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Introduction of mesoscale fuel performance modeling tool: MARMOT

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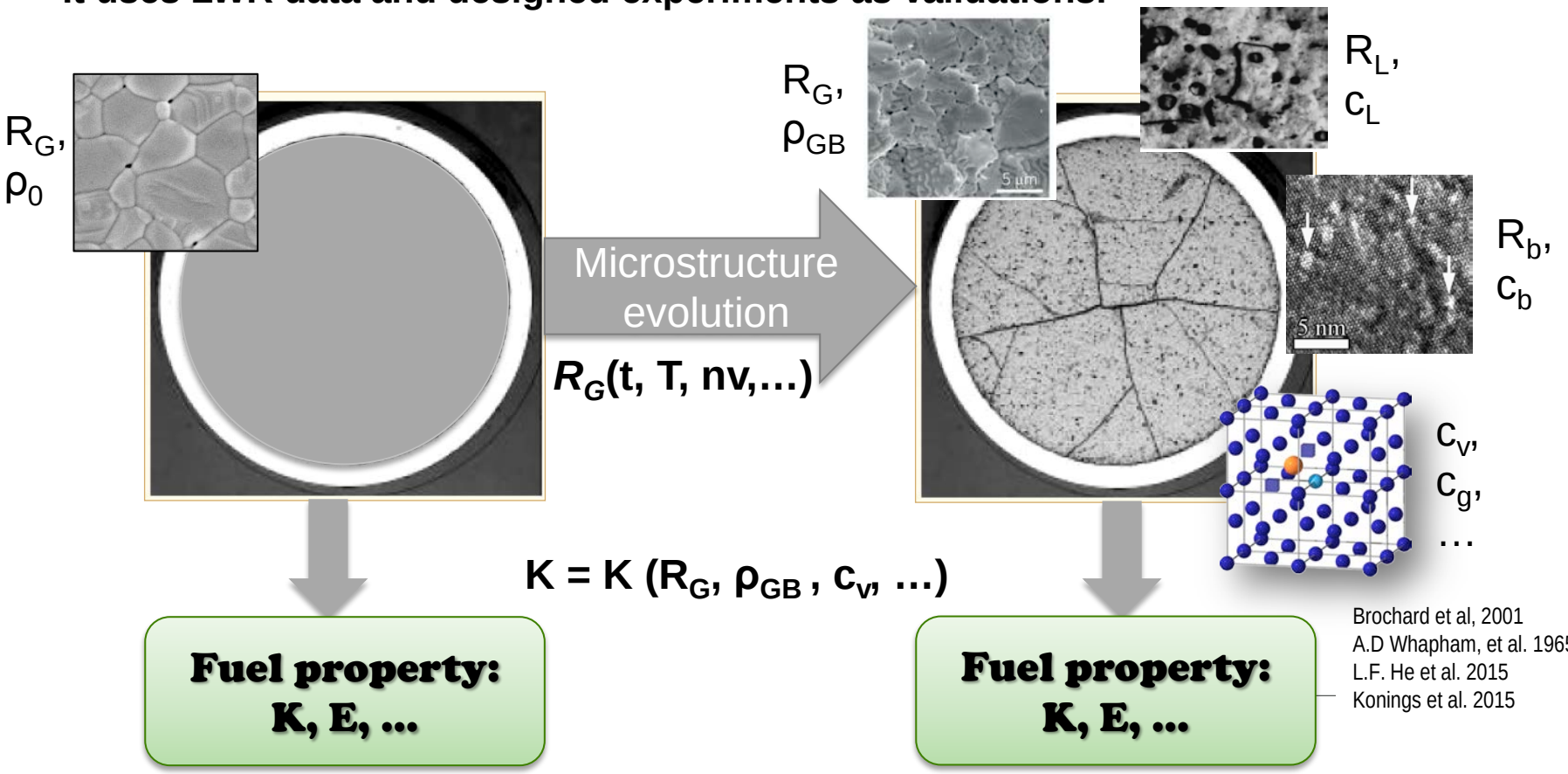
The NEAMS MBM approach: microstructure-based fuel performance modeling

- The MBM approach models the coevolution of microstructure and properties.
- It starts with identifications of state variables to represent microstructure.
- It centers on mechanistic models to evolve microstructure and properties.
- It uses LWR data and designed experiments as validations.



Brochard et al, 2001
A.D Whapham, et al. 1965
L.F. He et al. 2015
Konings et al. 2015

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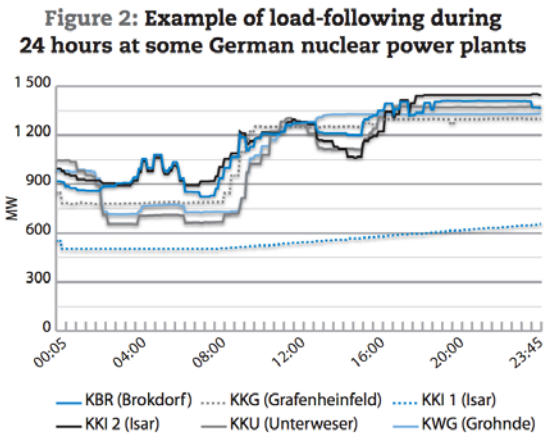
Why MARMOT

- Nuclear fuels and materials experience aging and degradation in extremely harsh environment combining chemistry, radiation, high temperature and high stress.
- This raises tremendous challenge to conventional fuel performance models which are correlated to burnup and temperature, by empirically fitting data for specific fuel types and operation conditions without fully addressing the physics.
- New approaches are desired that are based on common physics to enable explicit considerations of microstructure and operation conditions, therefore applicable for new fuel and reactor types, and various power histories.



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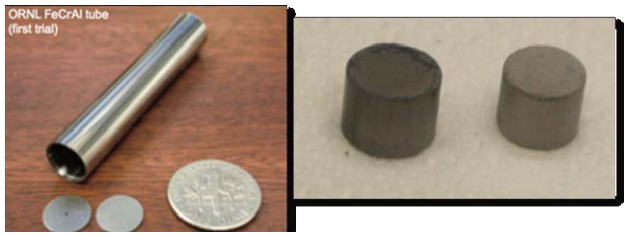
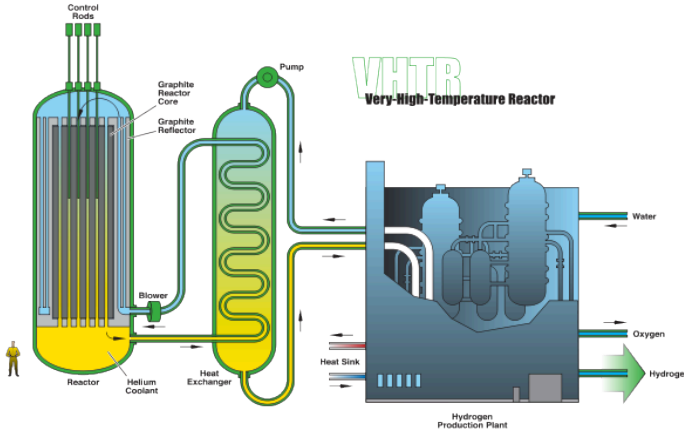


Accident tolerant fuel for LWRs



Next generation nuclear plants

[1] https://www.oecd-nea.org/nea-news/2011/29-2/nea-news-29-2-load-following-e.pdf

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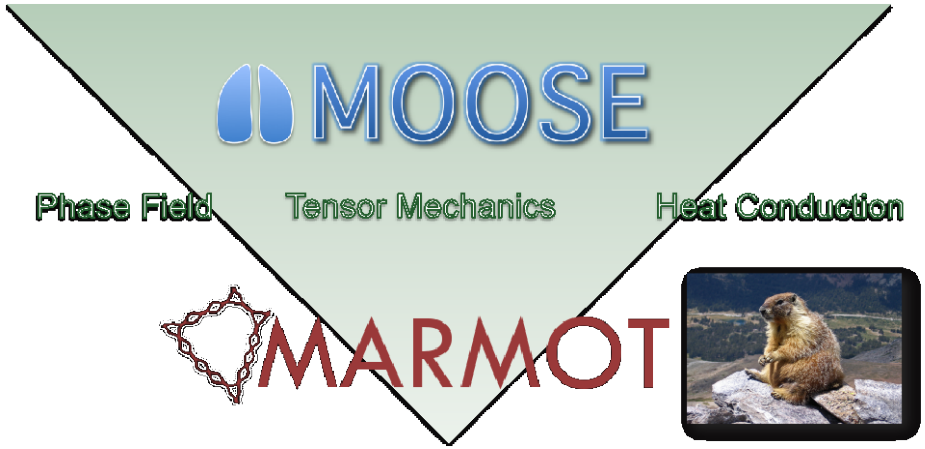
What is MARMOT

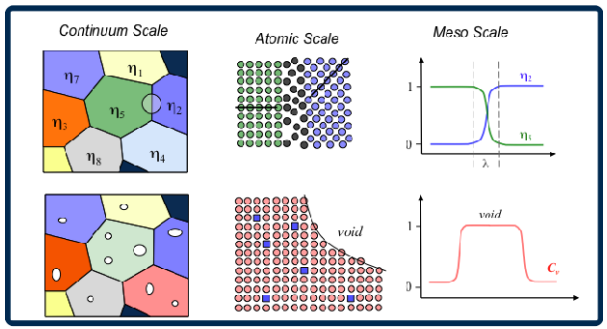
- MARMOT is a MOOSE based application for coevolution of microstructure and properties in nuclear materials.
- Typical MARMOT work involves substantial atomistic efforts using methods such as DFT, MD, TAD, MC etc.



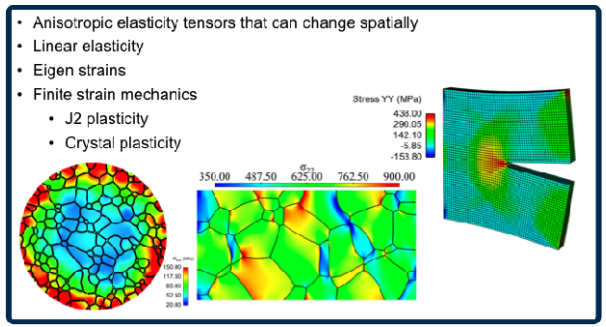
No physics

General capabilities

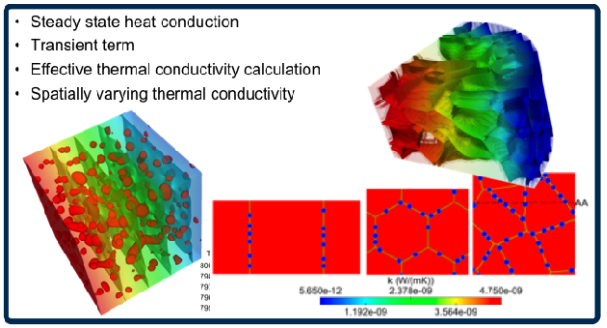
Nuclear-specific material physics



Mass transport
Microstructure evolution



Mechanical deformation



Heat transport

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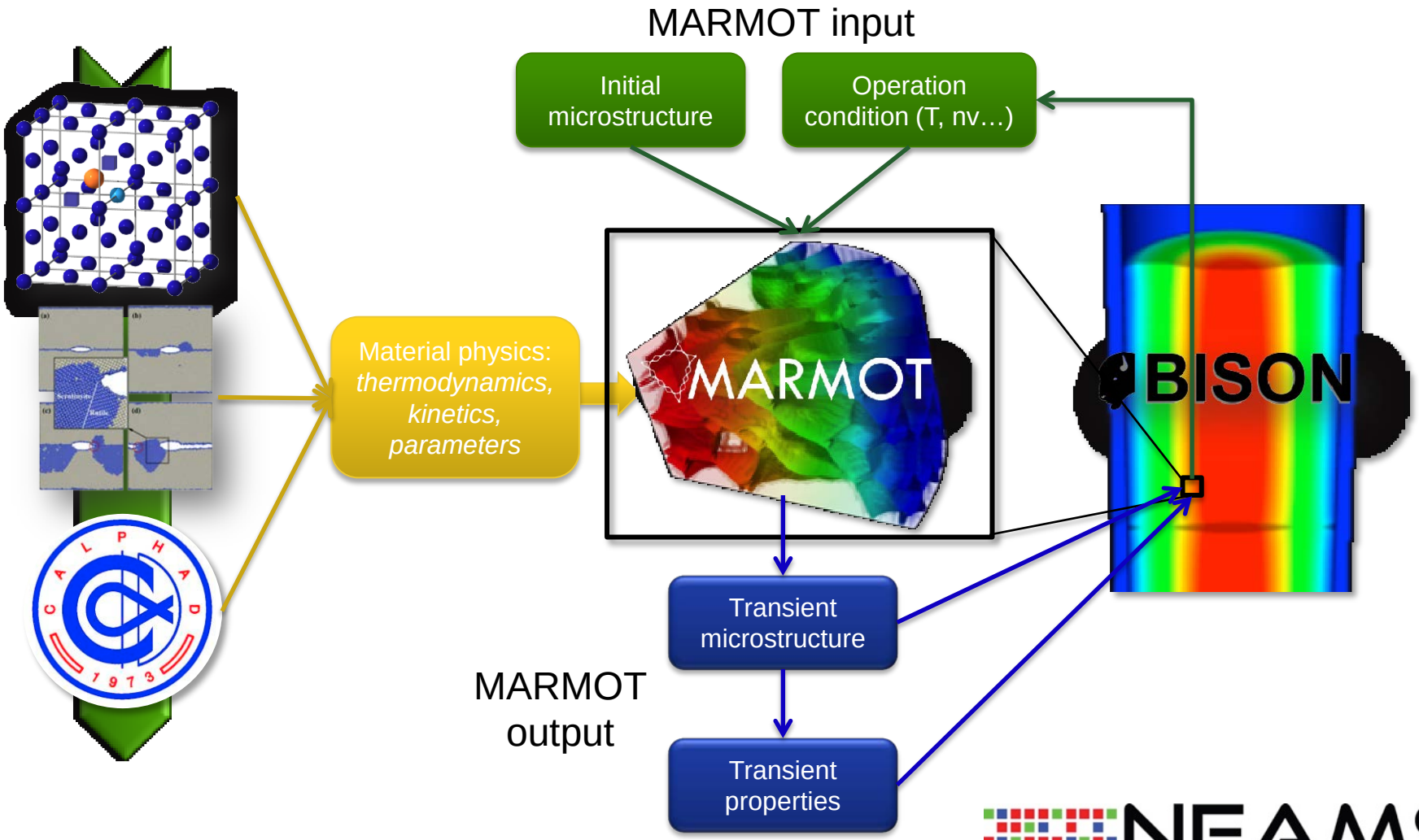
What MARMOT does



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What MARMOT currently has

- **UO2 fuel microstructure/chemistry and deformation:**
  - ***Grain growth***: GB energy and bubble pinning
  - ***Fission products evolution***: swelling, gas release, precipitates
  - Deformation: fracture and creep
  - Radiation damage and restructuring: HBS formation
  - Fuel sintering and densification
- **UO2 structure-property correlation:**
  - ***Thermal conductivity***
  - ***Fracture toughness***
- **Cladding:**
  - Hydrogen transport in Zircaloy
  - Hydride formation and evolution
- **Other fuels:**
  - U3Si2 fuel: gas bubble swelling, heat transport
  - UZr/UMo phase evolution and constituent redistribution

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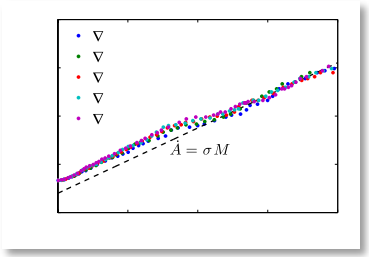
Microstructure evolution example: grain growth

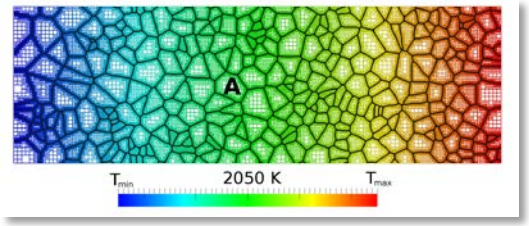
$$\frac{dD}{dt} = k\left(\frac{1}{D} - \frac{1}{D_m}\right)$$

$D(t, P_{DF}(\gamma_{GB}, \Delta T), M(T, c_{im}, \rho), P_r(\rho, r_b, f_c))$

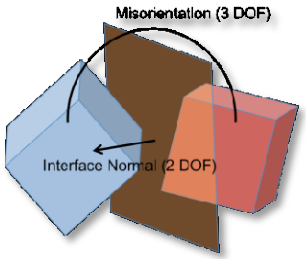
Driving force:

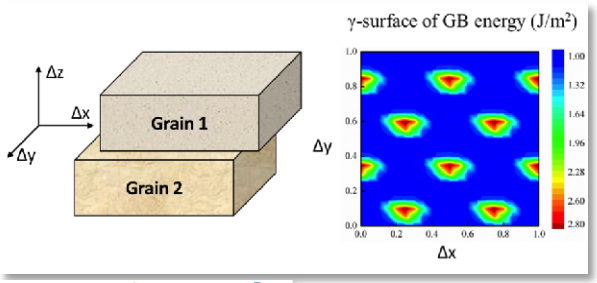
- Competitive driving forces

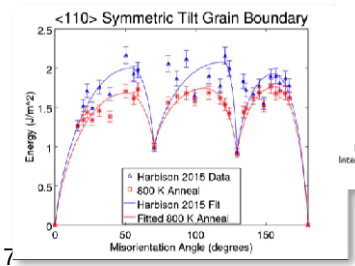


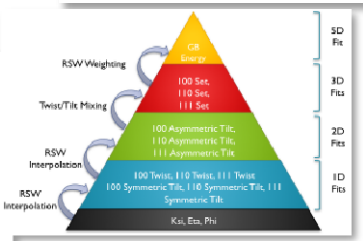


- A 5D GB energy model for UO2

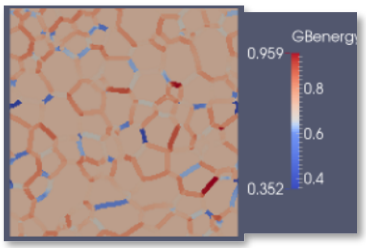








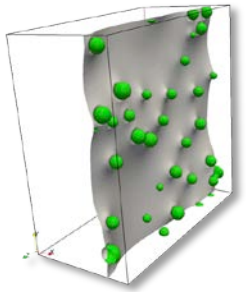
$$\varepsilon = \frac{1+\sum w_{hkl}(d_3)\varepsilon_{hkl}(\xi,\eta,\phi)}{1+\sum w_{hkl}(d_3)}\varepsilon_{RGB}$$

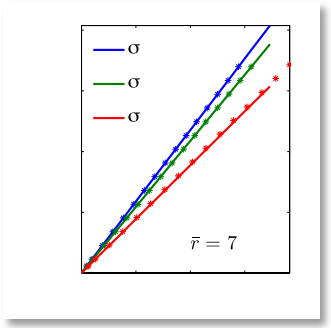


Resistive force:

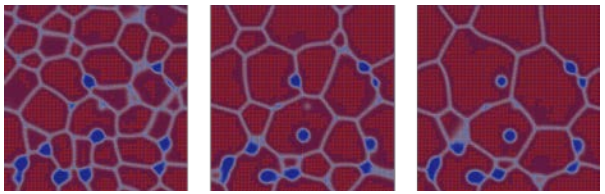
- Pinning of mobile and immobile particles

$$\bar{P}_r^{max} = \left(1 + \frac{\sigma_r^2}{\bar{r}^2}\right)^{-1} W\frac{\gamma_{GB} f_c}{\bar{r}}$$





- Grain growth with evolving porosity



$$\frac{n_p M_b}{2\pi L_{cyl}}[R(t)-R(0)] + \frac{M_p}{2}[R^2(t)-R^2(0)] = -\gamma_b M_b M_p t\,.$$

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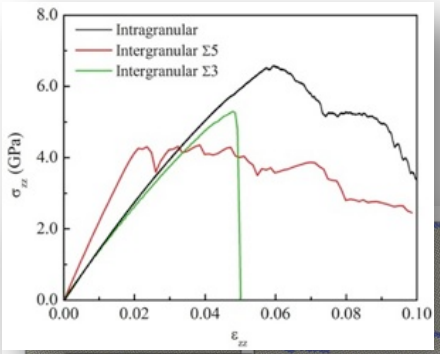
Structure-property relationship example: fracture toughness

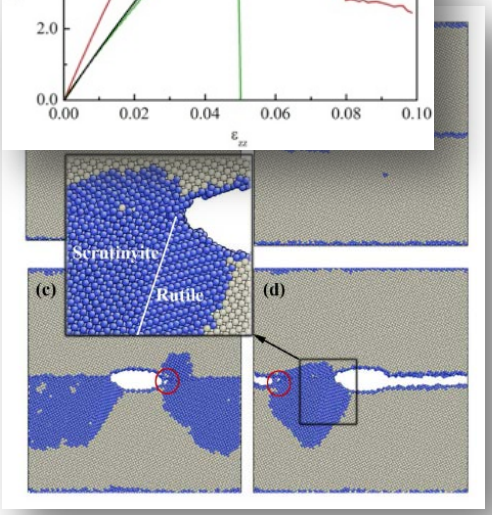
- Fuel fracture impacts thermal transport and fission gas release
- It is impacted by temperature, stress, grain size d, and grain boundary fractional coverage f_c

Fracture Stress

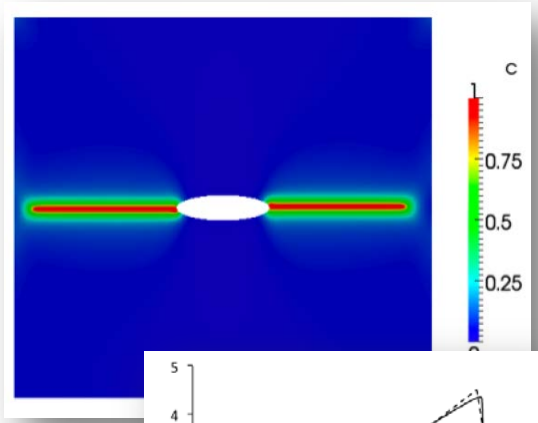
$$\sigma_f(G_c, f_c, D)$$

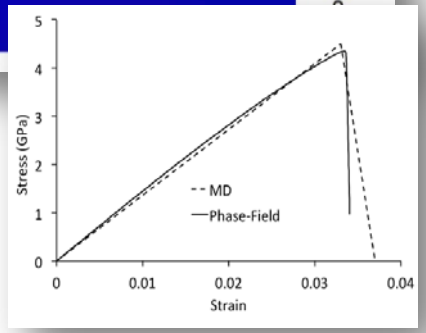
Fracture Energy from molecular dynamics



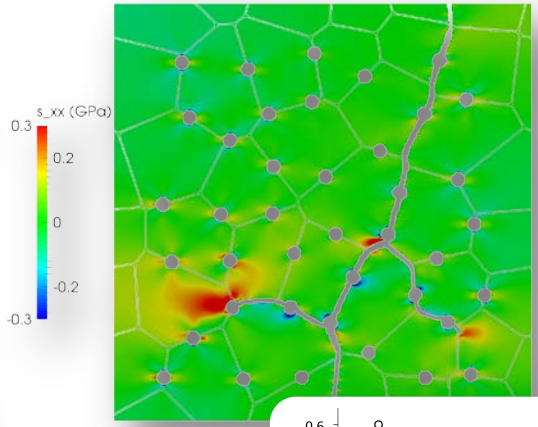


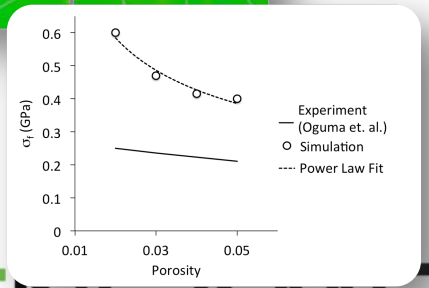
Parameterization of phase field fracture





Impact of microstructure: fractional coverage and grain size





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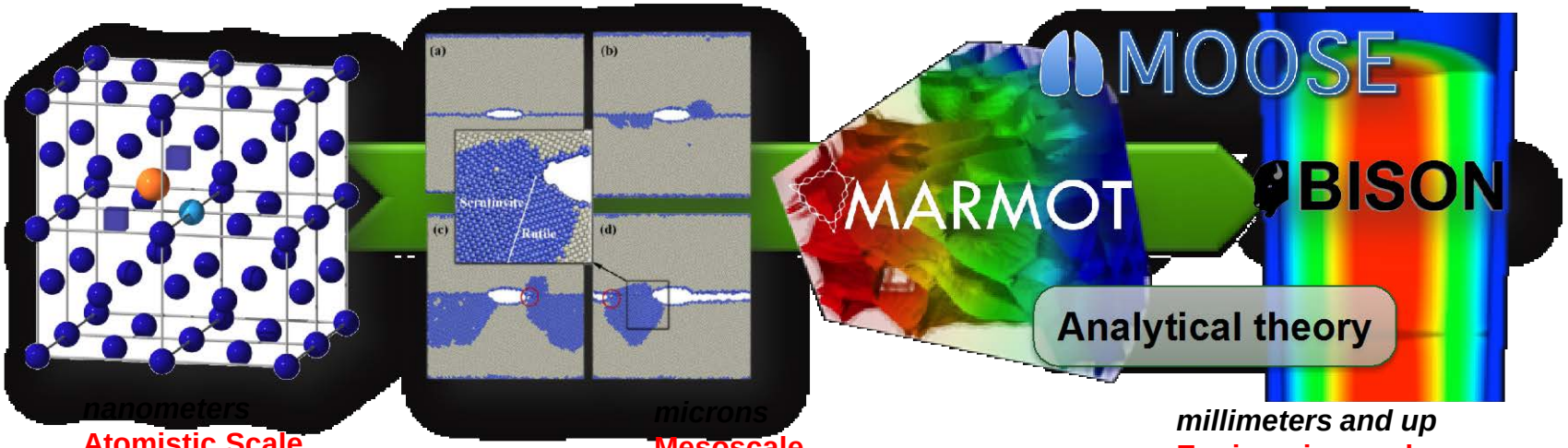
MARMOT validations

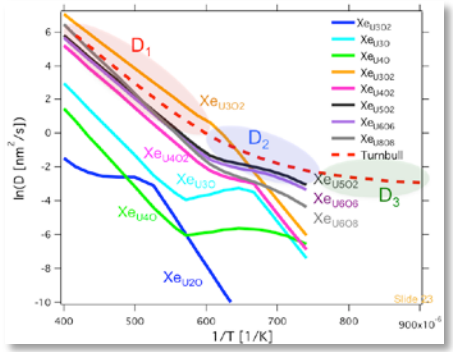
- MARMOT can be validated at different levels and scales, by using reactor operation data and well-designed experiments.
- Validations are being pursued within NEAMS and via NEUP projects.



nanometers

Atomistic Scale

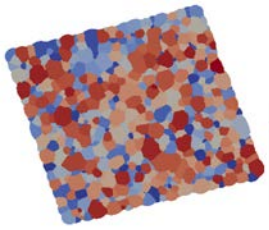
- Parameter measurements
- High resolution characterization



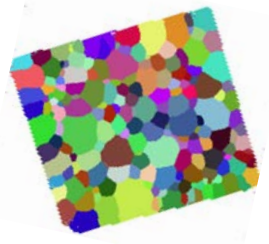
microns

Mesoscale

- Microstructure characterization
- Property measurement



Simulation

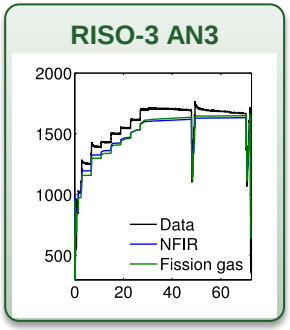


Experiment

millimeters and up

Engineering scale

- Reactor data



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Quality assurance and computation needs

- Similar to BISON, MARMOT follows the QA procedure adopted for MOOSE applications.
- A rigorous review and regression process is applied for new code implemented.
- Extensive tests are available to cover over 85% of all code.

- MARMOT can be run on any Linux / macOS installation. Depending on the complexity of the problems, parallel simulations on high performance computing facilities or serial run on single CPU may be utilized.

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Access, training and support

- **A licensing process is on going, after which a standard way of obtaining access will be worked out.**
- **At this moment, contact Daniel Schwen at daniel.schwen@inl.gov for MARMOT access.**
- **A public MARMOT website is under construction. https://moose.inl.gov/AnimalsPortal/**

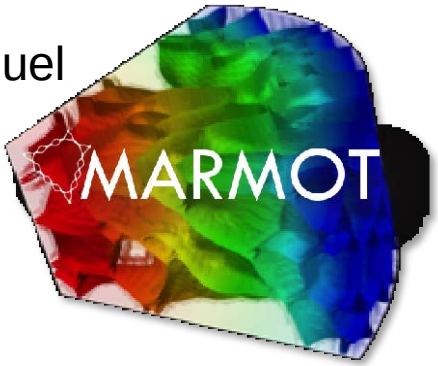
- **Training is provided regularly, usually held with MOOSE training.**
  - March 2015, Orlando
  - June 2015, Idaho Falls
  - February 2016, Nashville
  - April 2016, KAPL

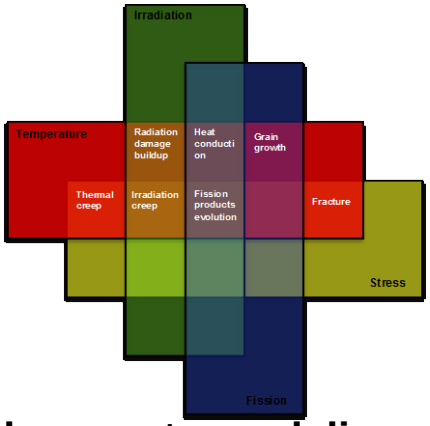
- **Support is available via the MOOSE user group (moose-users@googlegroups.com) since MARMOT relies heavily on the MOOSE modules.**

How MARMOT may help to resolve some gaps

- **FR: Atomistic modeling tools for fuels and materials. (See David's talk)**
- **FHR: High-fidelity simulation of key degradation mechanisms for structures and fuels that limit life and determine replacement frequency.**

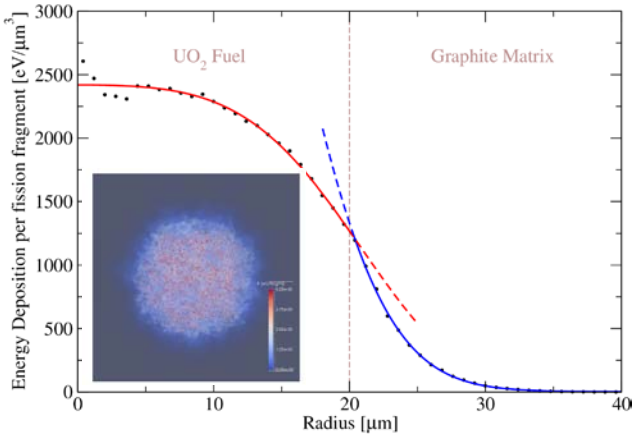
Fuel

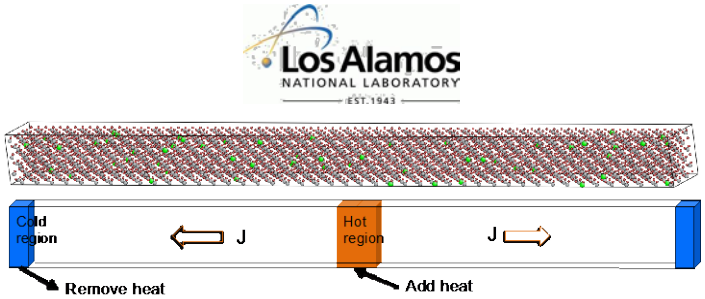




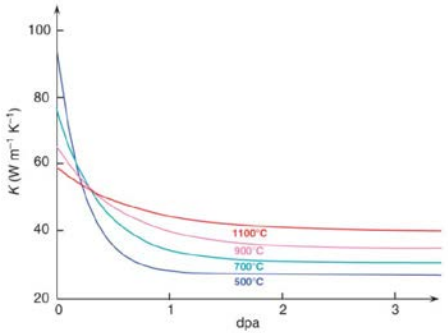
Structural materials

- **HTGR: Graphite material property modeling coding as a function of temperature and dose is required for prediction of graphite life time**





Bonal JP et al., MRS Bulletin, 34, 28-34, 2009



RAM

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Summary

- MARMOT is a mesoscale tool for materials aging and degradation in harsh environments. It is an excellent example of integrating lower-length-scale physics for engineering scale material responses.
- MARMOT focuses on the development of materials models that describe microstructure evolution and structure-property correlation.
- So far the development has focused on oxide fuels in LWRs. But the general capabilities have great potential to be extended to other fuels or materials, particularly those without sufficient operating data.
- The development of MARMOT has led publications of over 30 journal publications.
- MARMOT currently has users from over 20 institutes.

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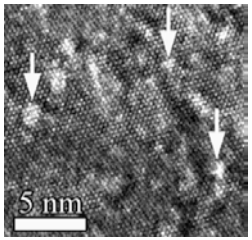
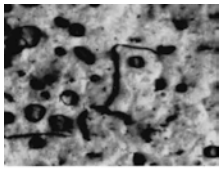
What MARMOT does: the more complex reality

Adapted from Rashid (2011) and Beyer et al. (1975)

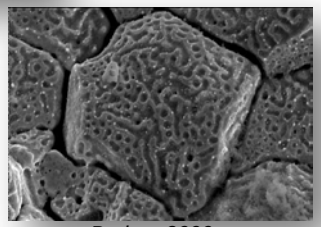
L.F. He et al. 2015



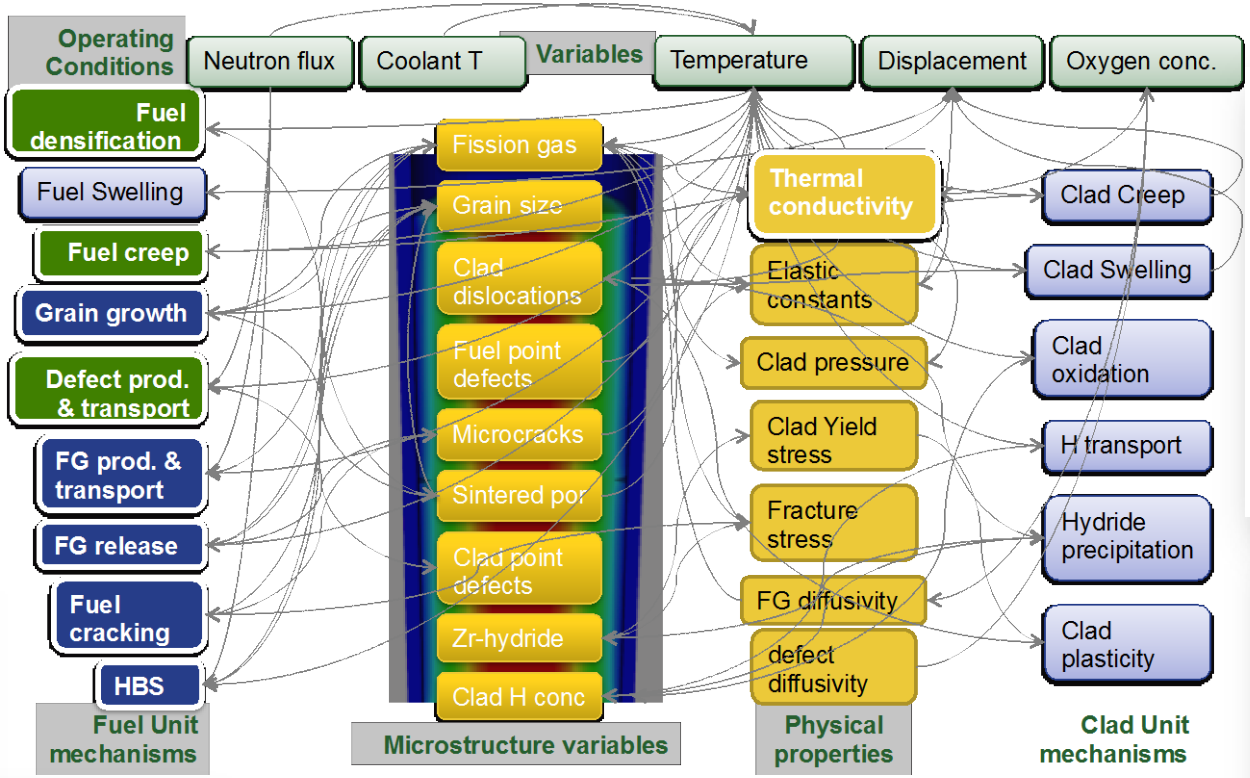
A.D Whapham, et al. 1965



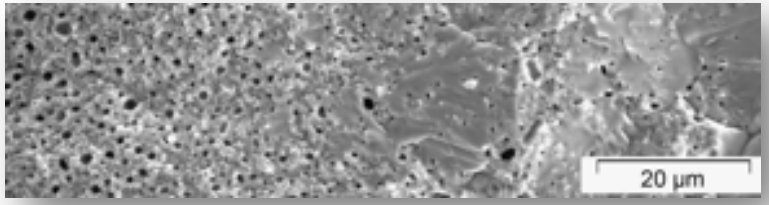
Brochard et al, 2001



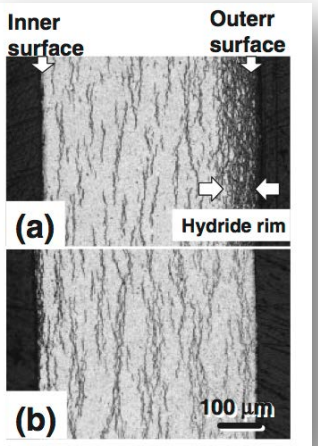
Brohan 2000

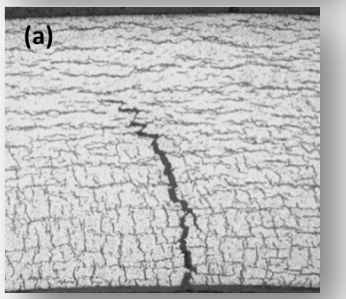


J. Noirot et al. 2008



From Nagase and Fuketa, 2005





Chu et al., 2008