Multiscale Investigation of Fission Gas for the Development of Fuel Performance Materials Models

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Idaho National Laboratory

Presentation Summary:

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

- The US Department of Energy Nuclear Energy Advanced Modeling and Simulation Program (NEAMS) seeks to rapidly create and deploy "science-based" verified and validated modeling and simulation capabilities essential for the design, implementation, and operation of future nuclear energy systems.
- In this talk, I will summarize NEAMS-funded efforts to develop advanced materials models for fuel performance using multiscale modeling and simulation.
- Outline:
  1. MOOSE-BISON-MARMOT
  2. MOOSE summary
  3. BISON summary
  4. MARMOT summary
  5. Example of multiscale model development

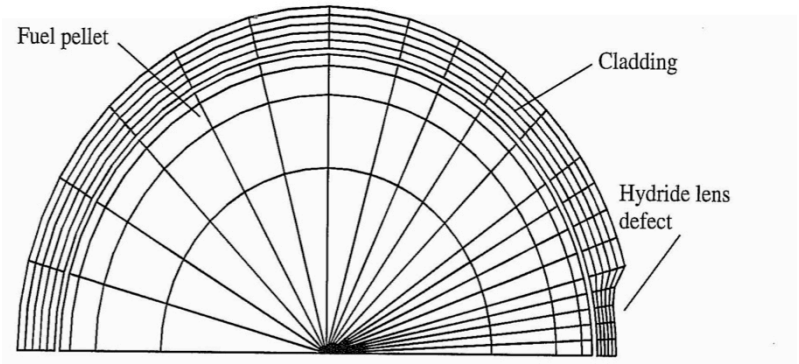
LWR Fuel Behavior Modeling – U.S. State of the Art

- Fuel performance codes are used today for determination of operational margins by calculating property evolution.
- However, current US industry standard codes (e.g. FRAPCON and FALCON) have limitations in three main areas:

Numerical Capabilities
- Serial
- Inefficient Solvers
- Loosely Coupled
- High Software Complexity

Geometry representation
- 1.5 or 2-D
- Smeared Pellets
- Restricted to LWR Fuel

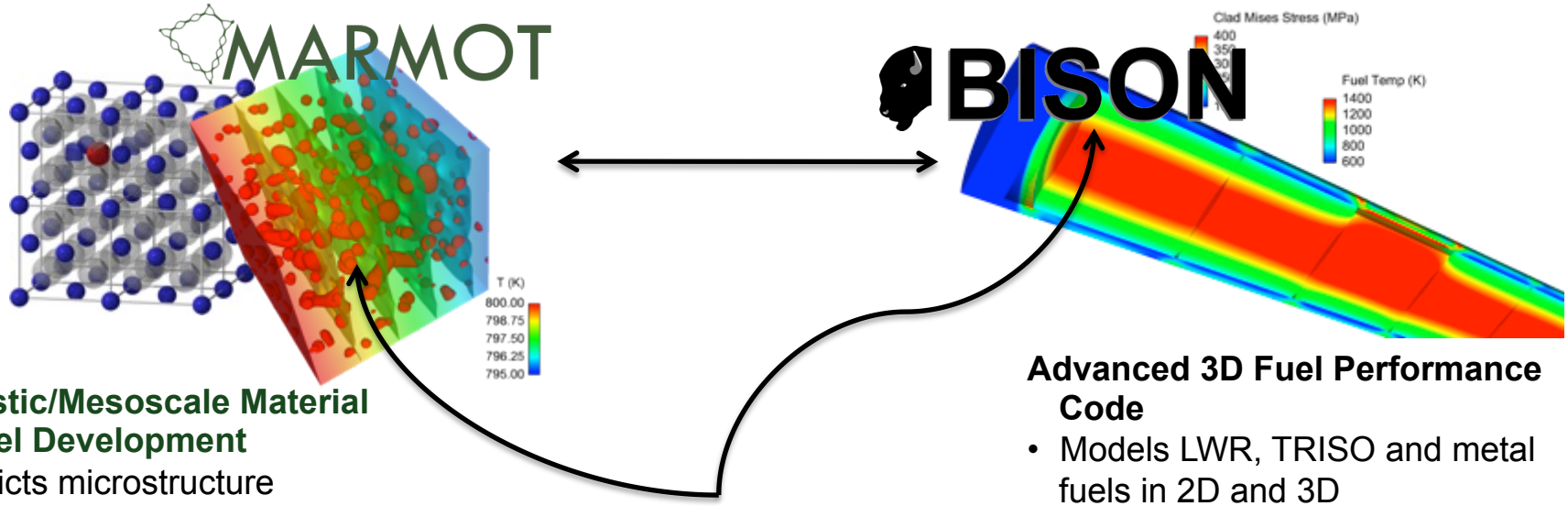
Materials models
- Empirical
- Models only valid in limited conditions
- Limited applicability in accident scenarios



FALCON model to investigate clad failure due to defect

MOOSE-BISON-MARMOT

- The MOOSE-BISON-MARMOT codes address current limitations in numerical capabilities, geometry representation and materials models.



Atomistic/Mesoscale Material Model Development

- Predicts microstructure evolution in fuel
- Used with atomistic methods to develop multiscale materials models

Advanced 3D Fuel Performance Code

- Models LWR, TRISO and metal fuels in 2D and 3D
- Steady and transient reactor operations

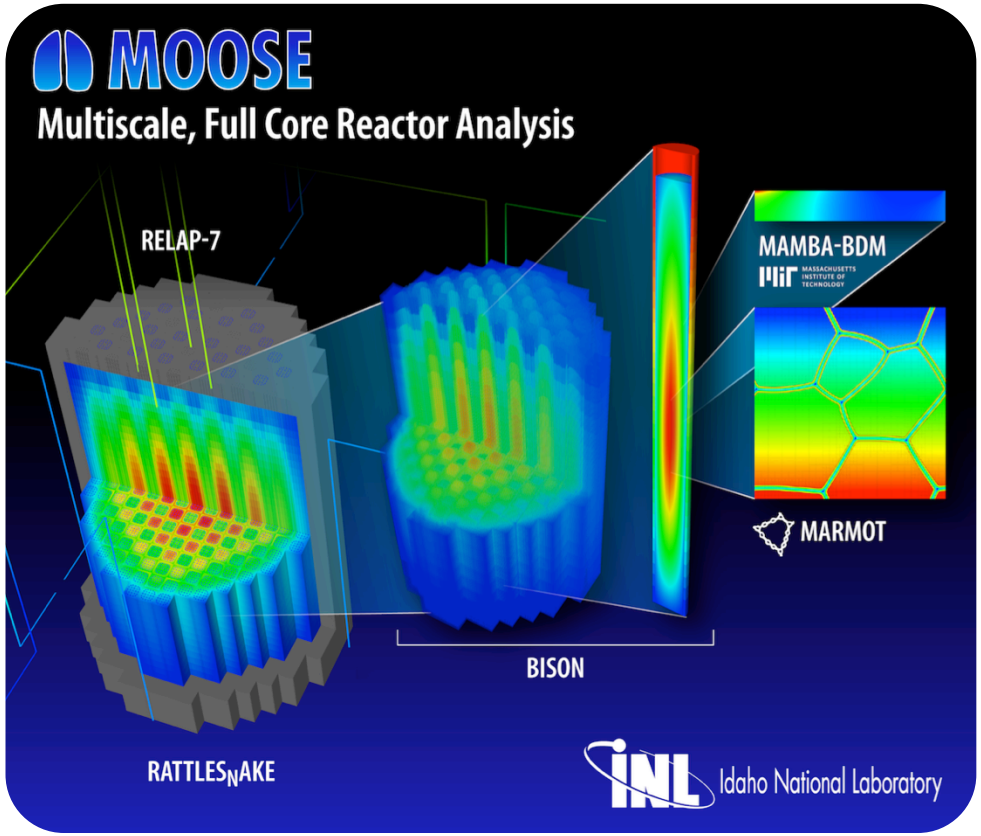
MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework allowing rapid development of FEM-based applications

Multiphysics Object-Oriented Simulation Environment

- A finite element based framework for solving systems of partial differential equations
- Employs an object-oriented approach to allow for rapid development of new simulation tools (Meets NQA-1 requirements)
- Code development focuses on implementing physics rather than numerical issues
- Comes with the Extended Library of Kernels (ELK) with various physics modules.



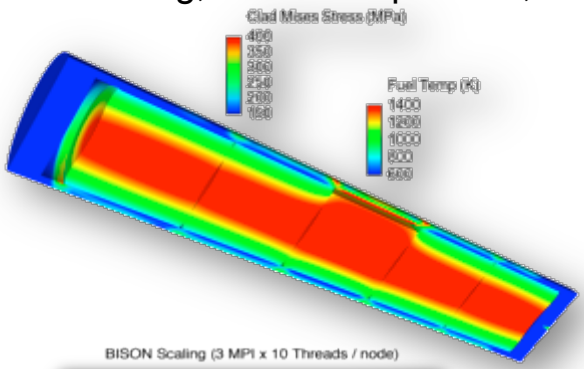
- Utilizes the Jacobian-free Newton–Krylov (JFNK) method to enable the implicit solution of large nonlinear systems of coupled physics equations
- Ecosystem of 27 applications (including MARMOT) that have been used to model a wide range of problems

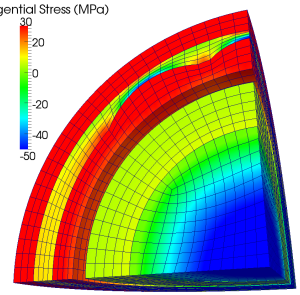
Licensed Laboratories - Industry Partners - Universities

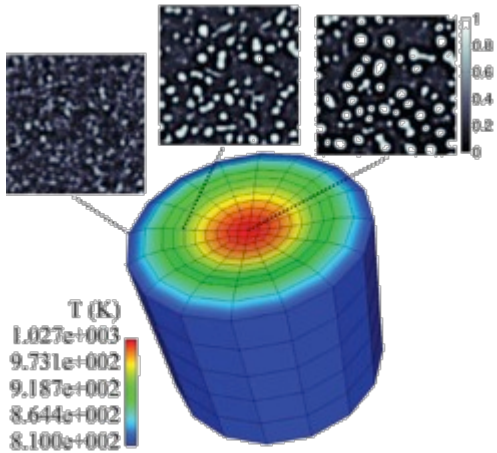
BISON *Fuel Performance Code*

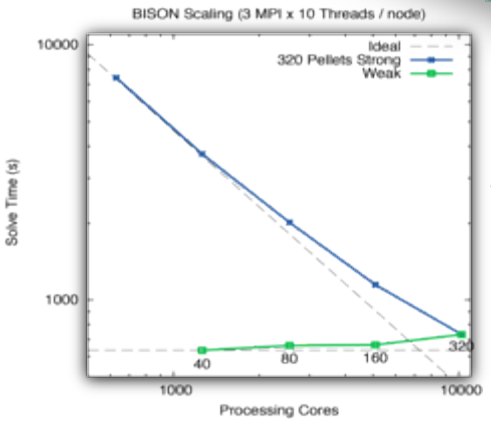
Solution method: Implicit finite element solution of the coupled thermomechanics and species diffusion equations using the MOOSE framework

Multiphysics constitutive models: large deformation mechanics (plasticity and creep), cracking, thermal expansion, densification, radiation effects (swelling, thermal conductivity, etc.)

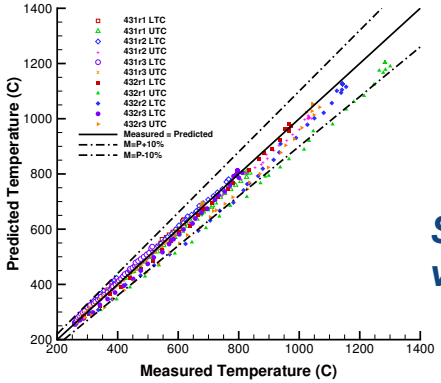








Massively parallel, has been run on 1 - 12,000 cpus.



Substantial experimental validation is underway

R. L. Williamson, J. D. Hales, S. R. Novascone, M. R. Tonks, D. R. Gaston, C. J. Permann, D. Andrs and R. C. Martineau, "Multidimensional Multiphysics Simulation of Nuclear Fuel Behavior," *Journal of Nuclear Materials*, **423**, 149 (2012)

MARMOT

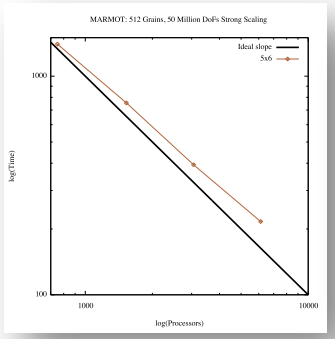
Mesoscale Multiphysics Simulation Tool

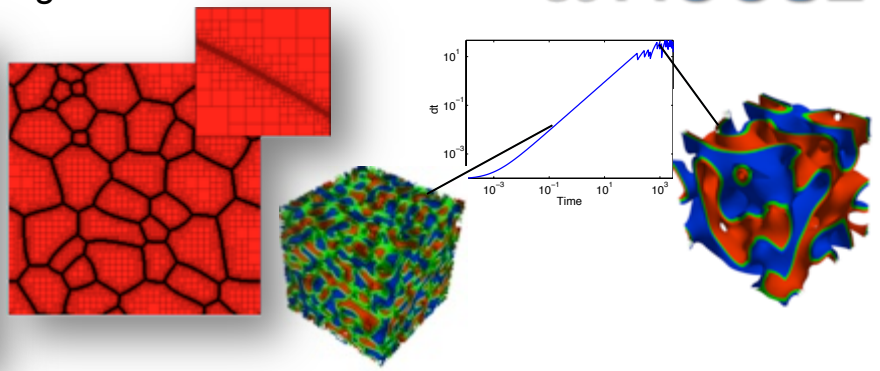
- MARMOT predicts coevolution of microstructure and physical properties due to applied load, temperature, and radiation damage

Technique: Phase field coupled with large deformation solid mechanics and heat conduction solved with implicit finite elements using INL's MOOSE framework

All models implemented in MARMOT are:

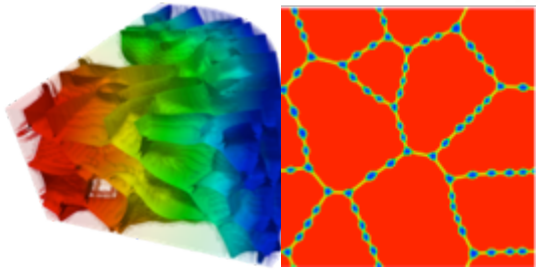
- 1D, 2D or 3D
- Massively parallel, from 1 to 1000's of processors
- Able to employ mesh and time step adaptivity
- Easily coupled to additional physics from the Extended Library of Kernels (ELK)





MARMOT is being used at various labs and Universities:

Argonne NATIONAL LABORATORY · Los Alamos NATIONAL LABORATORY · Pacific Northwest NATIONAL LABORATORY · The University of Wisconsin Madison · BYU Idaho · Michigan

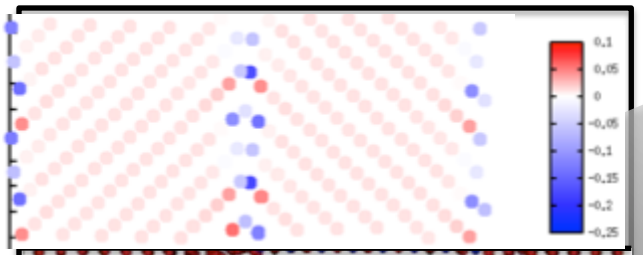


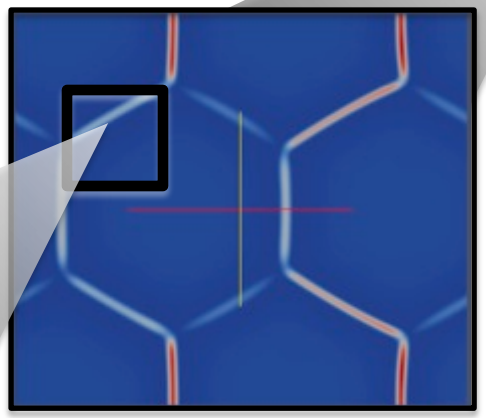
Physical models include:

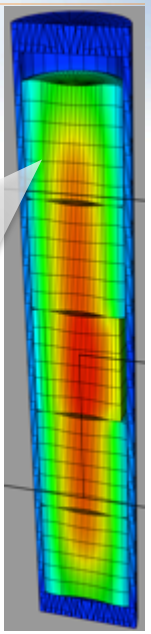
- GB migration/grain growth
- Species redistribution, phase separation
- Void/Bubble growth and coalescence
- Coupling between phase field and plasticity

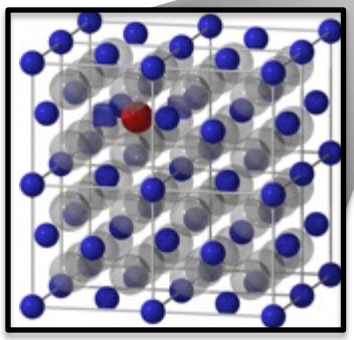
Multiscale Materials Modeling Approach

Modeling Approach: *Physics-based materials models are developed using a hierarchical multiscale approach ranging from the atomistic to the macroscale*









1st Principles Simulations

- Identify important bulk mechanisms
- Determine bulk material parameter values

Molecular Dynamics Simulations

- Investigate role of idealized interfaces
- Determine interface properties

Mesoscale Simulations (MARMOT)

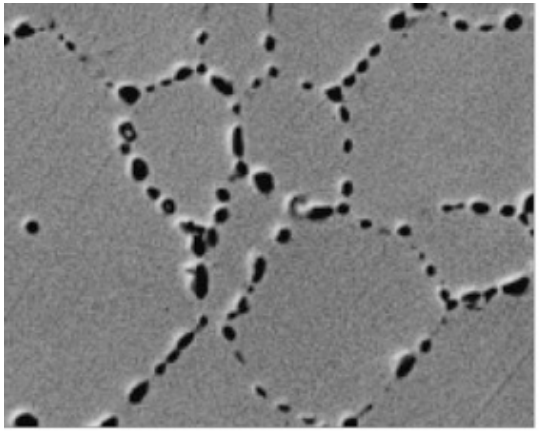
- Predict and define microstructure state variable evolution
- Determine effect of evolution on material properties

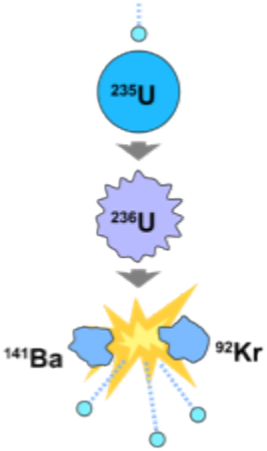
Fuel Performance Code (BISON)

- Predict fuel performance during operation and accident conditions

Effects of Gaseous Fission Products

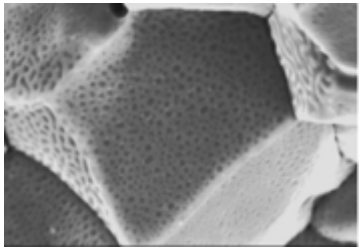
- We demonstrate our multiscale approach by focusing on fission gas behavior, due to its large impact on the fuel performance.
- Gaseous fission products and point defects are constantly generated within the fuel during reactor operation



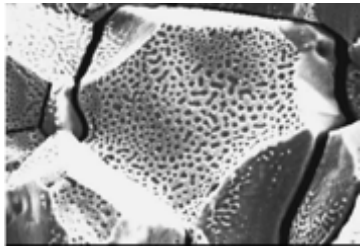


Fission gas effects fuel performance by:

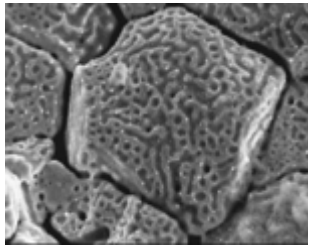
- Fission product swelling
- Degradation of thermal conductivity
- Fission gas release (increases plenum pressure and decreases gap thermal conductivity)



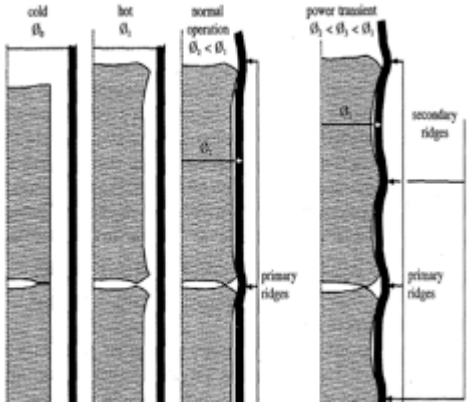
Nucleation



Growth

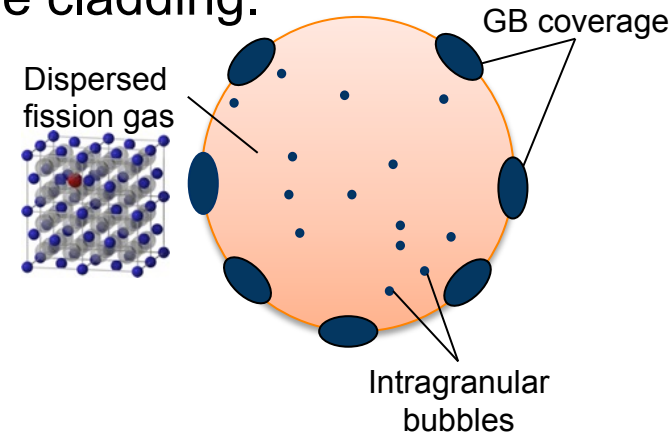


Percolation



Fission Gas Evolution Model

- BISON Fission gas evolution model predicts the migration of the fission gas to GBs and its eventual release into the gap between the fuel and the cladding.



- Model approximates the gas diffusion using a 1D spherical domain (grain)
- Gas is divided into three types
  - Dispersed intragranular gas migrating towards GB.
  - Trapped gas in small intragranular bubbles.
  - Gas in GB bubbles that can be released.

$$\frac{\partial C_t}{\partial t} = D_{eff}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_t}{\partial r}\right) + \beta$$

$$\frac{dN_{gb}}{dt} = -\frac{6N_{gb}^2}{3+4N_{gb}A_{gb}}\frac{dA_{gb}}{dt}$$

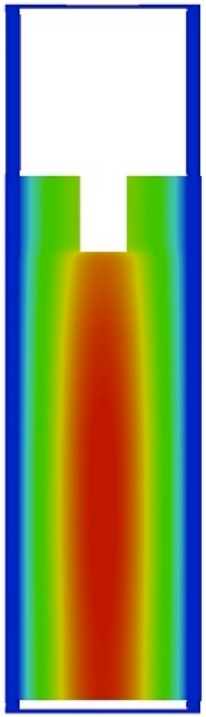
$$p_{ig} = N_{ig}\left(\frac{4}{3}\pi R_{ig}^3\right)$$

$$C_b = \frac{g}{g+b}C_t$$

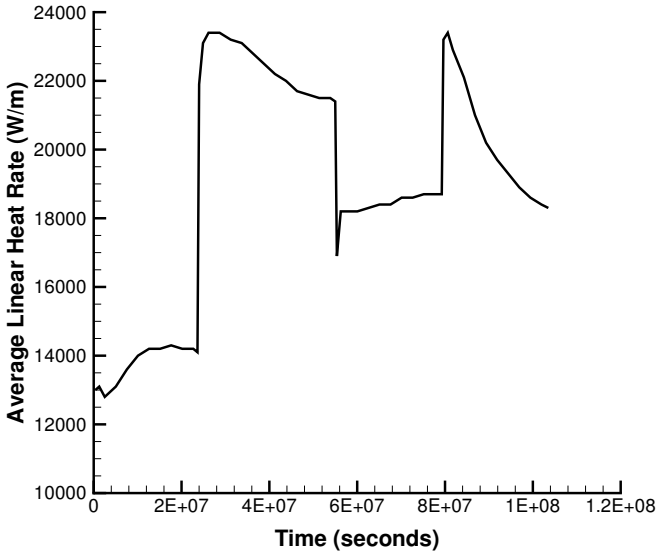
- Gas in GB bubble begins to release once the GB coverage reaches a set percolation threshold of 0.5.

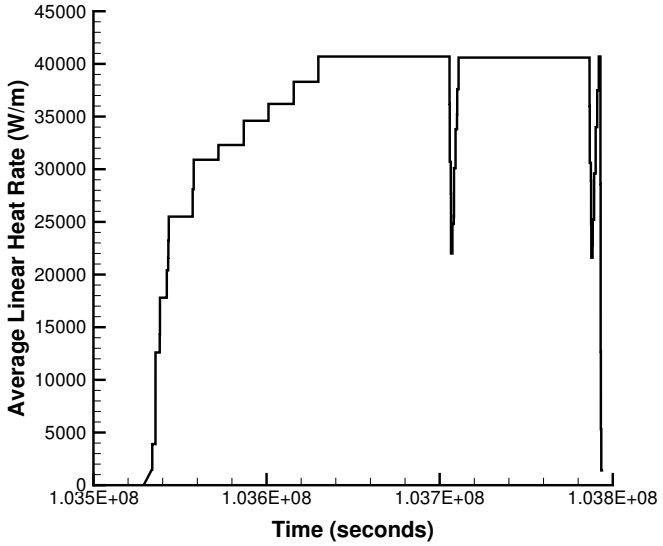
Validation: RISO-3 AN3

- Model has been validated against a series of assessment cases, including the RISO-3 AN3 test:
  - Fuel pin CB8 was base irradiated in the Biblis A PWR for four cycles
  - Re-fabricated fuel pin was shortened and instrumented with a fuel centerline thermocouple and pressure transducer.
  - CB8-2R was ramp tested at the Riso DR3 water-cooled HP1 rig
  - Assumed short rod length through base irradiation for simulation
  - Modeled as 2D-RZ axisymmetric with smeared pellets

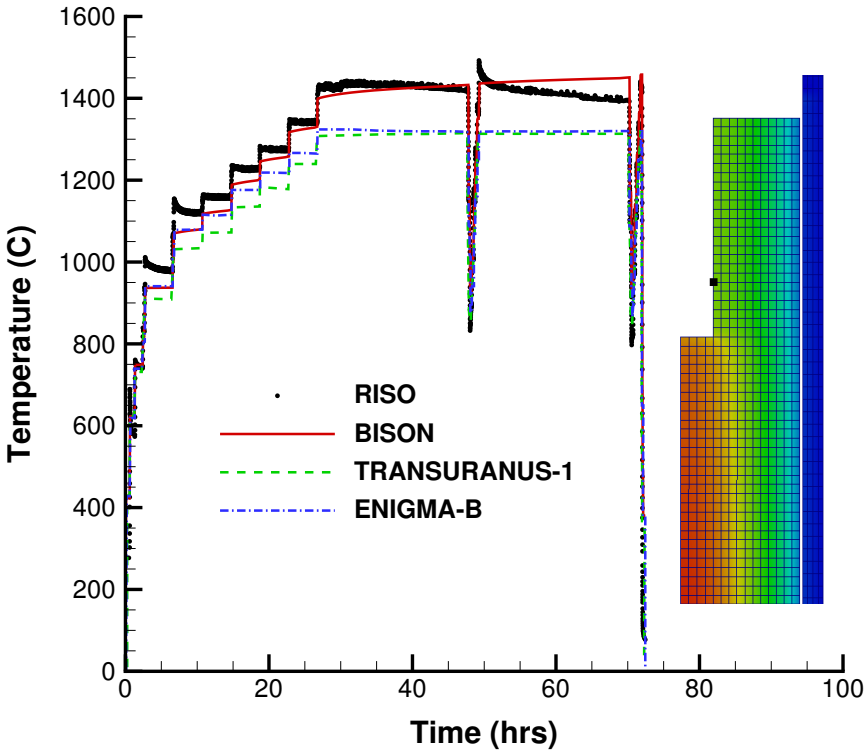


Aspect ratio scaled 10x

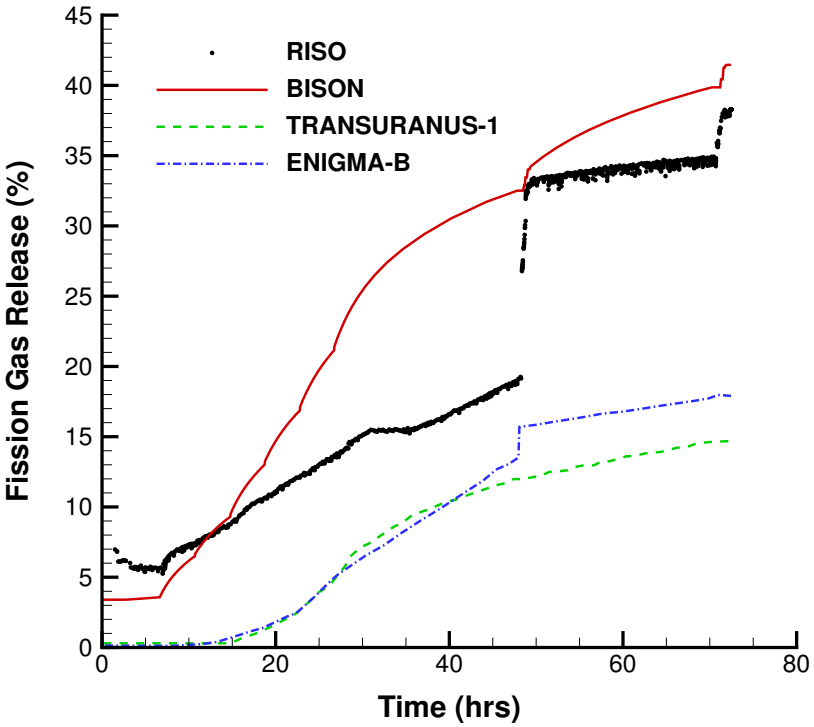




Comparisons During Power Ramp – Riso AN3



Fuel Centerline Temperature

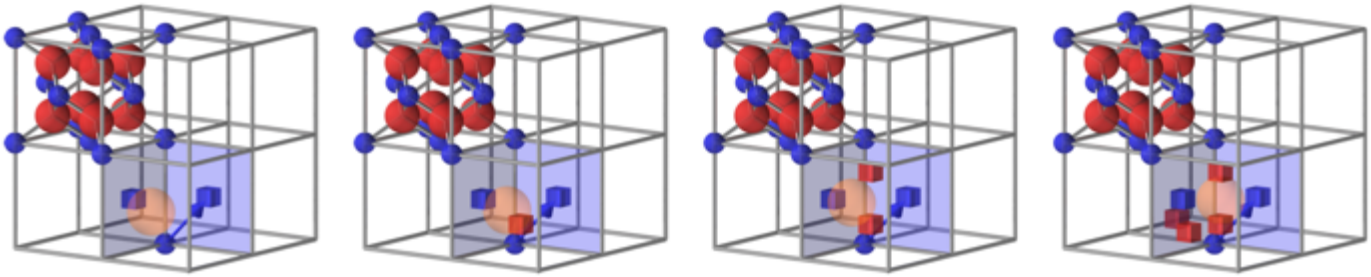


Fission Gas Release

We will now demonstrate how we are improving this model through the use of multiscale modeling and simulation.

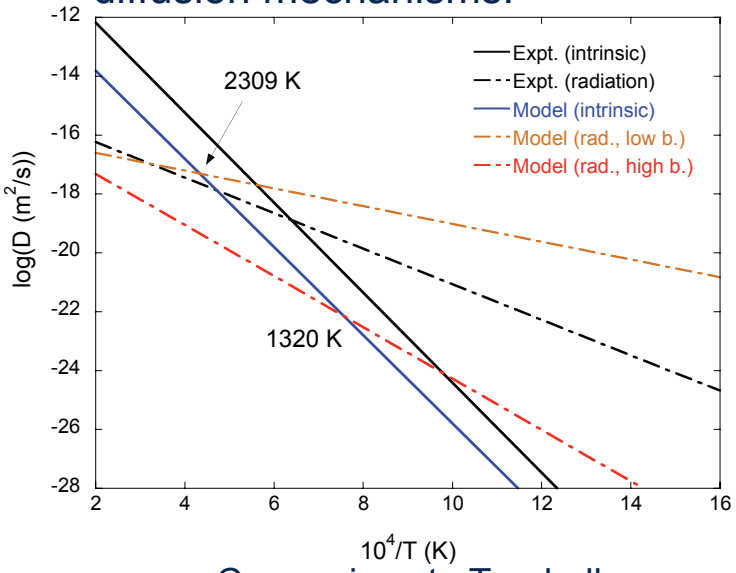
Fission Gas Diffusivity Investigation

- Density functional theory (DFT) is being used to investigate the diffusion constants of fission gas (Xe) in UO_2.

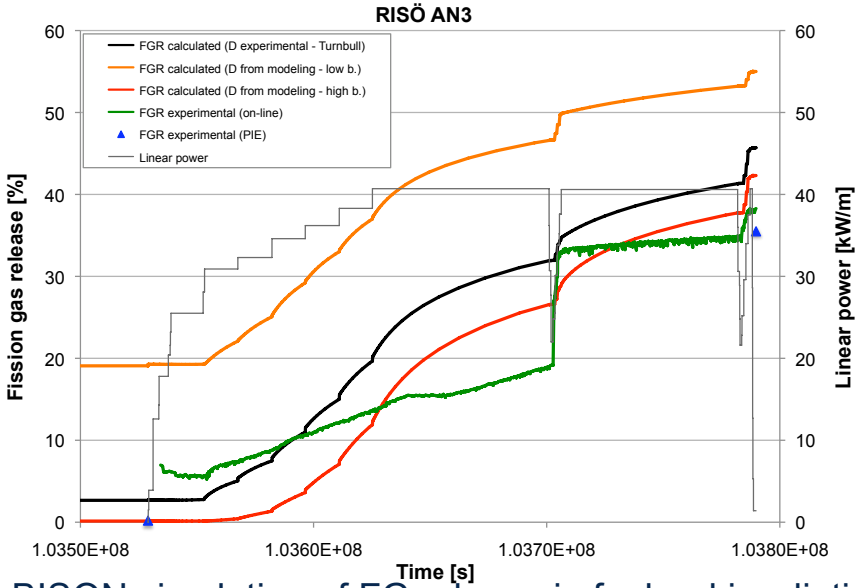


DFT calculations were conducted at LANL

Mechanisms and values of diffusivity are calculated for intrinsic and radiation diffusion mechanisms.



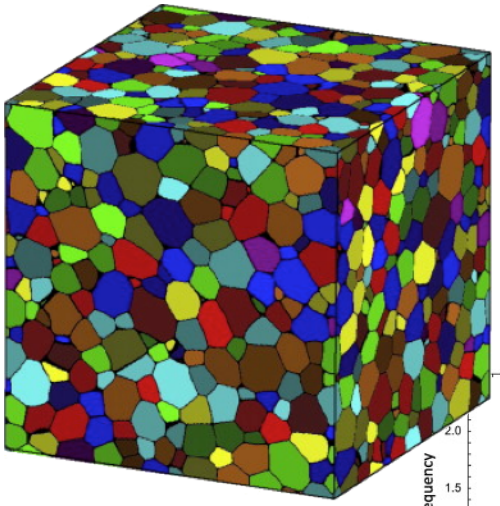
Comparison to Turnbull



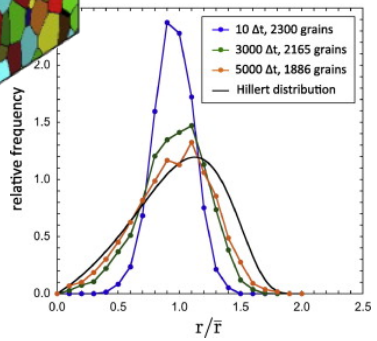
BISON simulation of FG release in fuel rod irradiation experiment from Risö 3 project

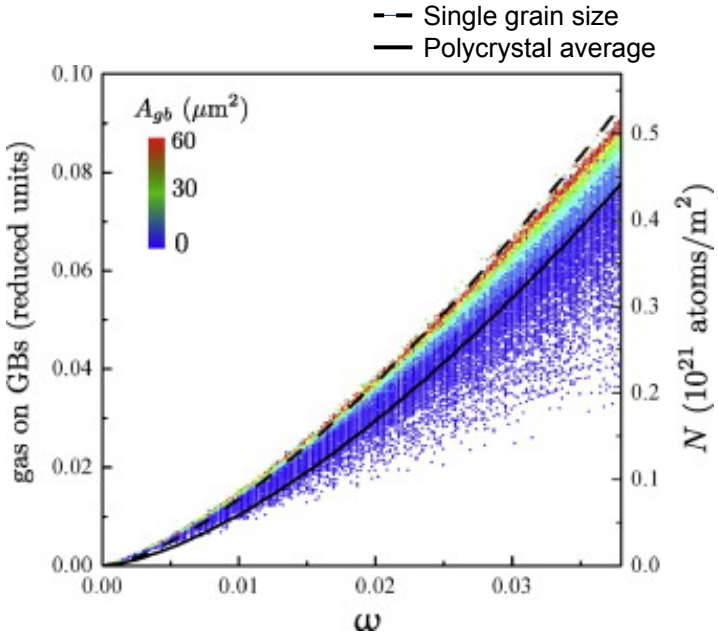
Impact of Grain Size Distribution on Fission Gas

- Typical gas release models assume all grains have the same grain size.
- 3D simulations were used to investigate the impact of the grain size distribution on the fission gas release.



Grain structure created using normal grain growth simulation, giving a more realistic grain size distribution

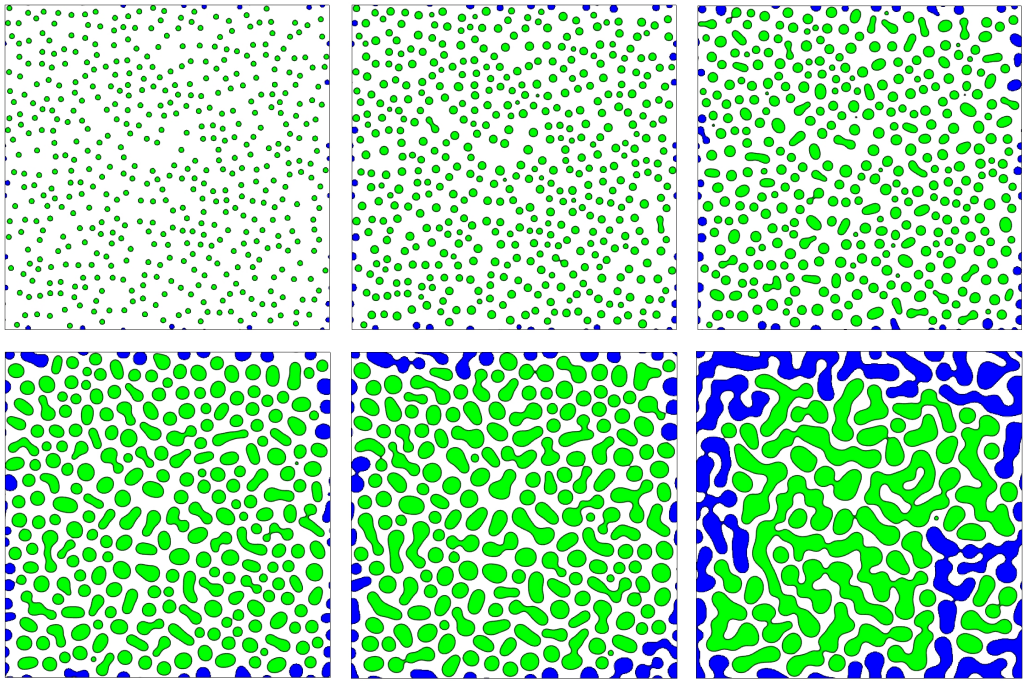


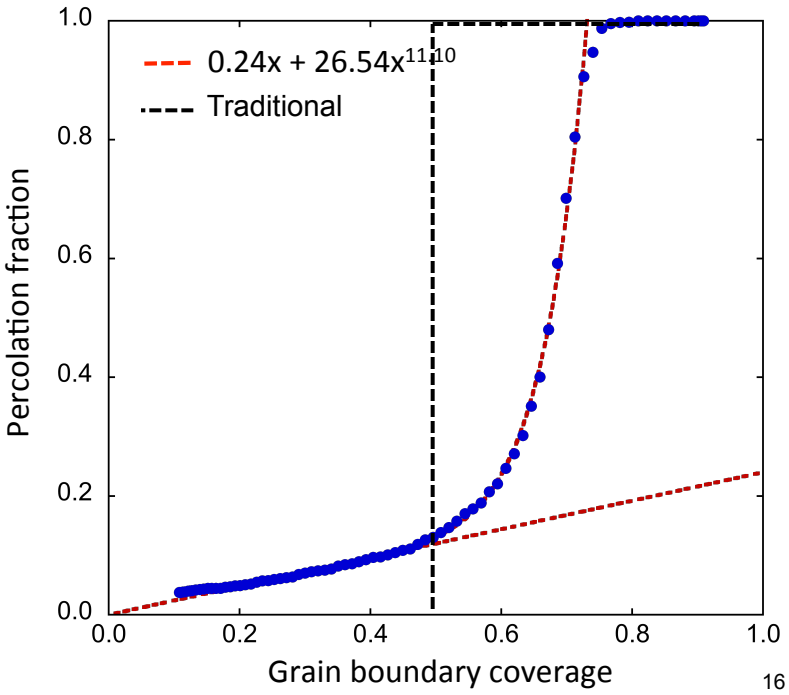


Fission gas migration simulation was conducted in 3D grain structure and the total gas on the GB was compared to the spherical grain model.

Fission Gas Release

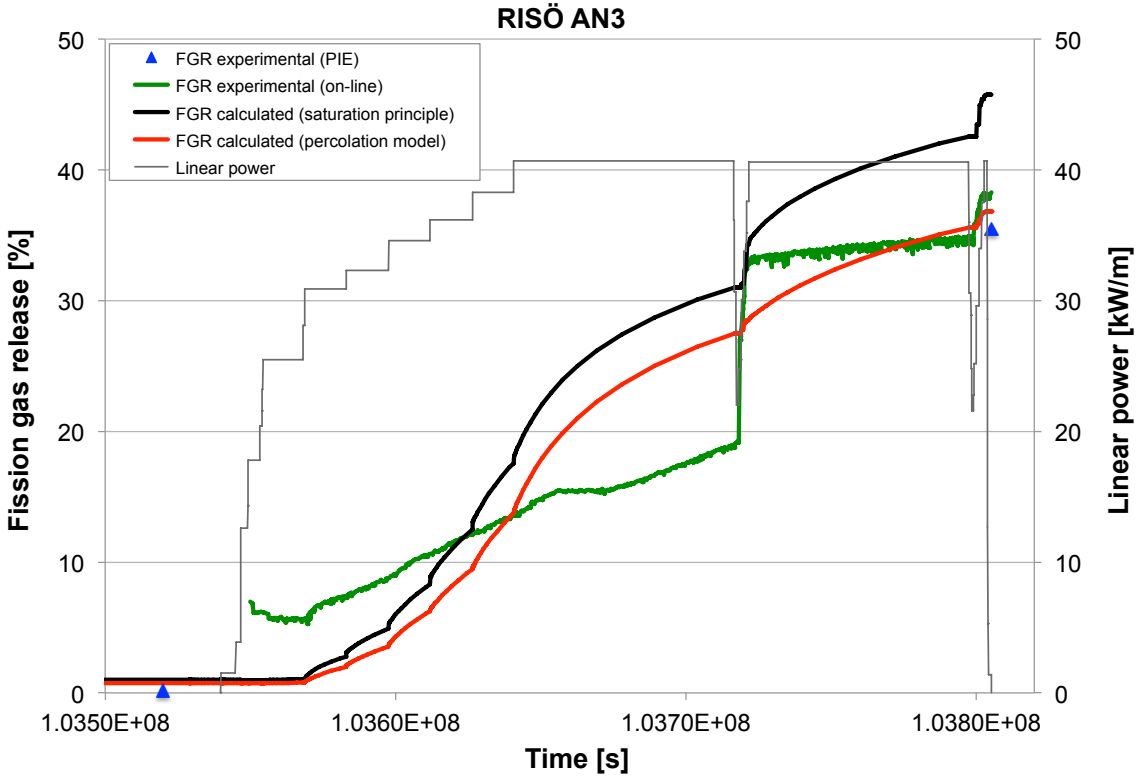
- Existing fission gas release model assumes no fission gas release until the GB fractional coverage reaches 50%. In reality, small amounts of gas are released at much smaller fractional coverages.
- We are using phase field simulations to develop a more realistic description of fission gas release.





Impact on Model Behavior

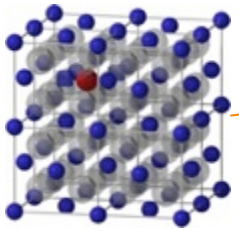
- We modified the fission gas model to consider the mesoscale-informed percolation model and repeated the RISO3 AN3 simulation:

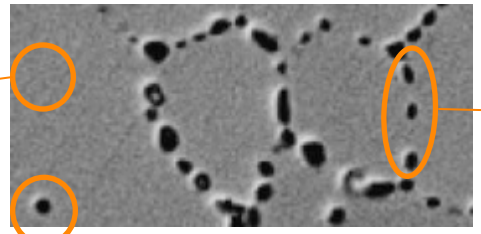


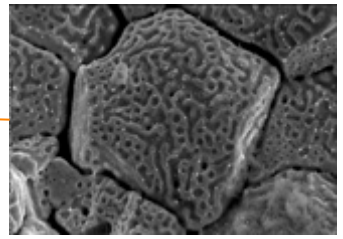
Fission Gas Thermal Conductivity Model

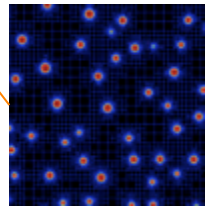
- Accounts for dispersed gas, as well as intra- and intergranular bubbles

MD calculations were conducted at LANL



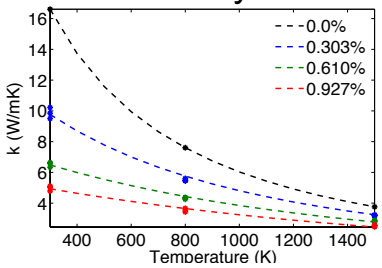


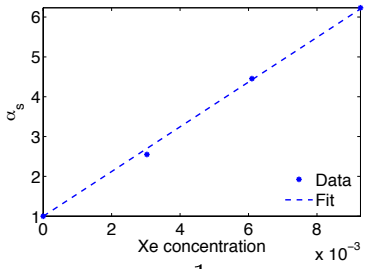




Dispersed fission gas

MD simulations are used to quantify impact of dispersed fission gas on thermal conductivity.





$$k_0' = \frac{1}{7.5408\alpha_s + 17.692t + 3.6142t^2} + \frac{6400}{t^{5/2}} \exp\left(\frac{-16.35}{t}\right),$$

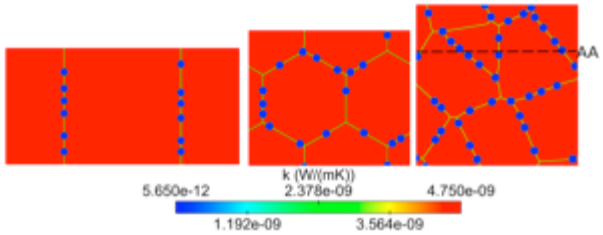
Intragranular bubbles

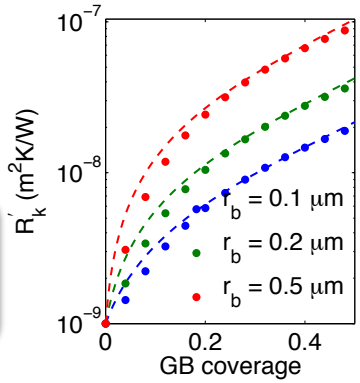
Maxwell-Euken equation used to account for intragranular bubbles:

$$\kappa_{ig} = \frac{1 - p_{ig}}{1 + \frac{p_{ig}}{2}}.$$

The three equations are combined according to: $k = \kappa_{ig}\kappa_{GB}k_0'(T)$

Intergranular (GB) bubbles



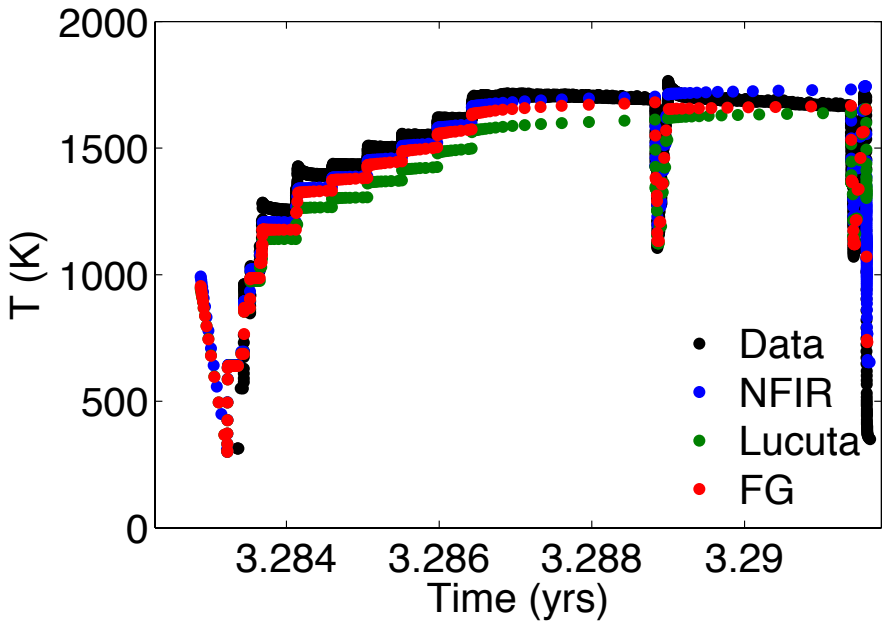


MD and mesoscale heat conduction are used to parameterize constitutive model.

$$\frac{1}{R_k'} = \frac{1}{A_{GB} + A_{bub}} \left(\frac{A_{GB}}{R_k^0} + \frac{A_{bub}}{R_{bub}} \right)$$

Impact of Fission Gas Model Behavior

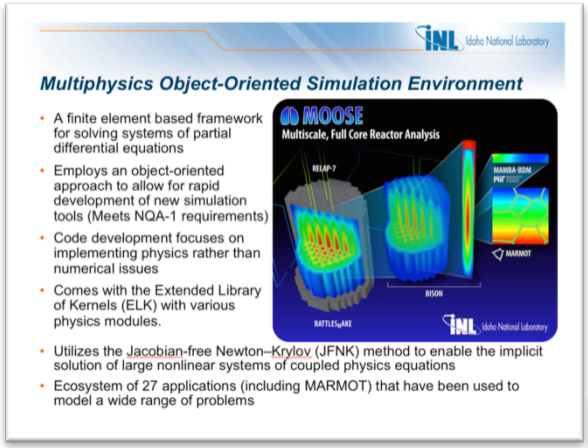
- RISO3 simulation was repeated using our thermal conductivity model coupled to the fission gas release model

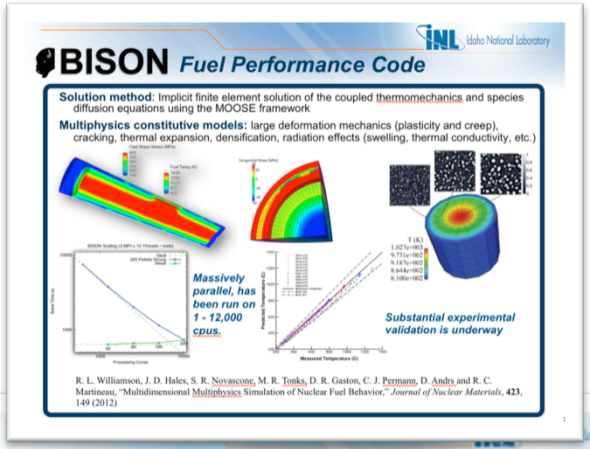


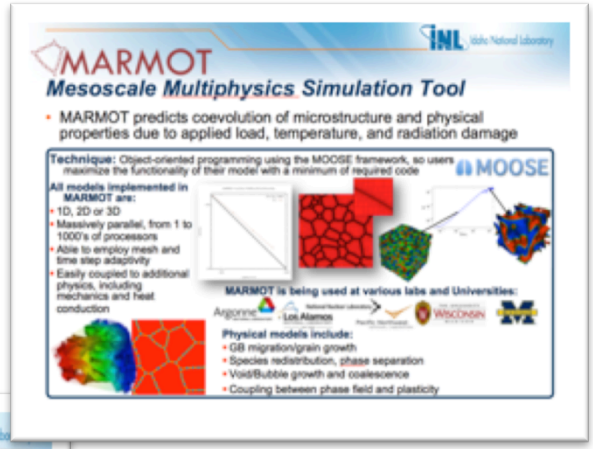
Fuel Centerline Temperature

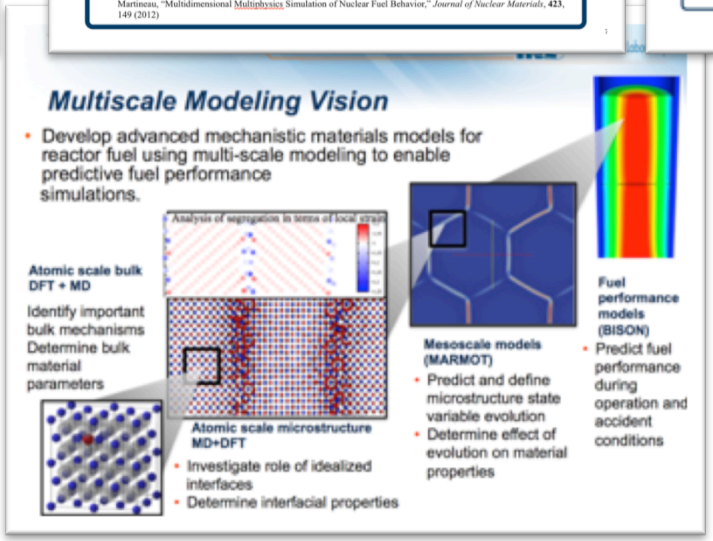
Summary

- MOOSE-BISON-MARMOT provides an advanced fuel performance modeling capability, using multiscale modeling and simulation to develop









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