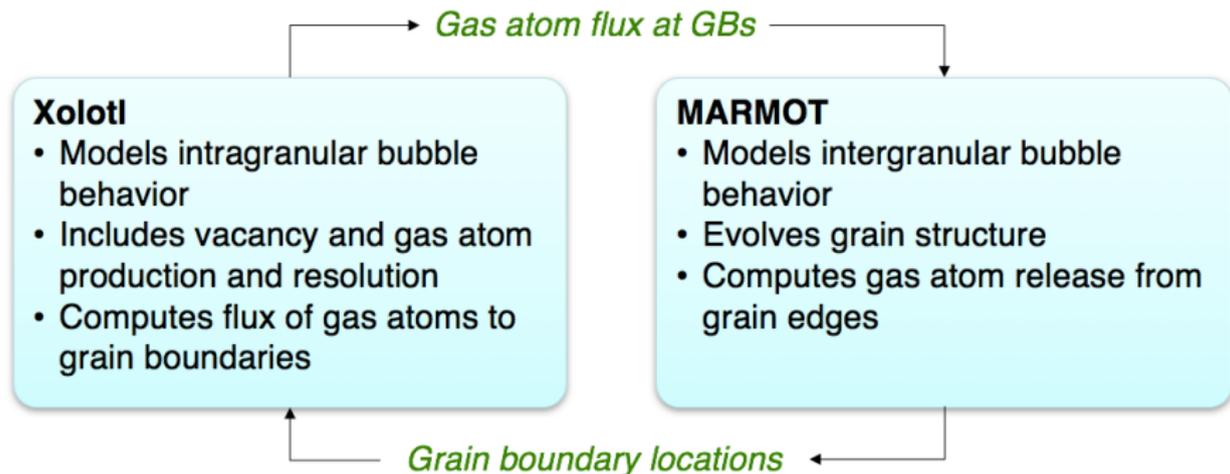
Generated a database of Xe bubbles re-solving into smaller Xe clusters by the passage of a fission fragment through MD simulations.

We are currently developing a simplified model to include in Xolotl.



Coupling with MARMOT

MARMOT uses phase field coupled with large deformation solid mechanics and heat conduction to predict the coevolution of microstructure and properties in nuclear materials.



- Coupling will be managed by the multi-app system in MOOSE
- The codes will each converge separately and then pass information

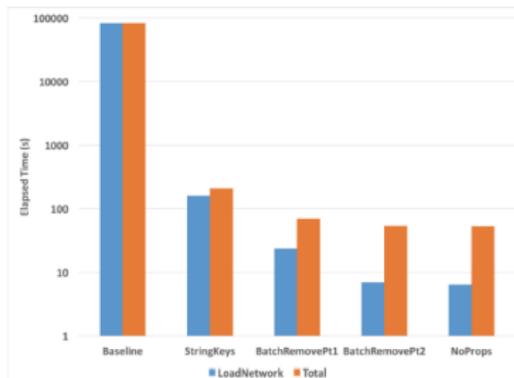
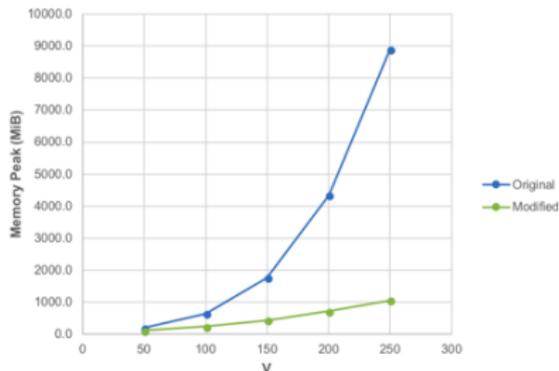
* M. Tonks (UFL)

Code Development

- **Grouping:** Use of a moment method to gather neighboring clusters together, average and first moments are then tracked:

$$C^i = L_0^i + \sum_{n,m \in i} [d_n^i L_{He}^i + d_m^i L_V^i]$$

- **Optimization:** Involvement with computer scientists to improve the performances, recent work was incorporated in PETSc



- **Dynamic Solver:** Work on having an extending cluster network with time.

Conclusion

- ▶ Benchmarks against other simulations proved successful
- ▶ Strong involvements with computer scientists to have a performant and reliable code
- ▶ Currently coupling Xolotl with other physics codes to reach experimental timescales

Thank You!

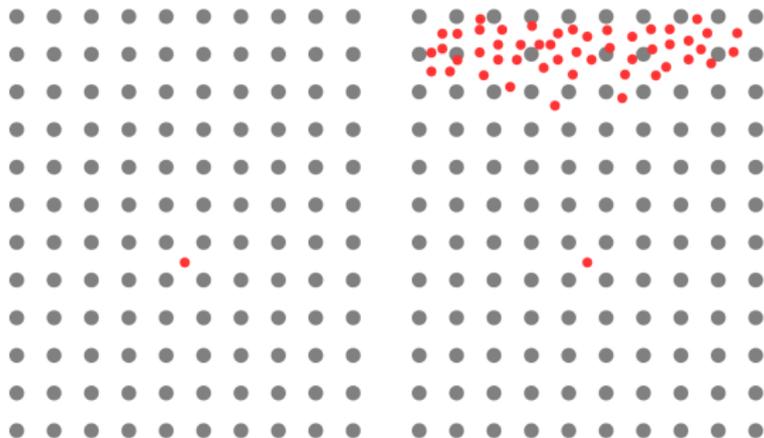
This work is supported by the US DOE under the Scientific Discovery through Advanced Computing program.

Back-Up

Attenuation

The effect of the modified trap-mutation in MD simulations seems to be attenuated with higher fluence.

The parameters obtained from small scale MD simulations are computed with no pre-existing helium concentration near the surface and their strengths are weakened when the layer of helium start building up.



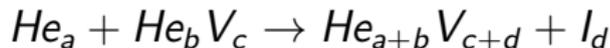
⇒ Attenuate these parameters in Xolotl too:

$$k_{\text{TM}} = e^{-A \cdot C_{\text{He}}} \times k_{\text{TM}}$$

Surface Evolution

Different physical processes contribute to the surface evolution under irradiation.

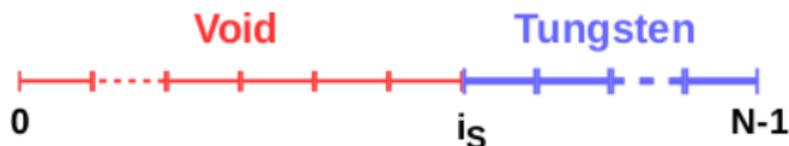
- ▶ **Trap mutation and loop punching:** When the bubble grows



These self-interstitials can then move to the surface and create adatoms (increase height).

- ▶ **Sputtering:** Tungsten atoms are ejected by incoming energetic particles (decrease height).
- ▶ **Re-deposition:** These tungsten atoms can then travel back to the material after ionization in the plasma sheath (increase height).

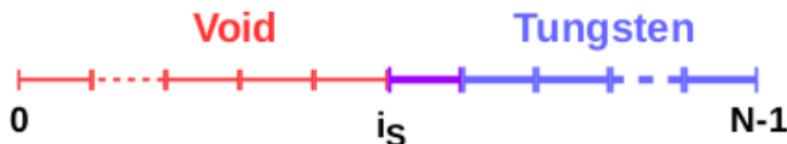
Surface Evolution in Xolotl



- ▶ No reaction, diffusion, or anything on the void grid points, concentrations are forced to 0.0
- ▶ On the tungsten side, classic ADR equations
- ▶ Count the number of interstitials diffusing from the $i_S + 1$ grid point to the i_S grid point to account for adatoms from trap mutation
- ▶ Remove the number of sputtered atoms given by the sputtering yield (given by FTriDyn)
- ▶ Profile of implanted interstitial for re-deposition is given by FTriDyn with energetics from GTR

Surface Evolution in Xolotl

- ▶ When the interstitial flux at the surface reaches a given threshold (corresponding to the tungsten density), move the surface



- ▶ Re-initialize all the processes that are depth dependent (helium and re-deposition flux profiles, near-surface advection, near-surface trap mutation, ...)
- ▶ The surface can move up or down, by one or many grid points per time step

Moment Grouping Method

In Xolotl the grouping method for now is a moment scheme:

- ▶ Normal clusters that are neighbors are grouped in a super cluster (for instance $\text{He}_{13 \rightarrow 16} \text{V}_{13 \rightarrow 16} \Rightarrow \text{He}_{14.5} \text{V}_{14.5}$)
- ▶ Only the concentration of the super cluster is tracked (instead of the many normal clusters that compose it) taking

$$C^i = L_0^i + \sum_{n,m \in i} [d_n^i L_{He}^i + d_m^i L_V^i]$$

- ▶ There are 3 equations for each super cluster (L_0^i, L_{He}^i, L_V^i)

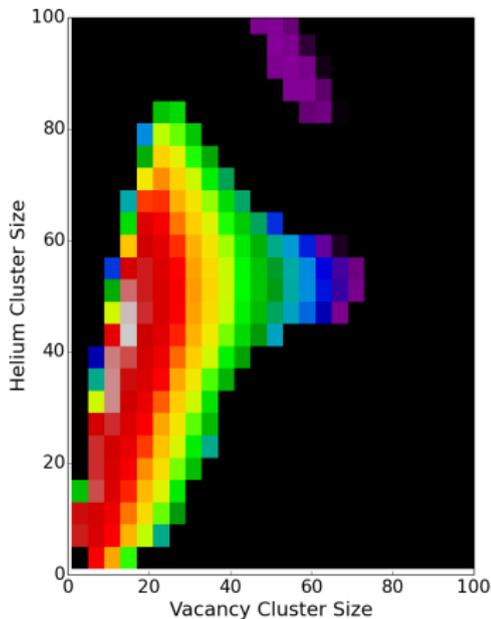
Modelling Simul. Mater. Sci. Eng. 25 (2017) 015008

Dynamic Solver in Xolotl

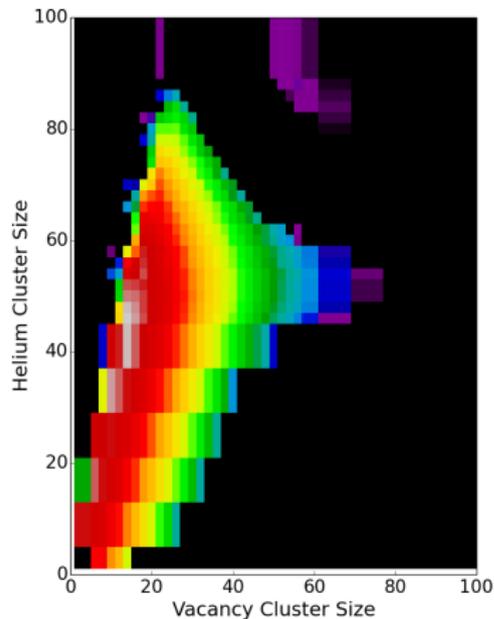
Extend the network and update the grouping with time:

- ▶ Start with small network ($100He \times 100V$)
- ▶ When the edge clusters have a concentration higher than a threshold times the total concentration, stop the solver
- ▶ Copy the solution, create a new network X times larger, define new bounds for the grouping (function of previous moments), start the solver from the new solution
- ▶ Loop until we are happy

Dynamic Solver in Xolotl: Concentration Copy



End of Loop



Reinitialization