U.S. DEPARTMENT OF ENERGY | Nuclear Energy

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program

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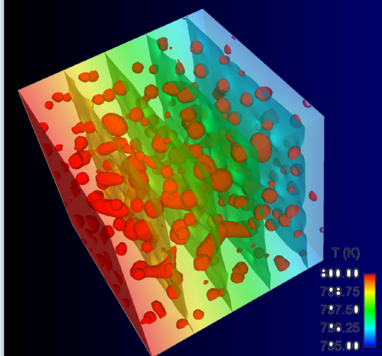
NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

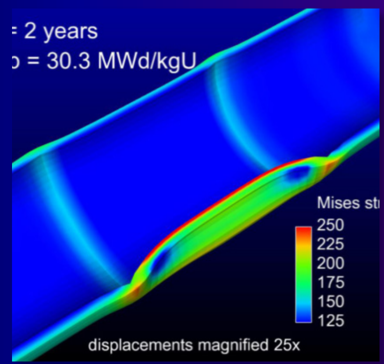
Presented at the 12th Annual Materials Modeling and Simulation for Nuclear Fuels Meeting
University of Chicago
October 15, 2013

What is NEAMS?

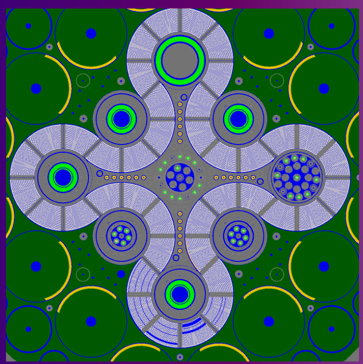
*The NEAMS Pellet-to-Plant Simulation Toolkit***



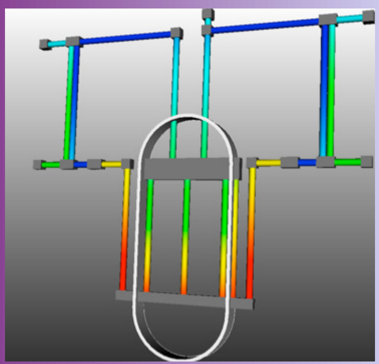
MARMOT (Pellet)



BISON (Pin)



SHARP (Core)



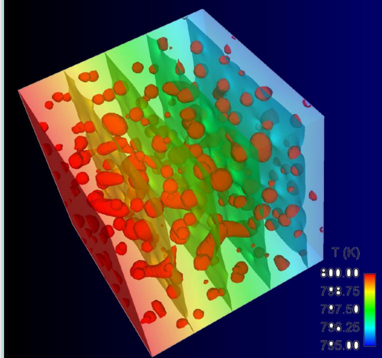
RELAP-7 (Plant)

Objective	Develop and validate predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems.
Value Proposition	The NEAMS Pellet-to-Plant ToolKit will provide insights that cannot be achieved through experimentation alone.

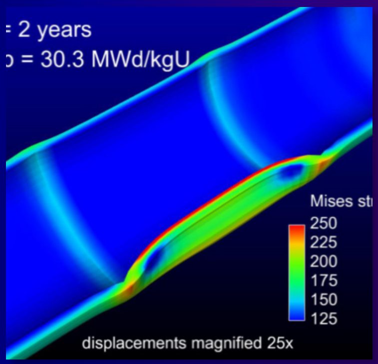
***Pellet-to-Plant = Fuel Performance + Reactor Performance + Balance of Plant*

We manage NEAMS as two connected product lines

Fuels Product Line

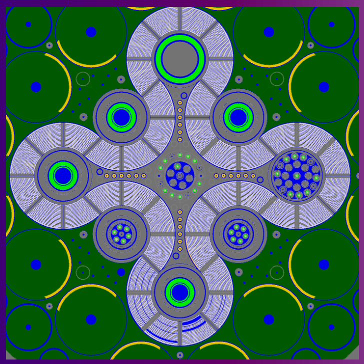


MARMOT (Pellet)

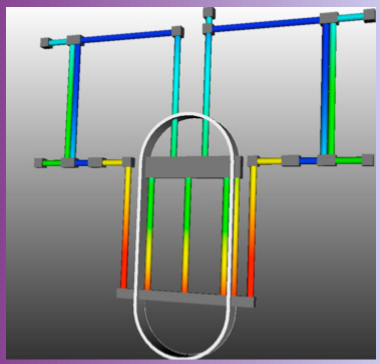


BISON (Pin)

Reactors Product Line



SHARP (Core)



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Fuels Product Line

Fuels Challenge Problems

- **For a full-size fuel pin, predict cladding integrity during steady-state reactor operation and anticipated, operational transients**

① **Oxide fuel in LWR (UO_2 in Zircaloy cladding)**

- ☑ Fuel swelling/fission gas release
- ☑ Cladding creep
- ☑ Pellet-cladding mechanical interaction
- ☑ Cladding corrosion/hydriding
- ➔ **Failure prediction** (with uncertainty estimate)

Champion: **Industry/CASL**

② **Metallic/oxide fuel in SFR (U-Pu-Zr/MOX in SS cladding)**

- ☑ Restructuring, constituent redistribution, solid fission product transport
- ☑ Fuel swelling/fission gas release
- ☑ Cladding creep
- ☑ Fuel-cladding mechanical interaction
- ☑ Fuel-cladding chemical interaction
- ➔ **Failure prediction** (with uncertainty estimate)

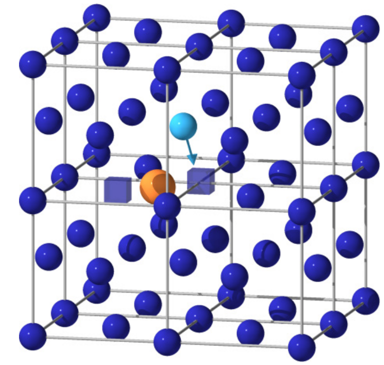
Champion: **FCRD**

Example of multiscale approach: fission gas release

- **Various methods employed at different scales to investigate the different stages of FG release:**
  0. Diffusion of individual FG atoms in bulk UO_2+nucleation growth and resolution of intergranular bubbles.
  1. Xe segregation, clustering and bubble nucleation
  2. Bubble growth and coalescence
  3. Percolation in polycrystalline networks

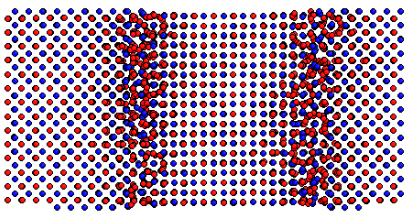
DFT and molecular dynamics

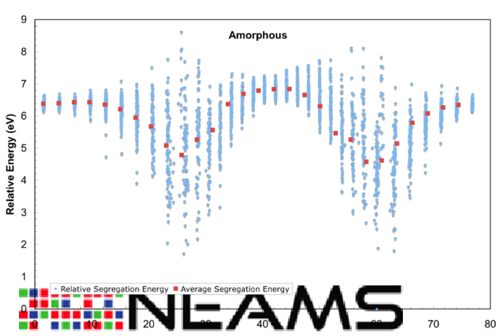
0.



Molecular dynamics

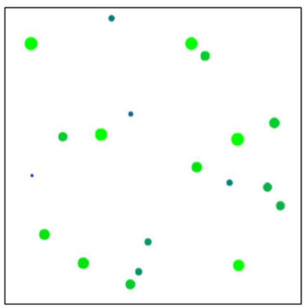
1.





Kinetic Monte Carlo

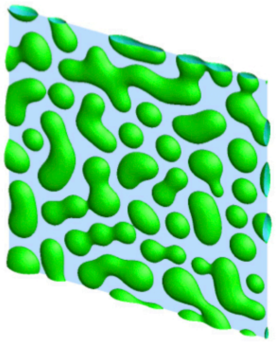
1.



Xe clustering vs. UO_2 boundary type

Phase Field Modeling

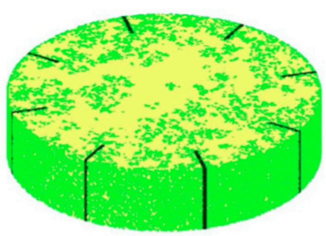
2.



Bubble growth and coalescence

Percolation Analysis

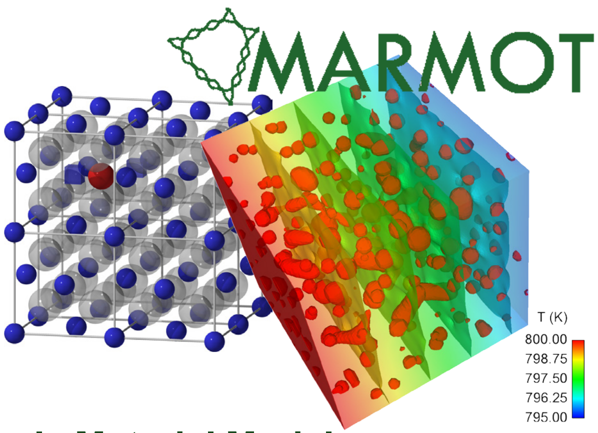
3.



Percolation in polycrystalline networks

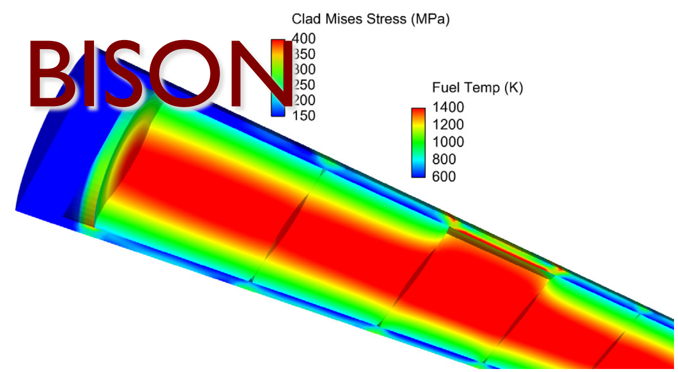
MBM: MOOSE-BISON-MARMOT

- **MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability**



Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models



Engineering-scale Fuel Performance Tool

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

MOOSE

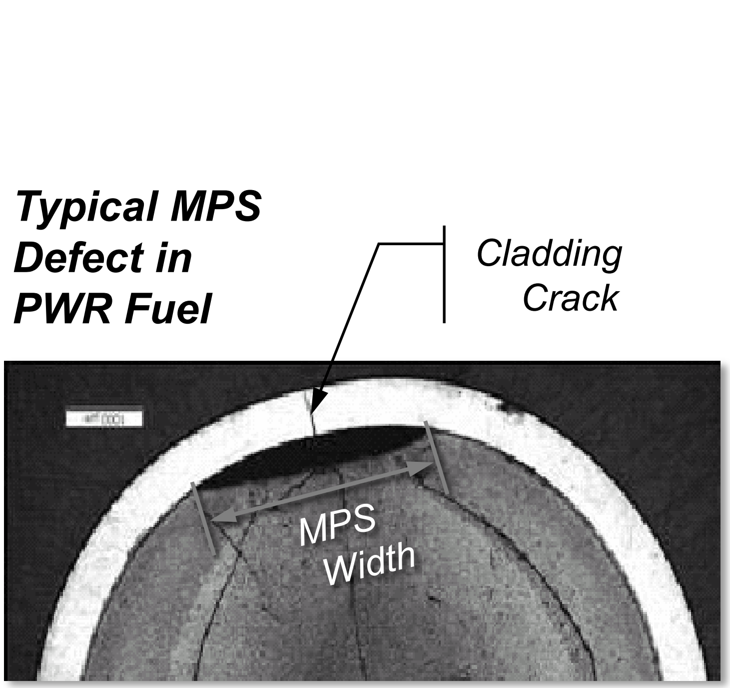
Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

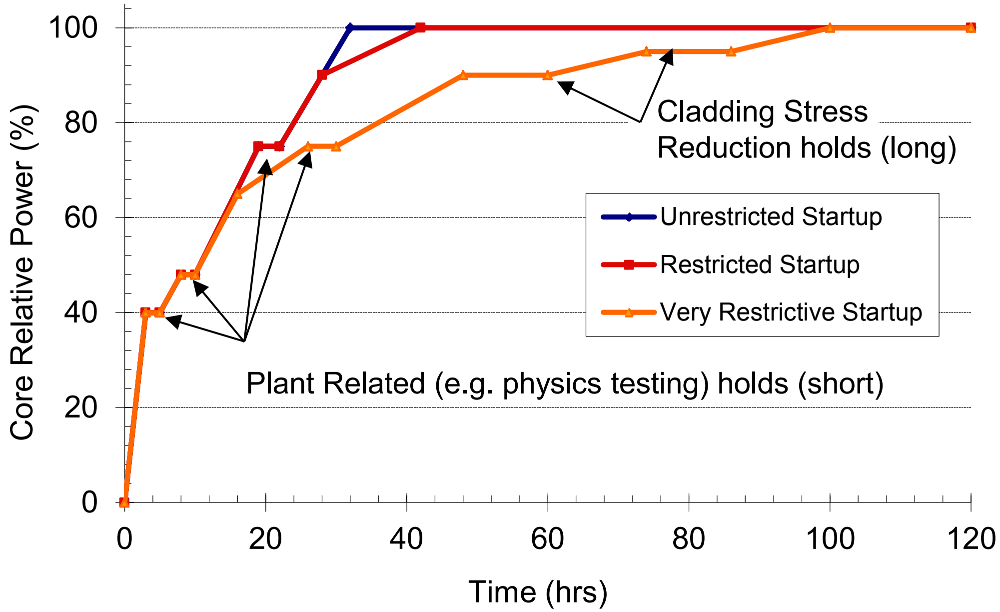
CHALLENGE PROBLEM: Missing Pellet Surface

- Missing Pellet Surfaces (MPS) cause cladding failure
- Increase in hoop stress outpaces thermal relaxation
- Causes reactor power-up restrictions
- **BISON** used to investigate MPS behavior in **3D** –

Typical MPS Defect in PWR Fuel

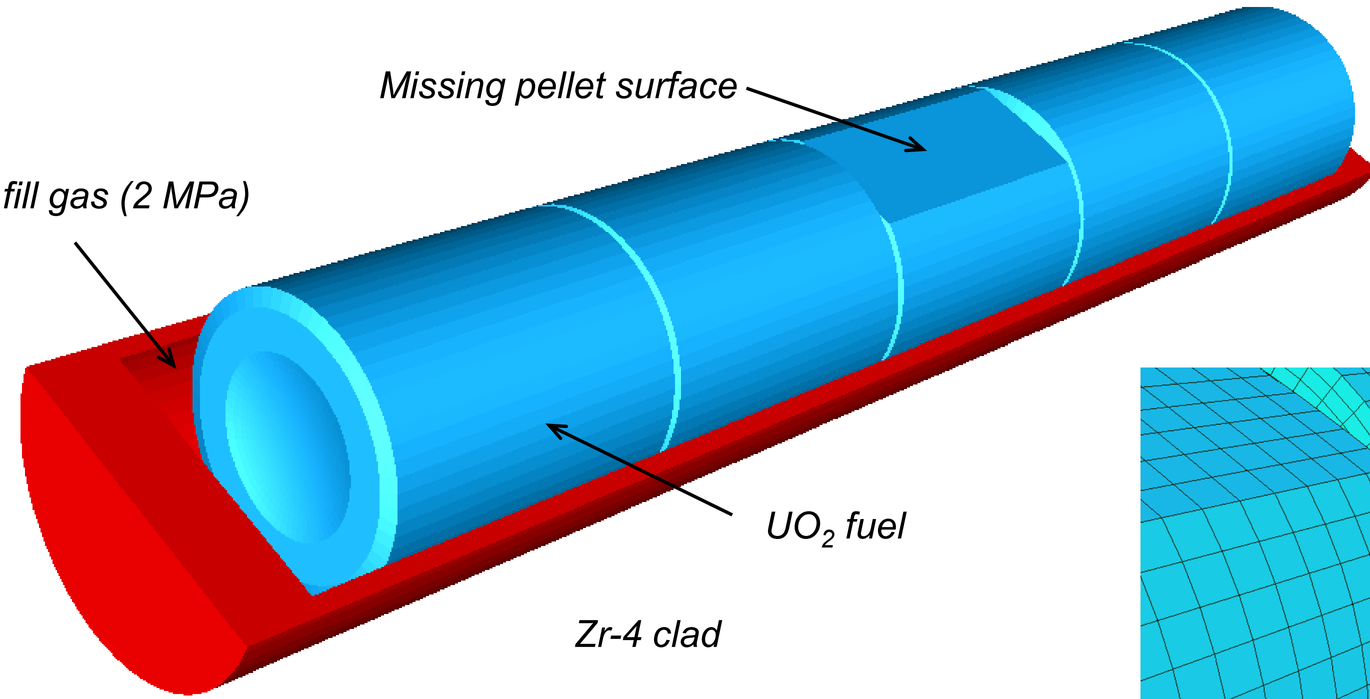


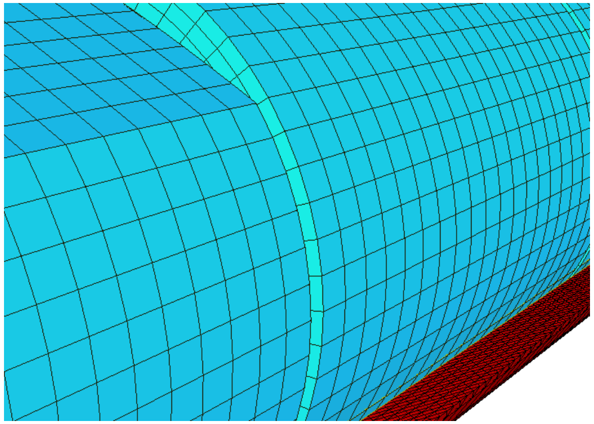
Reactor Power-Up Restrictions



Figures from Robert Montgomery (Anatech/PNNL)

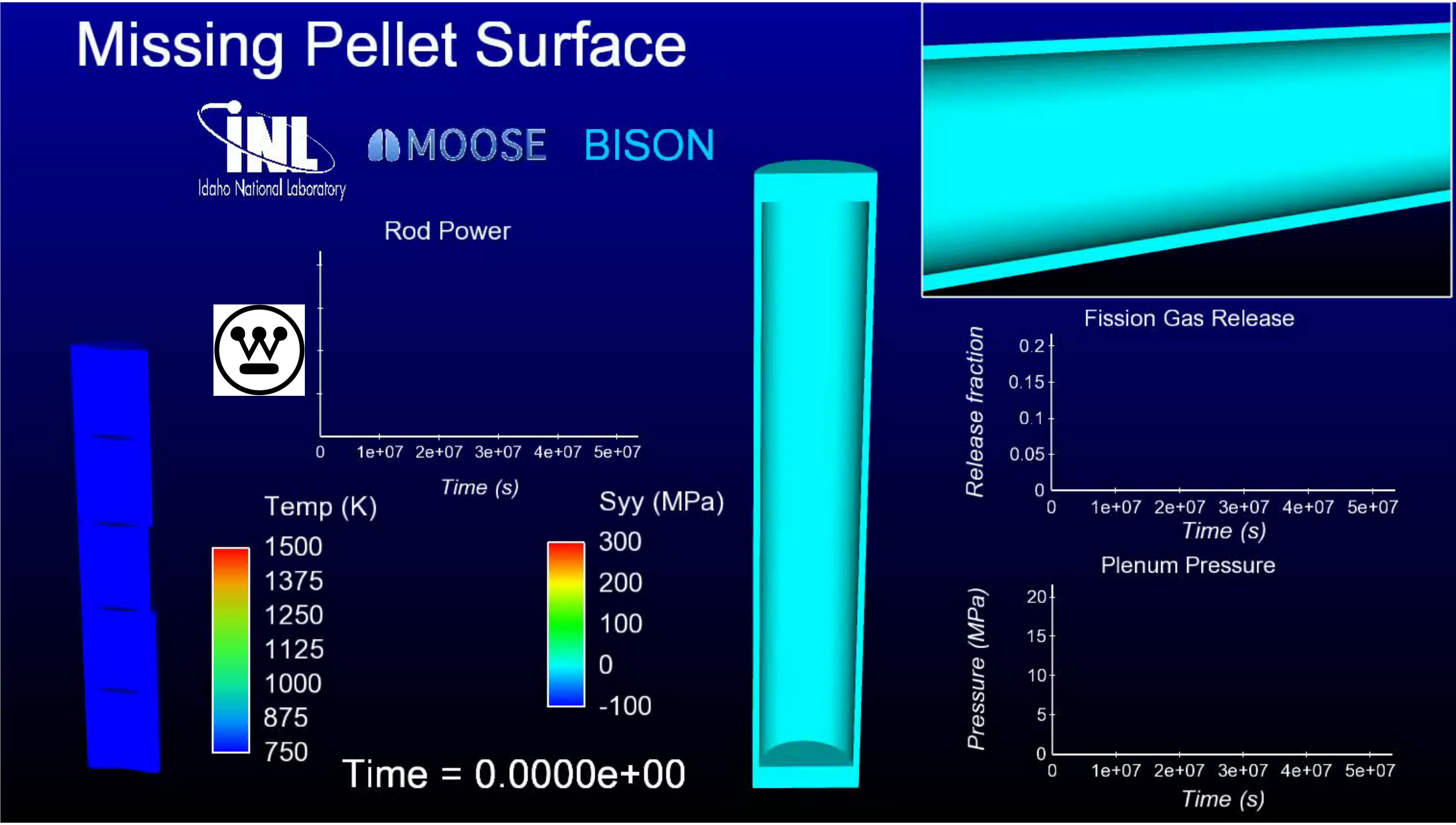
BISON Analysis of a Missing Pellet Surface





- Defective (MPS) pellet placed midway between four intact pellets
- High resolution **3D** calculation (250,000 elements, 1.1×10^6 dof) run on 120 processors
- Simulation from fresh fuel state with a typical power history, followed by a late-life power ramp

Effect of a Missing Pellet Surface



Unvalidated tools are worse than useless

- **Versatile tools must be validated for specific applications**
- **We are already validating**
- **End user participation is critical**
- **Validation is expensive, time-consuming**
- **But it is essential**
- **Plans are underway to further codify DOE/NE's approach**

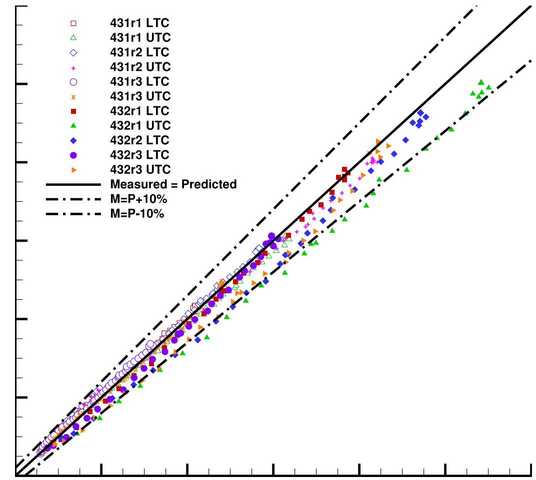
Validation = the process of certifying that the tool represents real world behavior in the regime it was intended

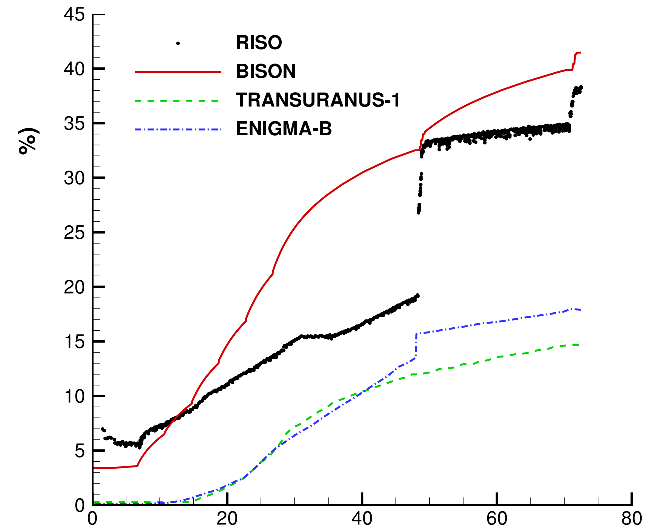
Current **BISON** Validation Activities

- **To date, focus of BISON validation activities has *primarily* been on:**
  - Experimental data sets (88 pins) used for Assessment and Validation of FRAPCON (**not** a comparison with FRAPCON code predictions, but with the experimental data used to validate the FRAPCON code)
  - Includes instrumented fuel pins with steady-state <u>and</u> ramp data relevant to:
    1) Fuel centerline temperature
    2) Fuel restructuring
    3) Gap conductance
    4) Fission gas release
    5) Pellet-cladding mechanical interaction
    6) Cladding elongation
  - Value in assessment against well-known, well-accepted (by NRC) experimental data

Experiment	Rod	FCT - BOL	FCT – TL	FCT - Ramps	FGR	Clad - Elong	Clad – Dia (PCMI)
IFA-431	[illegible]	X					
IFA-432	1, 2, 3	X					
IFA-513*	1, 6	X	X				
IFA-515.10	[illegible]	X	X				
IFA-597.3	7			X		X	
IFA-597.3*	8			X			
RISO-3*	AN3			X	X		
RISO-3*	AN4			X	X		
FUMEX-II	27(1)				X		
FUMEX-II	27(2a)				X		
FUMEX-II	27(2b)				X		
FUMEX-II	27(2c)				X		
RISO-3	GE7						X
OSIRIS	J12						X
REGATE							X
IFA-431 (3D)	4	X					

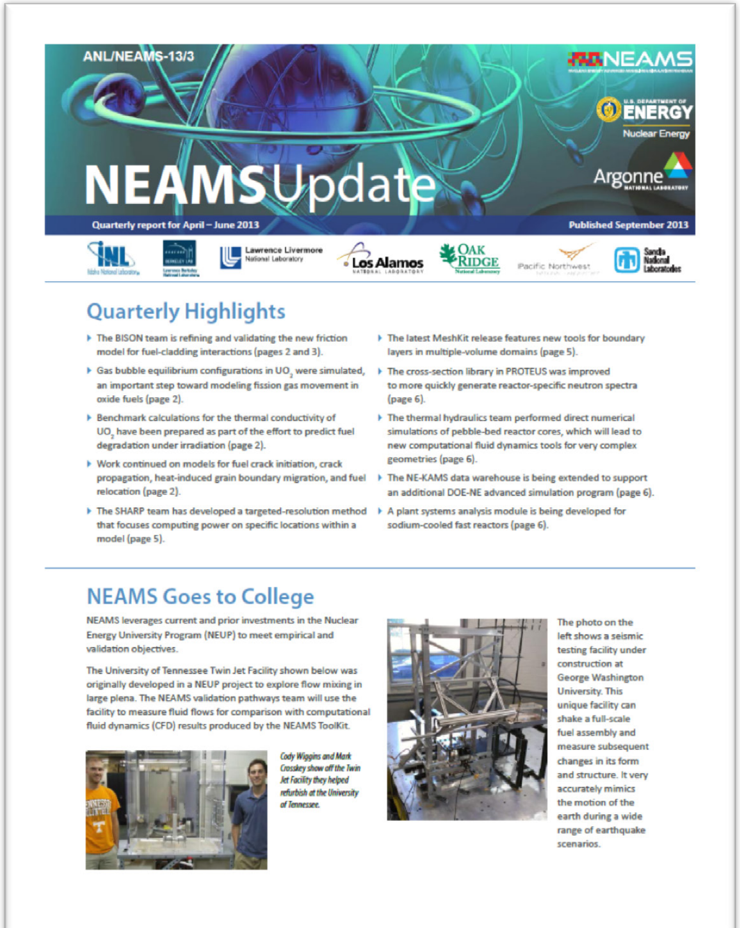
* "Early User" assessment problems





NEUP is one mechanism for providing validation capability

Staying informed about NEAMS



ANL/NEAMS-13/3

NEAMS Update

Quarterly report for April – June 2013

Published September 2013

Quarterly Highlights

- The BISON team is refining and validating the new friction model for fuel-cladding interactions (pages 2 and 3).
- Gas bubble equilibrium configurations in UO_2 were simulated, an important step toward modeling fission gas movement in oxide fuels (page 2).
- Benchmark calculations for the thermal conductivity of UO_2 have been prepared as part of the effort to predict fuel degradation under irradiation (page 2).
- Work continued on models for fuel crack initiation, crack propagation, heat-induced grain boundary migration, and fuel relocation (page 2).
- The SHARP team has developed a targeted-resolution method that focuses computing power on specific locations within a model (page 5).
- The latest MeshKit release features new tools for boundary layers in multiple-volume domains (page 5).
- The cross-section library in PROTEUS was improved to more quickly generate reactor-specific neutron spectra (page 6).
- The thermal hydraulics team performed direct numerical simulations of pebble-bed reactor cores, which will lead to new computational fluid dynamics tools for very complex geometries (page 6).
- The NE-KAMS data warehouse is being extended to support an additional DOE-NE advanced simulation program (page 6).
- A plant systems analysis module is being developed for sodium-cooled fast reactors (page 6).

NEAMS Goes to College

NEAMS leverages current and prior investments in the Nuclear Energy University Program (NEUP) to meet empirical and validation objectives.

The University of Tennessee Twin Jet Facility shown below was originally developed in a NEUP project to explore flow mixing in large plena. The NEAMS validation pathways team will use the facility to measure fluid flows for comparison with computational fluid dynamics (CFD) results produced by the NEAMS ToolKit.

Cody Wiggins and Mark Crosskey show off the Twin Jet Facility they helped refurbish at the University of Tennessee.

The photo on the left shows a seismic testing facility under construction at George Washington University. This unique facility can shake a full-scale fuel assembly and measure subsequent changes in its form and structure. It very accurately mimics the motion of the earth during a wide range of earthquake scenarios.

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