Simulation of Fission Gas in Uranium Oxide Nuclear Fuel

Multiscale MARMOT-Xolotl coupled framework for fission gas bubble growth simulations

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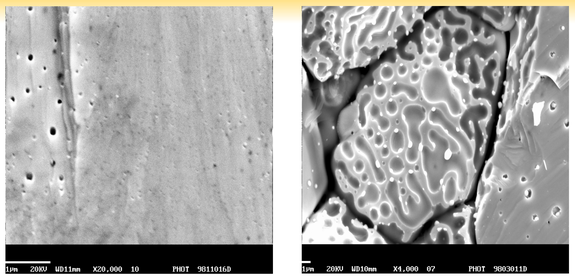
Introduction

- Fission gas bubble growth in nuclear fuel is a **multi-scale phenomenon**.
- The order of magnitude of length scale difference is up to 10^3.
  - Intragranular bubbles (~nm)
  - Intergranular bubbles (~µm)



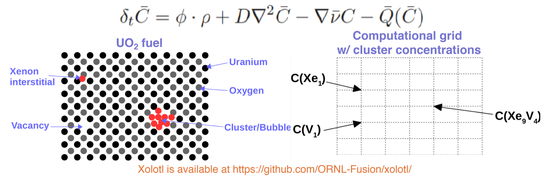
Multiscale approach

Intragranular bubbles

***Xolotl* cluster dynamics**

- Spatially-resolved, time evolution of clusters of atoms, vacancies, interstitials within material based on kinetics
- Bubble formation and evolution is major scientific focus (but not exclusive)

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

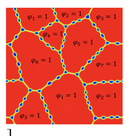


Xolotl is available at https://github.com/ORNL-Fusion/xolotl/

Intergranular bubbles

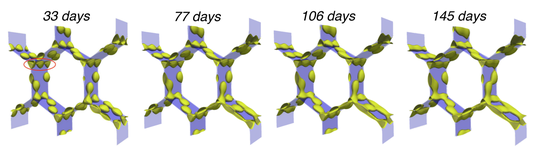
***MARMOT* phase-field modeling**

- Transport of gas atoms and U vacancies.
- Void growth and coalescence.
- Grain boundary migration.



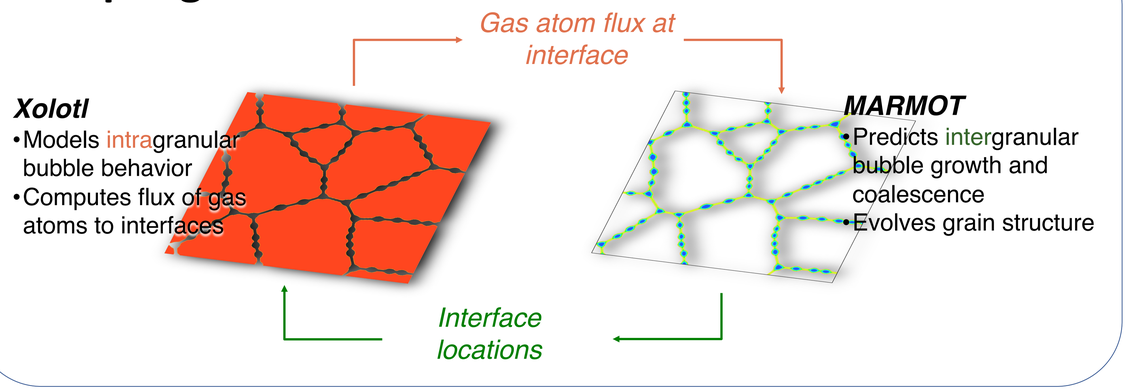
$$\frac{\partial \eta_{\alpha i}}{\partial t} = -L\left[m\left(\eta_{\alpha i}^3 - \eta_{\alpha i} + 2\eta_{\alpha i}\sum_{\beta}^{p_\beta}\sum_{j=1,\alpha i\neq\beta j}^{p_\beta}\gamma_{\alpha i\beta}\eta_{\beta j}^2\right) - \kappa\nabla^2\eta_{\alpha i} + \sum_{\alpha}\frac{\partial h_\alpha}{\partial \eta_{\alpha i}}\omega_\alpha\right]$$

$$\frac{\partial \mu_g}{\partial t} = \frac{1}{\chi_g}\left[\nabla\cdot(D_g\chi_g\nabla\mu_g) + s_g - \sum_{\alpha}\sum_{i=1}^{p_\alpha}\frac{\partial \rho_g}{\partial \eta_{\alpha i}}\frac{\partial \eta_{\alpha i}}{\partial t}\right]$$



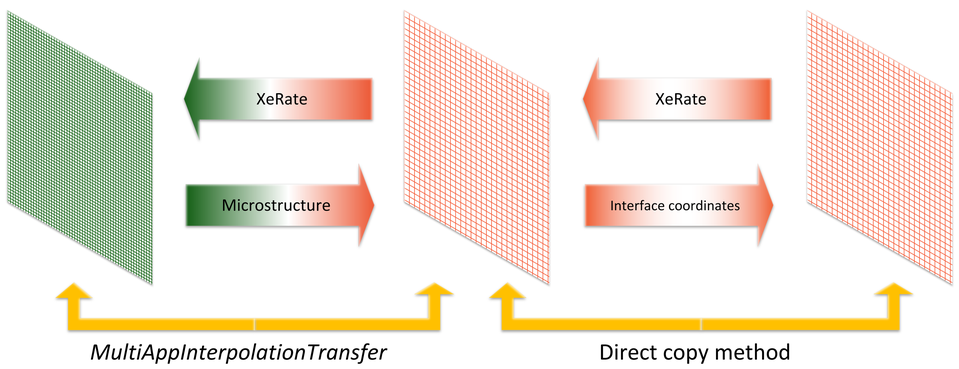
Larry K. Aagesen, Daniel Schewen, Michael R. Tonks, and Yongfeng Zhang, Computational Materials Science 161 (2019) 35-45

Coupling schematics



Code implementation

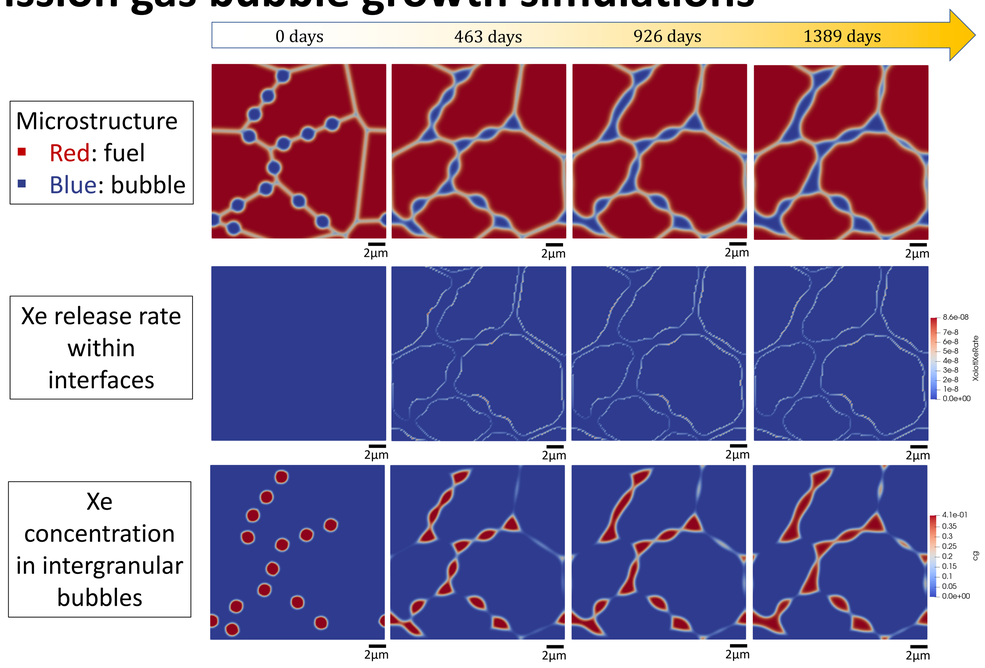
- **Managed by MOOSE MultiApp system**
  - Combine multiple MOOSE applications
  - Parallel computation
- ***Xolotl* becomes a MOOSE application**
- **Key components:**
  - (MasterApp) ***MARMOT*** phase-field solver
  - (SubApp) ***MOOSE-Xolotl wrapper***
  - (External library) ***Xolotl***
- **Parallel data transfer**



-Data transfer between nonidentical mesh
-Mesh adaptivity is available.

-Positions of every node should be identical.
-Parallelism is also identical for the efficiency.

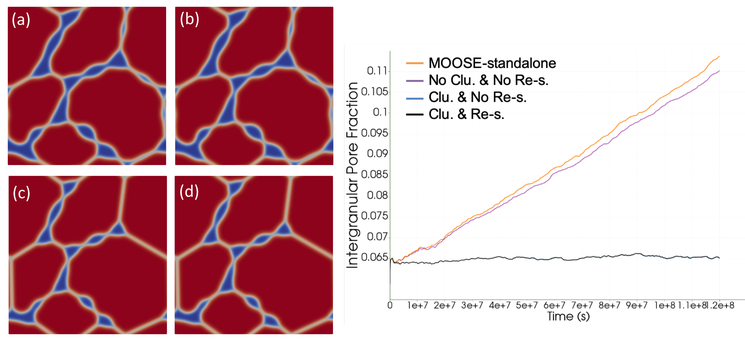
Fission gas bubble growth simulations



Microstructure* variation w.r.t. the considered physics:

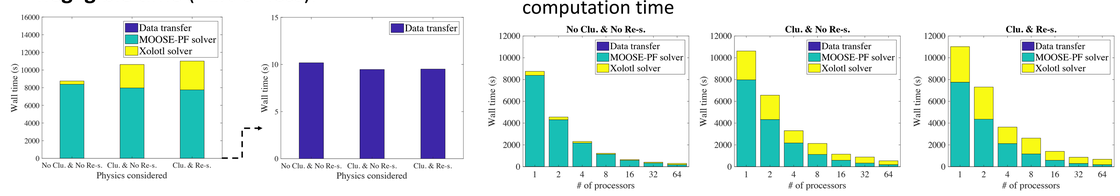
(a) Non-coupled, MOOSE standalone
(b) Coupled, No Clustering & No Re-solution
(c) Coupled, Clustering & No Re-solution
(d) Coupled, Clustering & Re-solution

*Time = 1389 days

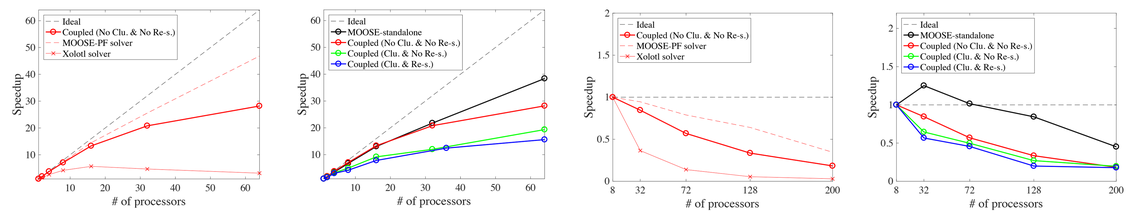


Code performance assessment

- **Division of computation time between codes**
  - The **data transfer** between coupled codes costs **negligible** time (~1% or less).
  - Addition of physics (clustering & re-solution) changes overall computation time and division
  - The # of processors is also a factor changing the division of computation time



- **The initial assessment of scalability of the coupled code was carried out.**
  - **Strong scaling**:
    - 2D, 125 x 125 elements with 126 x 126 nodes
    - # of DOF per node = 9*
    - Variable: # of processors
  - **Weak scaling**:
    - # of nodes per area of simulation domain: 32.1 µm^{-2} (fixed)
    - Problem sizes: (9 µm)^2, (18 µm)^2, (27 µm)^2, (36 µm)^2, (45 µm)^2
    - # of processors: 8, 32, 72, 128, 200



*If the clustering is considered, # of DOF = 1008

Code repository

- ✓ MOOSE: https://github.com/idaholab/moose
- ✓ MasterApp (***MARMOT***) and ***MOOSE-Xolotl wrapper***: https://github.com/eastglow-zz/coupling_xolotl
- ✓ ***Xolotl***: https://github.com/ORNL-Fusion/xolotl/tree/mooseApps-coupling

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