INL-MIS--18-50131-Revision-0

The Bison Nuclear Fuels Performance Application

Jason Hales

March 2018

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The
Bison Nuclear Fuels Performance Application

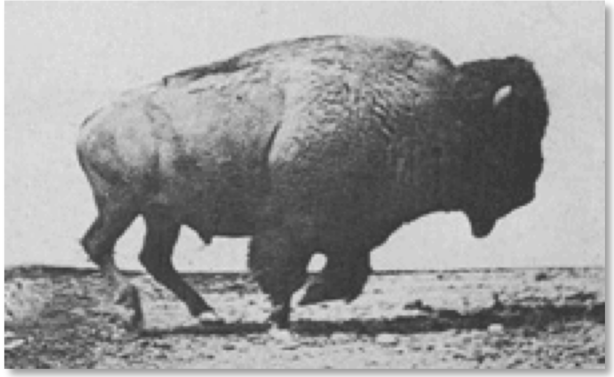
Jason Hales

12 March 2018

Portsmouth, UK

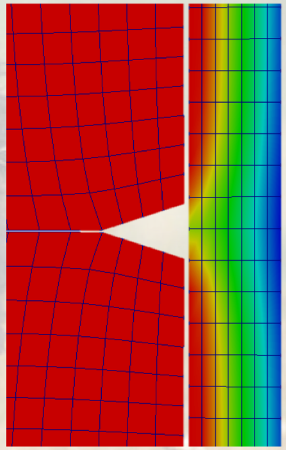
Bison: What is it?

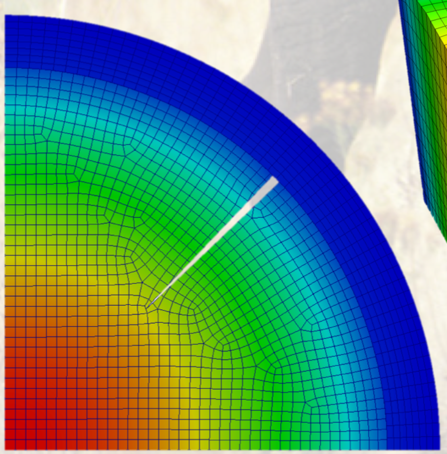
- Bison once numbered in the tens of millions and ranged over much of North America.
- Bison can weigh 1000+ kg and stand 1.8+ m high at the shoulder.
- Bison can jump 1.8 m vertically.
- Bison can run 60+ km/h.

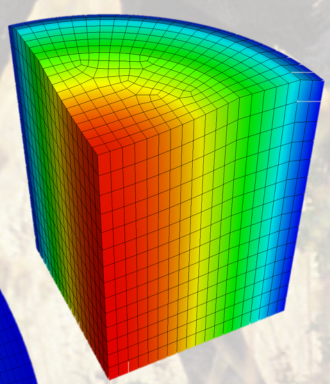


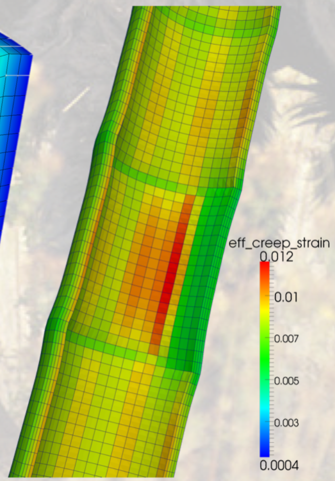
Bison: What is it?

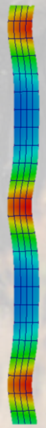
- **A finite element, thermo-mechanics code with material models and other customizations to analyze nuclear fuel**
  - Accepts user-defined meshes/geometries
    - 1D, 2D, or 3D
  - Runs on one processor or many
  - Analyzes a variety of fuel types
  - Couples to other analysis codes

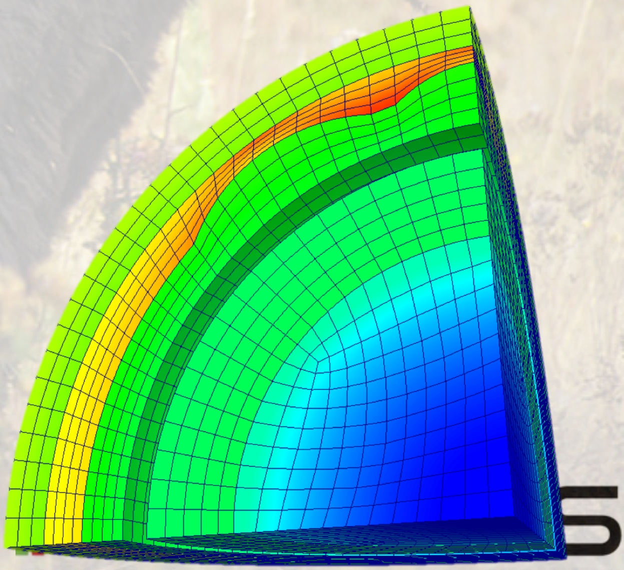






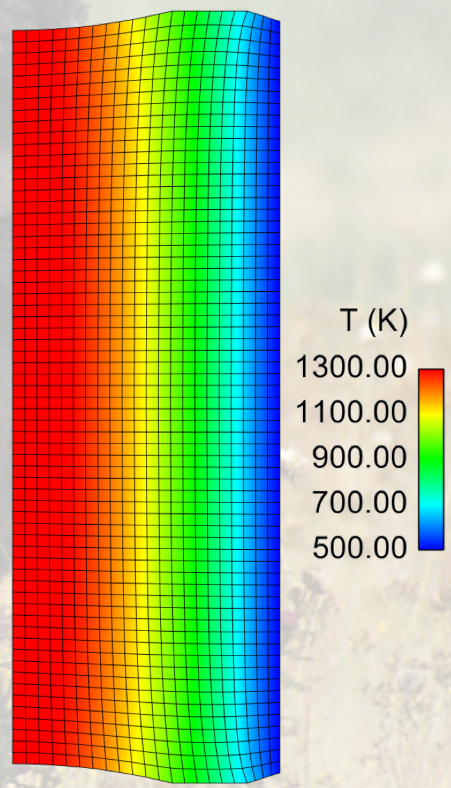






Bison Requirements and Limitations

- **Bison requires:**
  - An input file that describes thermal and mechanical material models, boundary conditions, initial conditions, power history
  - A mesh provided either directly in the input file or through a separate mesh file
- **Bison cannot currently model:**
  - Very high strain rate analyses (e.g., car crashes)
  - Structural elements (membranes, shells, beams)
  - Melting or flowing material
- **Bison is not:**
  - A thermal-hydraulics or CFD code
  - A neutronics code



Bison Governing Equations

- **Energy conservation (transient heat conduction with fission source)**

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + E_f \dot{F}$$

Fission density rate = f(**x**, t)

- **Species conservation (transient oxygen or fission product diffusion with radioactive decay)**

Fickian diffusion

Soret diffusion

$$\frac{\partial C}{\partial t} = \nabla \cdot D \left(\nabla C - \frac{CQ^*}{FRT^2} \nabla T \right) - \lambda C + S$$

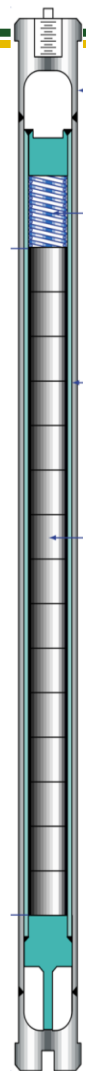
Radioactive decay

- **Momentum conservation (Cauchy's equation of equilibrium)**

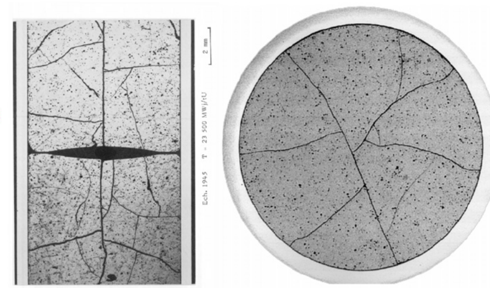
$$\nabla \cdot \mathbf{T} + \rho \mathbf{f} = 0$$

Fuel Behavior During Irradiation

At beginning of life, a fuel element is quite simple . . .

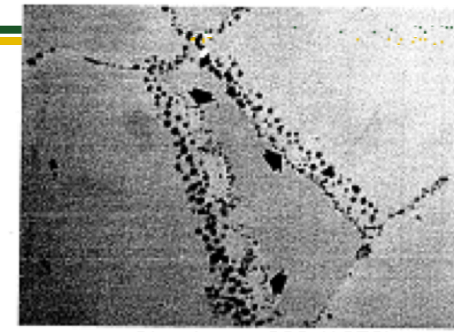


but irradiation brings about substantial complexity



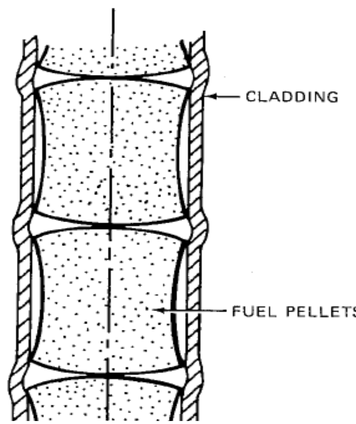
Michel et al, Eng Frac Mech, **75**, 3581 (2008)

Fuel Fracture



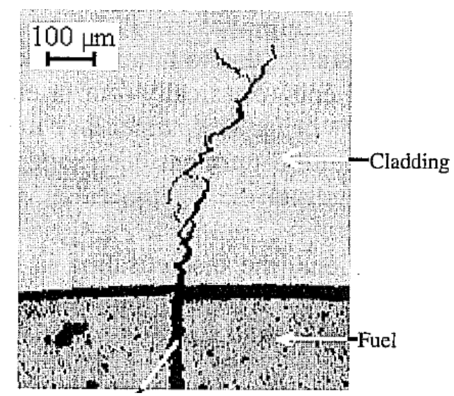
Olander, p. 323 (1978)

Fission gas



Olander, p. 584 (1978)

Multidimensional contact and deformation

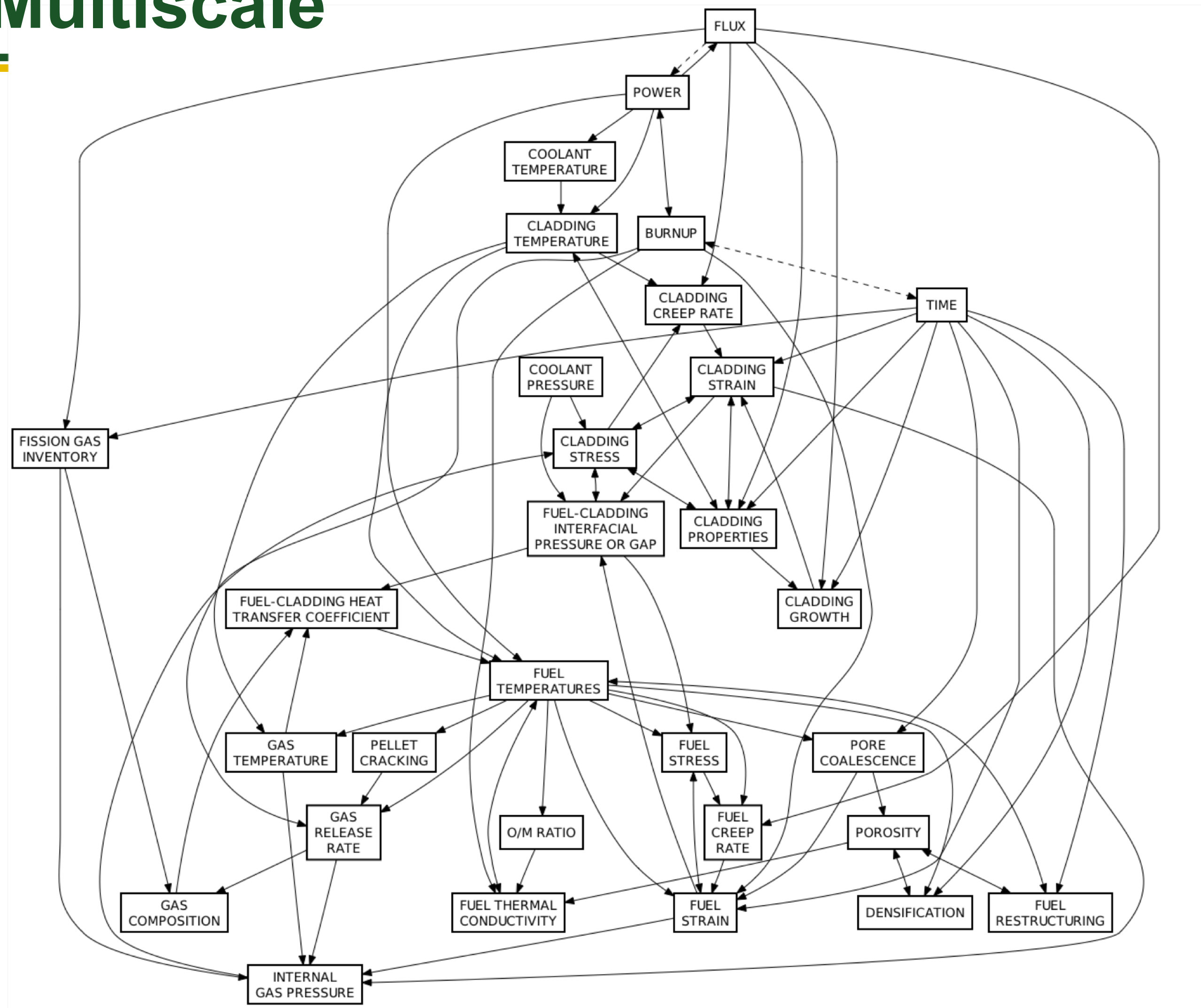


Bentejac et al, PCI Seminar (2004)

Stress Corrosion Cracking Cladding Failure

Fuel Behavior Modeling - Coupled Multiphysics and Multiscale

- **Multiphysics**
  - Fully-coupled nonlinear thermomechanics
  - Mass transport
  - Chemistry
  - Neutronics
  - Thermal-hydraulics
- **Multi-space scale**
  - Important physics operate at level of microstructure
  - Need real predictions at engineering scale
- **Multi-time scale**
  - Long, steady operation
  - Short power ramps
  - Rapid transients



Reproduced from Beyer et al., BNWL-1898, PNNL (1975)

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Bison Application: LWR Fuel

General Capabilities

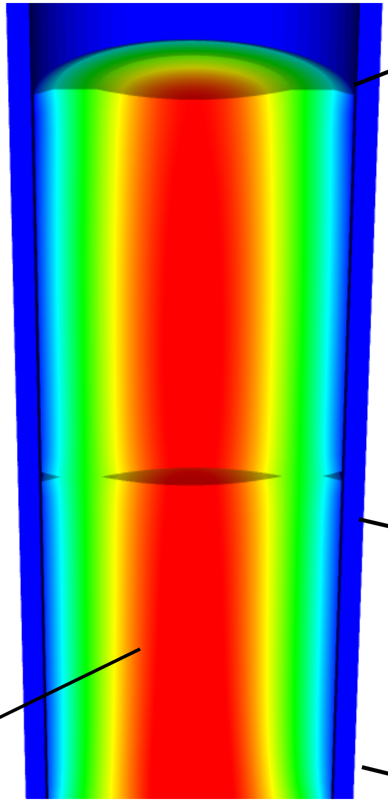
- Finite element based 1D spherical, 2D-RZ and 3D fully-coupled thermo-mechanics with species diffusion
- Linear or quadratic elements with large deformation mechanics
- Steady and transient operation
- Massively parallel computation
- Meso-scale informed material models

Gap/Plenum Behavior

- Gap heat transfer with $k_g = f(T, n)$
- Mechanical contact (master/slave)
- Plenum pressure as a function of:
  - evolving gas volume (from mechanics)
  - gas mixture (from FGR model)
  - gas temperature approximation

Oxide Fuel Behavior

- Temperature/burnup dependent conductivity
- Heat generation with radial and axial profiles
- Thermal expansion
- Solid and gaseous fission product swelling
- Densification
- Thermal and irradiation creep
- Fracture via relocation or smeared cracking
- Fission gas release (two stage physics)
  - transient (ramp) release
  - grain growth and grain boundary sweeping
  - athermal release



Temperature

Cladding Behavior

- Thermal expansion
- Thermal and irradiation creep
- Irradiation growth
- Gamma heating
- Combined creep and plasticity

Coolant Channel

- Closed channel thermal hydraulics with heat transfer coefficients

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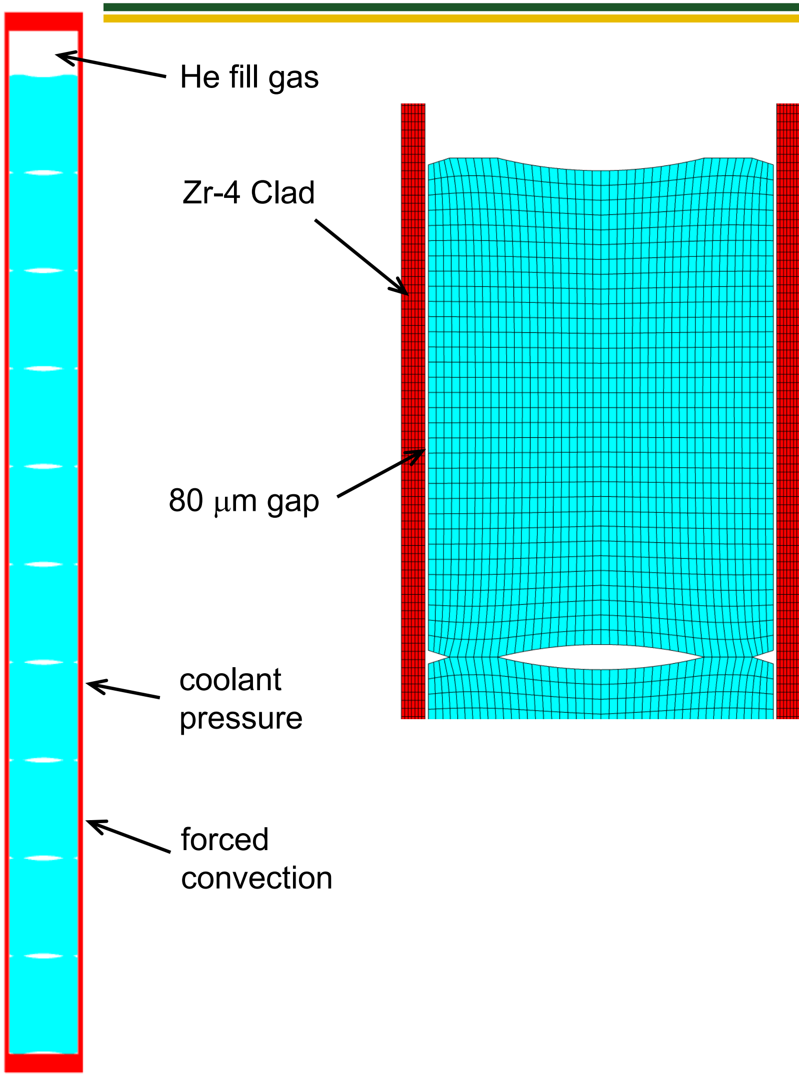
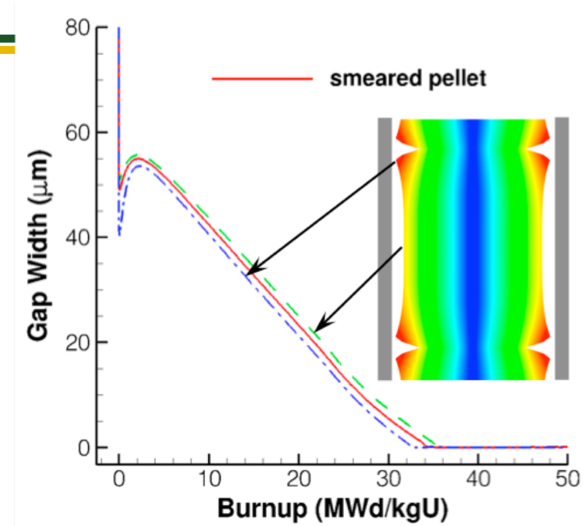
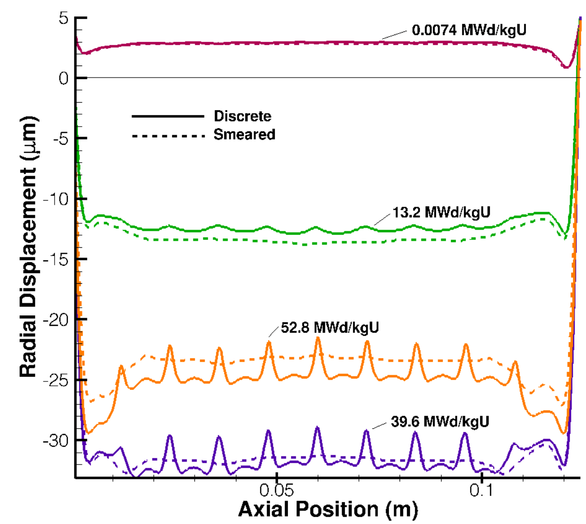
Discrete Pellet LWR Rodlet (2D-RZ multiphysics)







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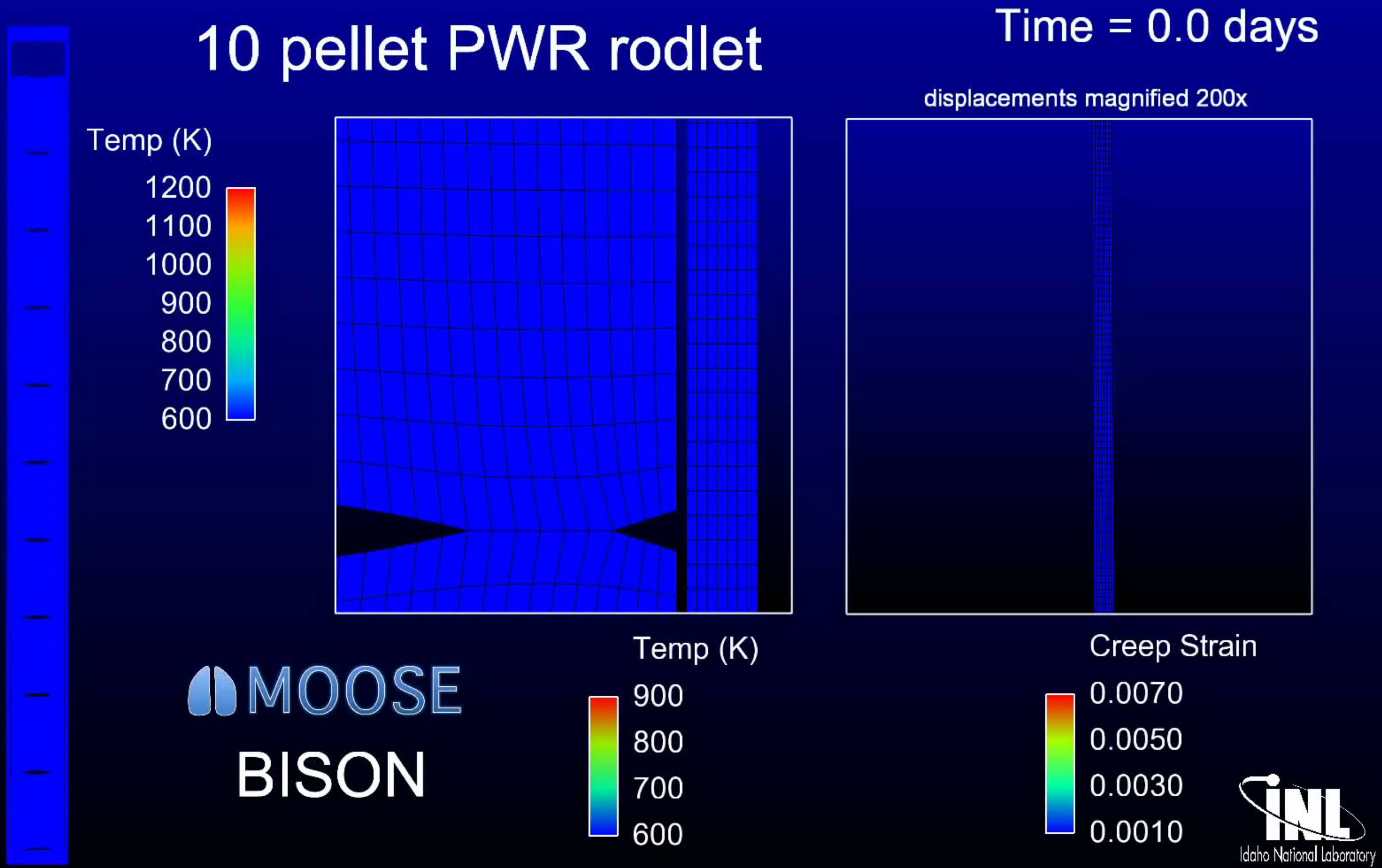
10 pellet PWR rodlet



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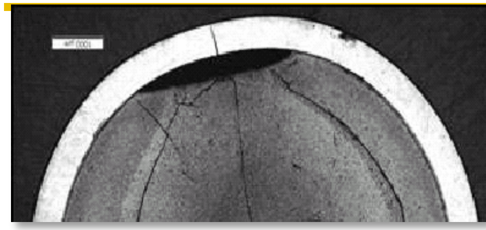
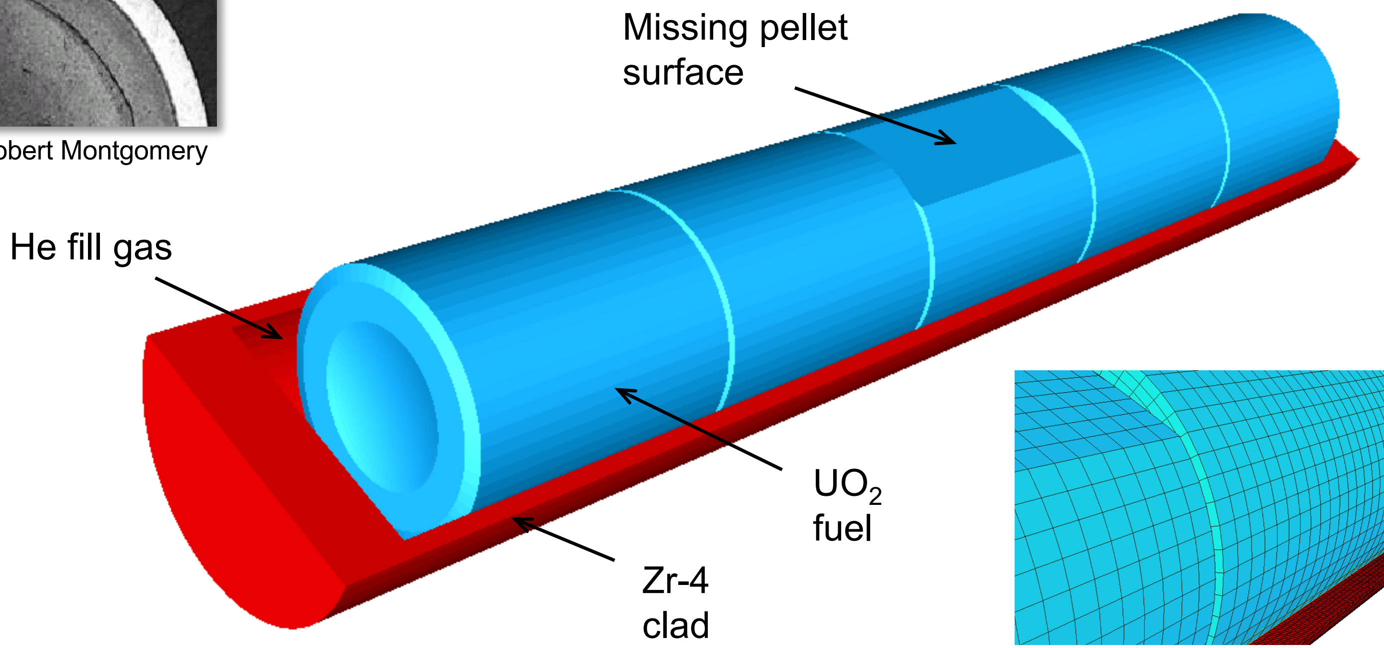
PCMI - Missing Pellet Surface Analysis



Micrograph from Robert Montgomery



- **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**

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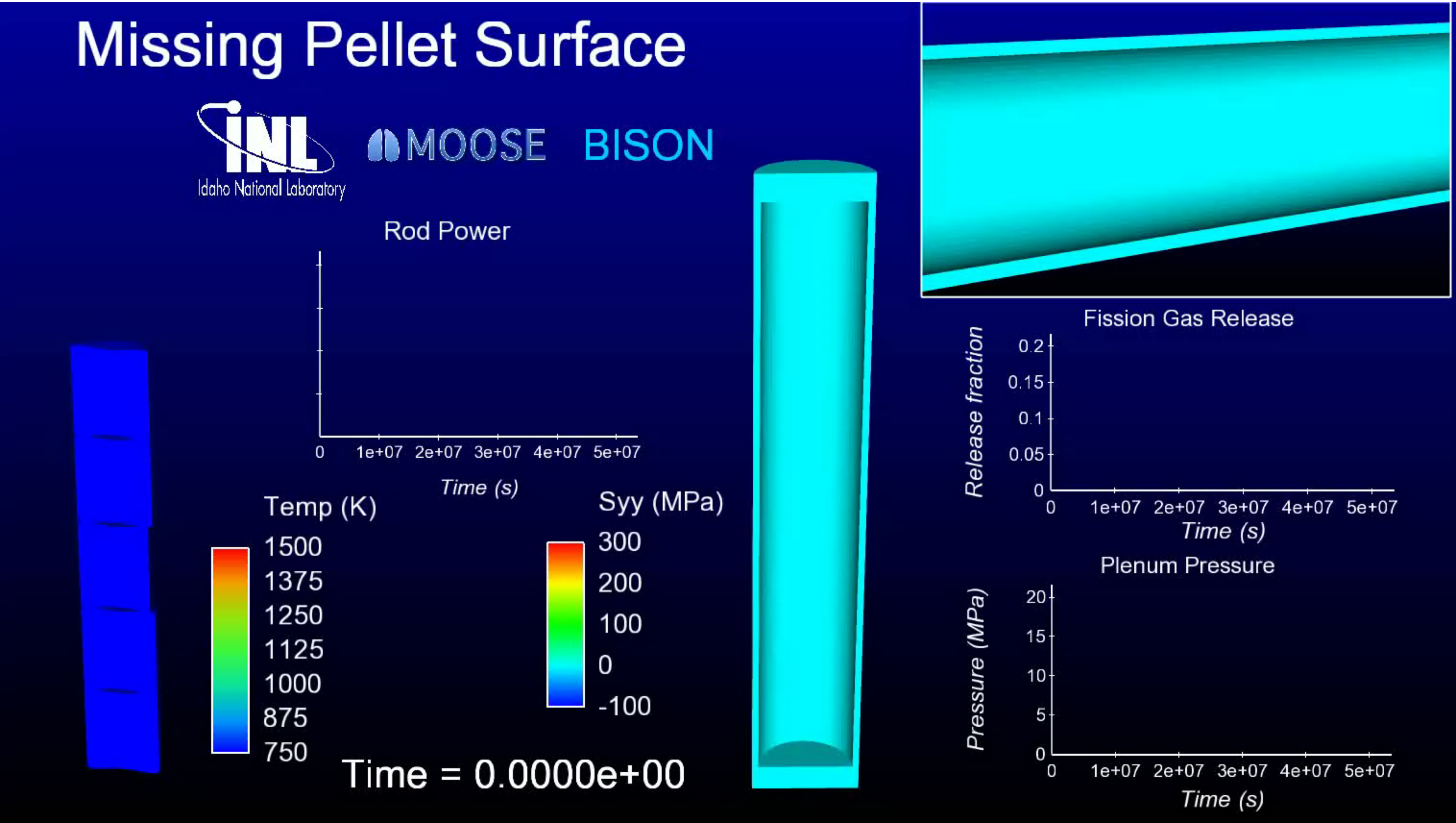
Animation – Missing Pellet Surface with Power Ramp



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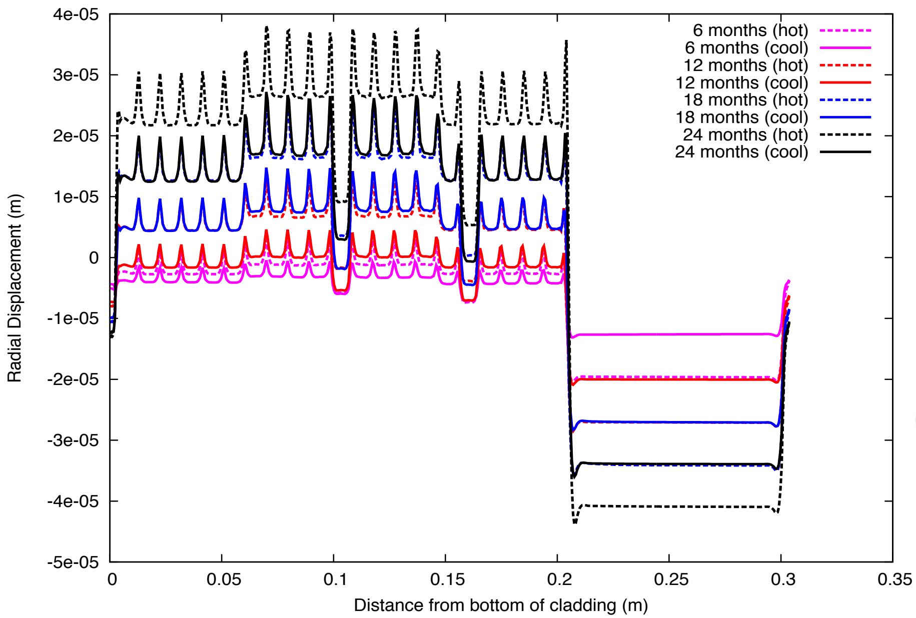
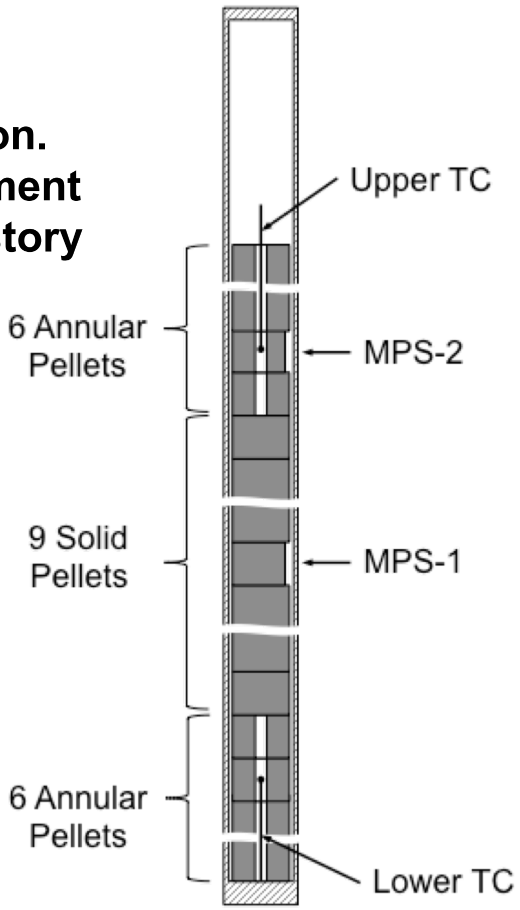
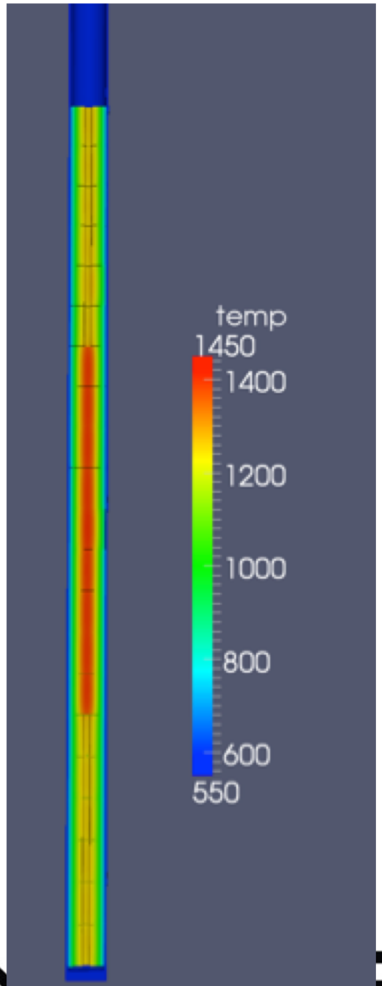
3D Halden MPS Experiment Design Using Bison

- Working with Halden to design unique 3D MPS experiment for Bison validation
- Generated 21 pellet model (full rod) and simulated behavior for two year irradiation.
- Calculations help determine final experiment configuration (defect size) and power history
- Experiment expected to start this year







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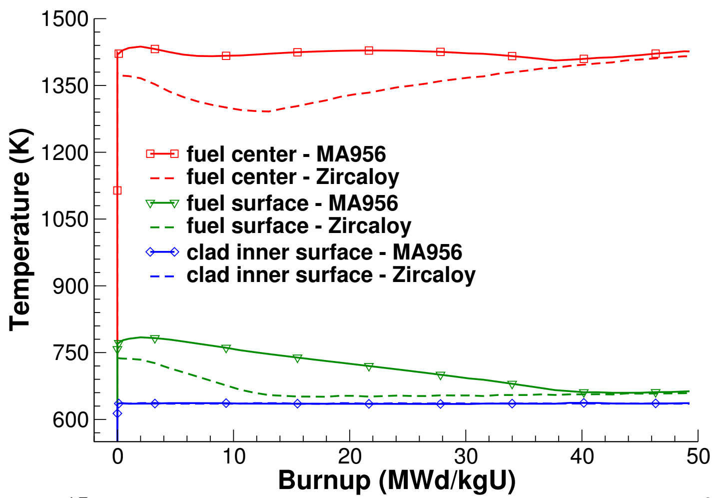
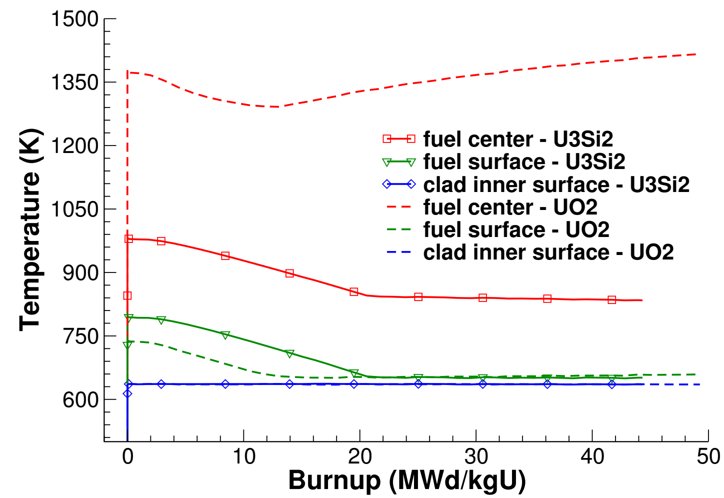
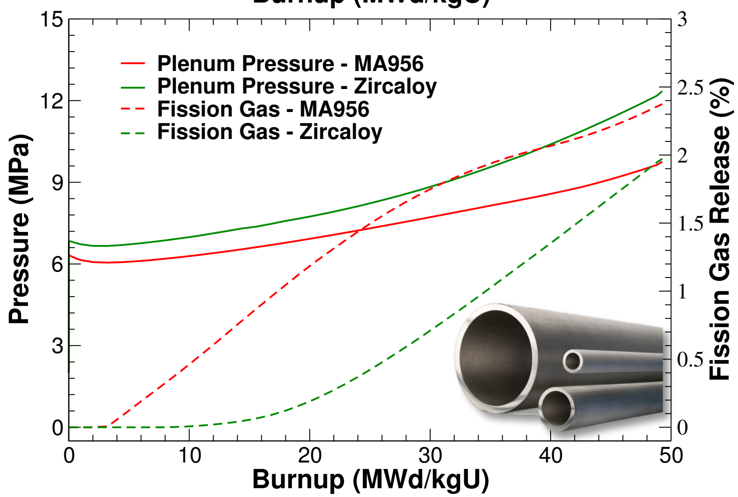
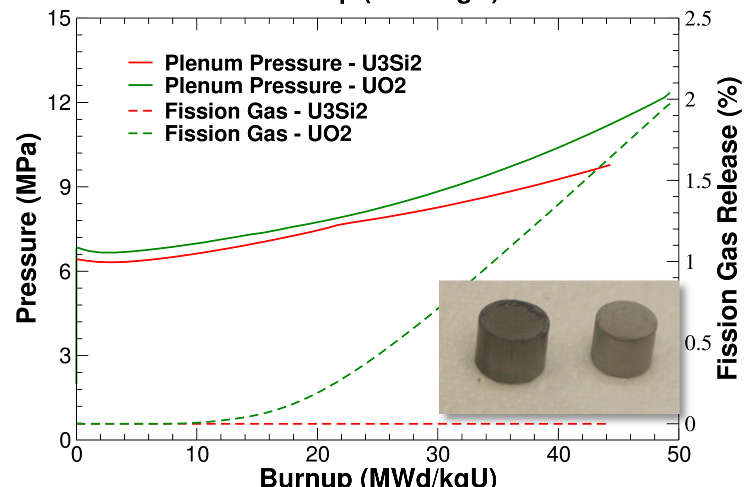
LWR Accident Tolerant Fuel









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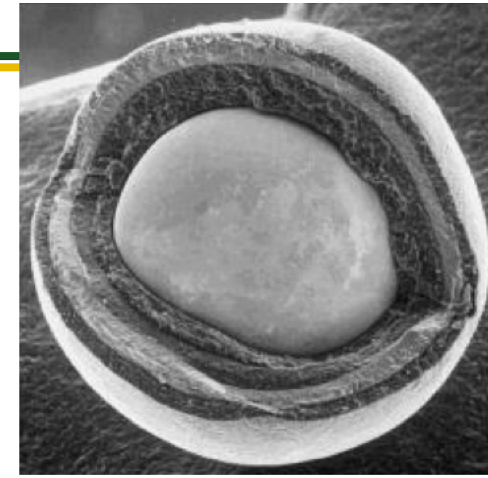
Bison Application: Particle Fuel

General Capabilities

- Finite element based 1D-Spherical, 2D-RZ and 3D fully-coupled thermo-mechanics with species diffusion
- Linear or quadratic elements with large deformation mechanics
- Elasticity with thermal expansion
- Steady and transient behavior
- Massively parallel computation

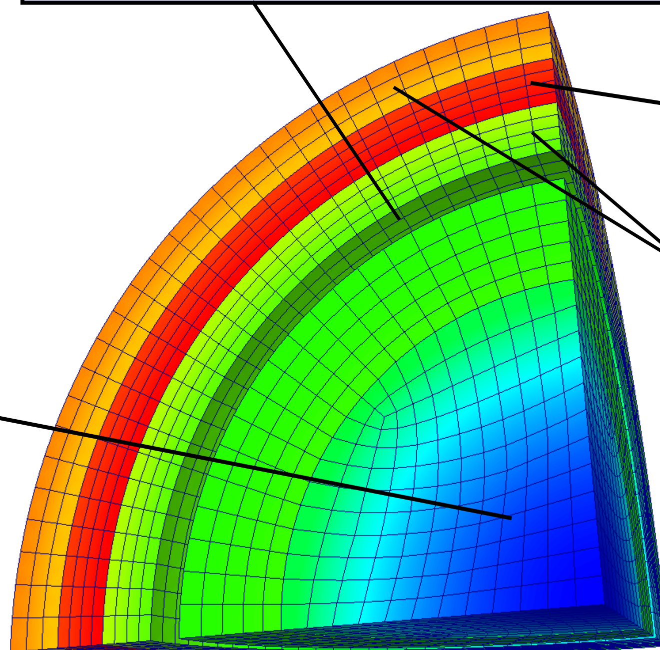
Gap Behavior

- Gap heat transfer with k_g= f (T, n)
- Gap mass transfer
- Mechanical contact (master/slave)
- Particle pressure as a function of:
  - evolving gas volume (from mechanics)
  - gas mixture (from FGR and CO model)
  - gas temperature approximation



Fuel Kernel

- Temperature/burnup/porosity dependent thermal conductivity
- Solid and gaseous fission product swelling
- Densification
- Thermal and irradiation creep
- Fission gas release (two stage)
- CO production
- Radioactive decay



Tangential Stress

Silicon Carbide

- Irradiation creep

Pyrolytic Carbon

- Anisotropic irradiation-induced strain
- Irradiation creep

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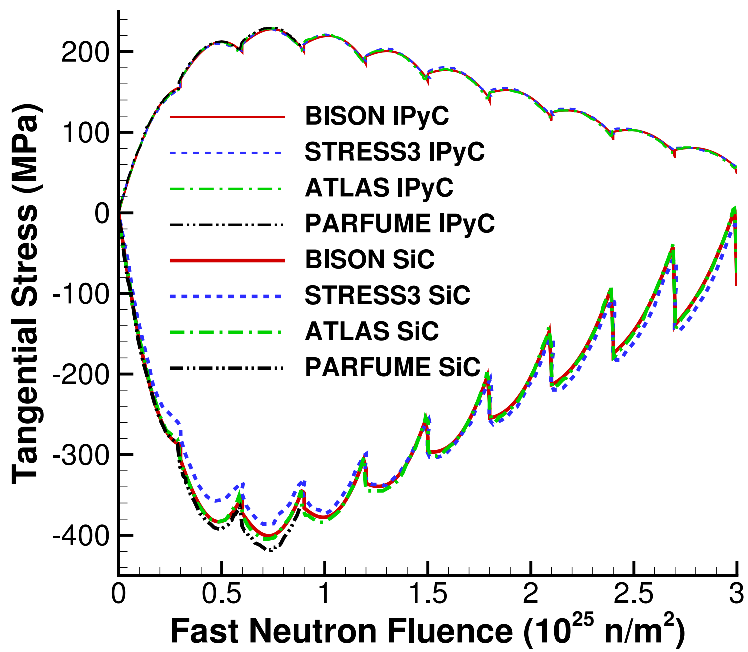
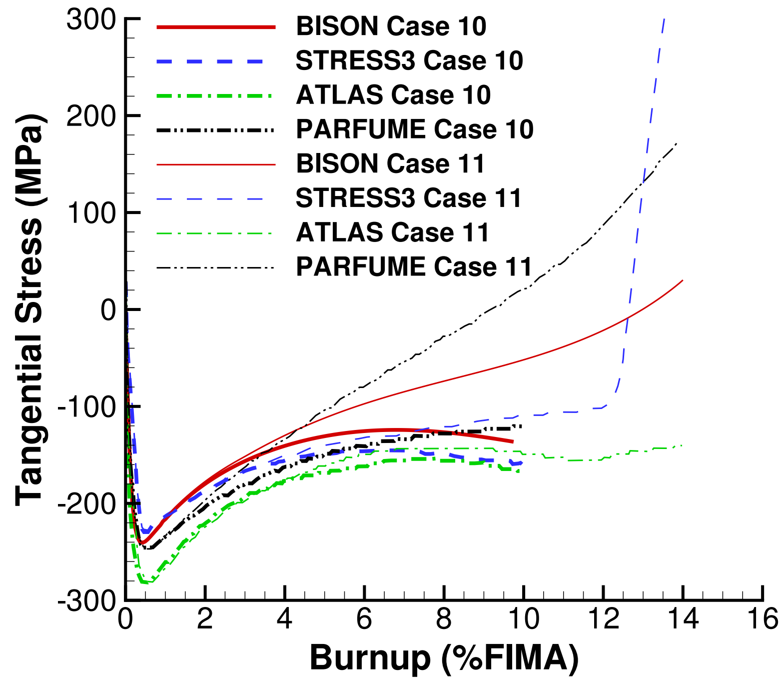
Evaluation of TRISO capability

- Bison compared against current 1D state-of-the-art codes: PARFUME (INL), ATLAS (French), STRESS3 (UK)
- Code comparisons are excellent, demonstrating Bison's ability to duplicate current state-of-the-art
- For spherical particles (1D spherical mode in Bison) run times of ~1 s are typical



Cyclic particle temperature as observed in pebble-bed reactor



Irradiations based on German HFR-K3 and HFR-P3 experiments

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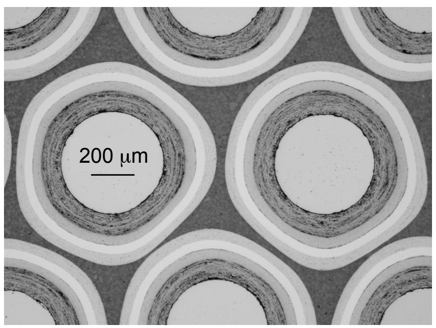
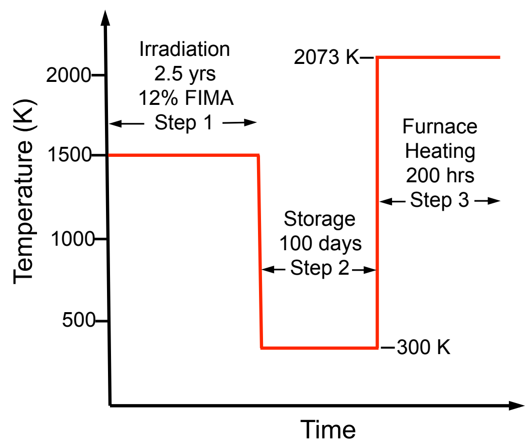
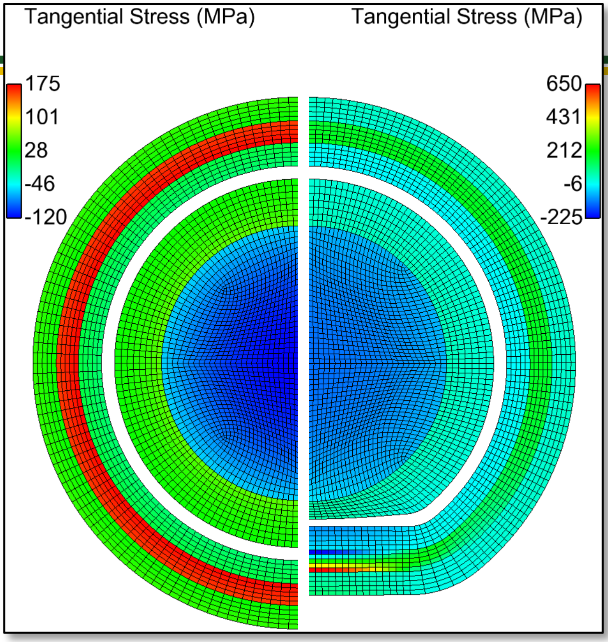
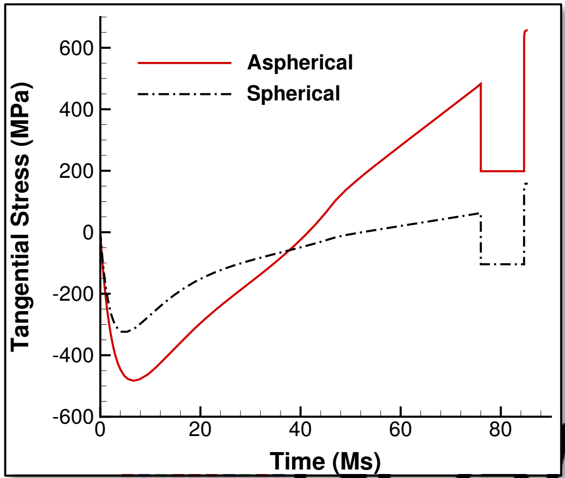
Simulation of Aspherical TRISO Particle

- Aspherical particles are fairly common
- Single facet aspherical particle problem has been solved in Bison assuming 2D axisymmetry



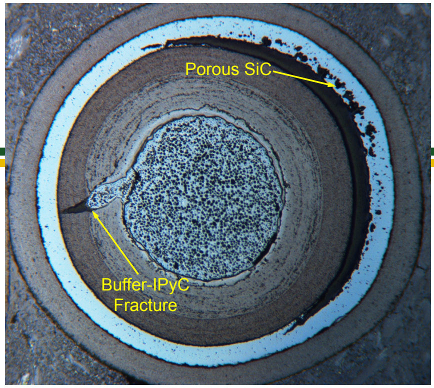




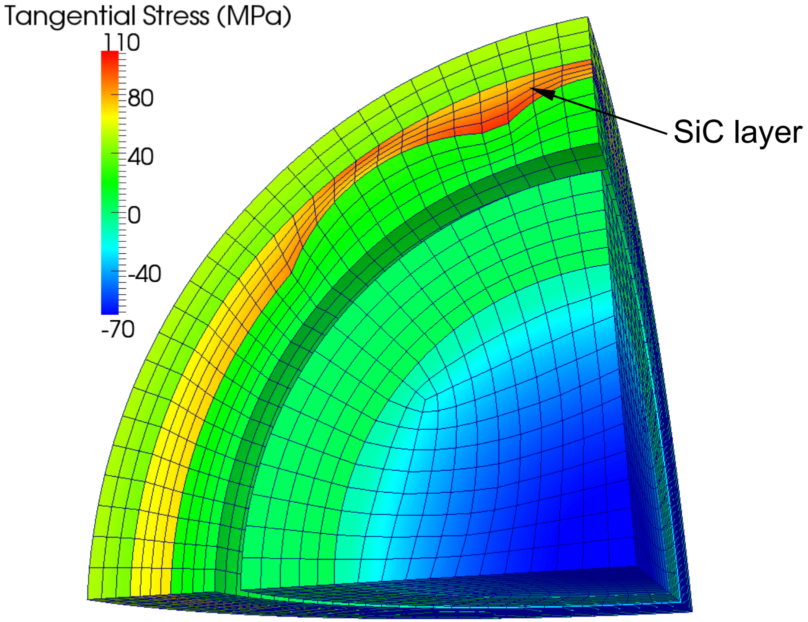


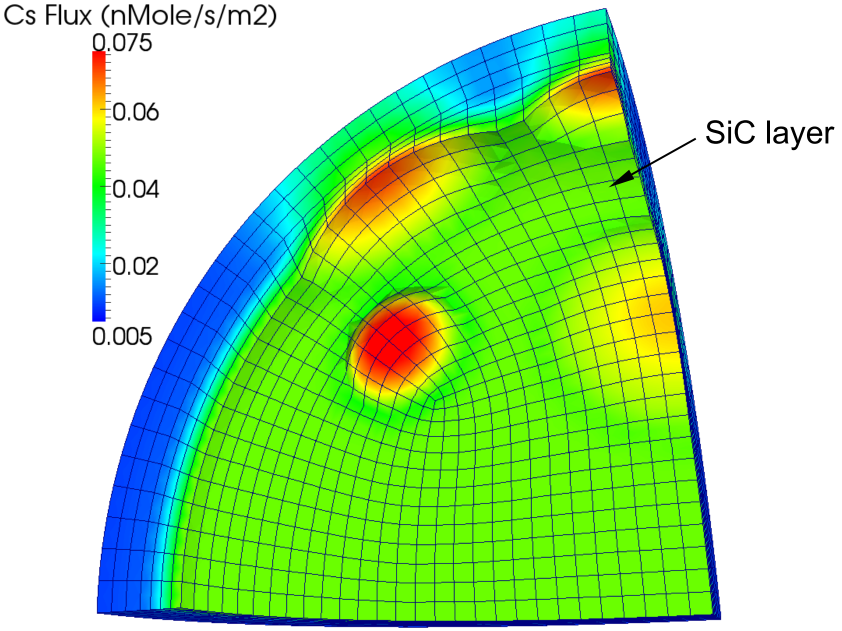
- During accident testing, asphericity raises peak tensile stress in SiC containment layer by almost 4x
- Typical run times of a few minutes on 8 processors
- Note: this model is for demonstration and does not represent a typical particle

3D Simulation of Thinned SiC Layer



- Localized thinning of SiC layer can occur due to soot inclusions or fission product interaction
- Bison 3D capability demonstrated on an eighth-particle with localized thinning of the SiC layer at random locations

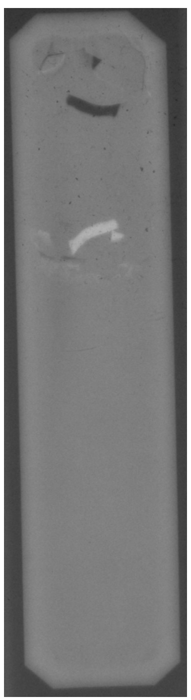


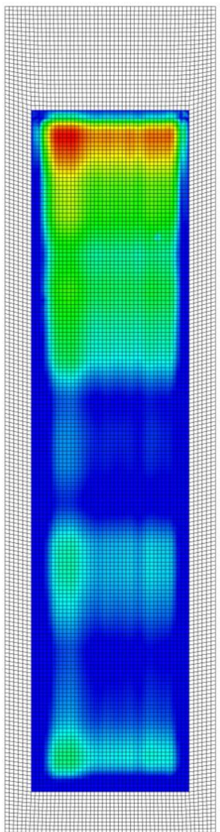


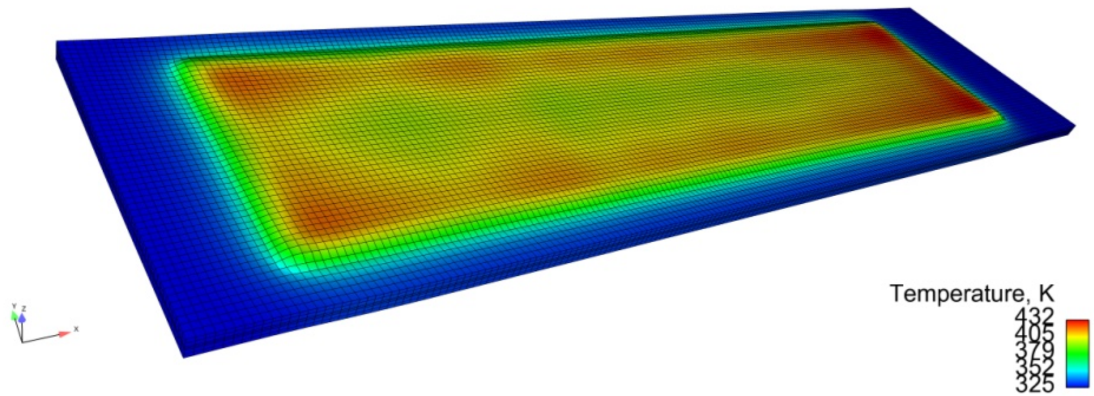
- Thinned SiC regions experience significantly higher tensile stress and greater cesium release; impossible to predict with 1D analysis
- Typical run times of a few hours on 8 processors

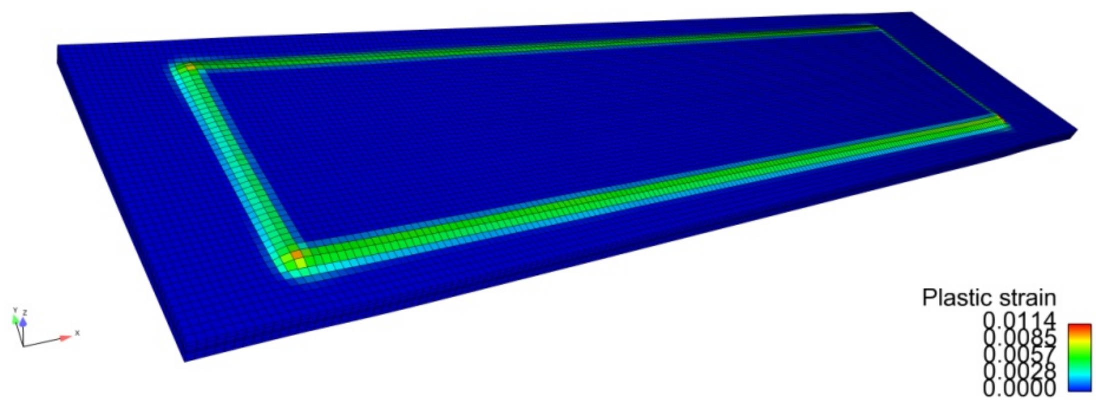
Bison Application: Plate Fuel

- **Bison has been used to analyze plate fuel for research reactors**





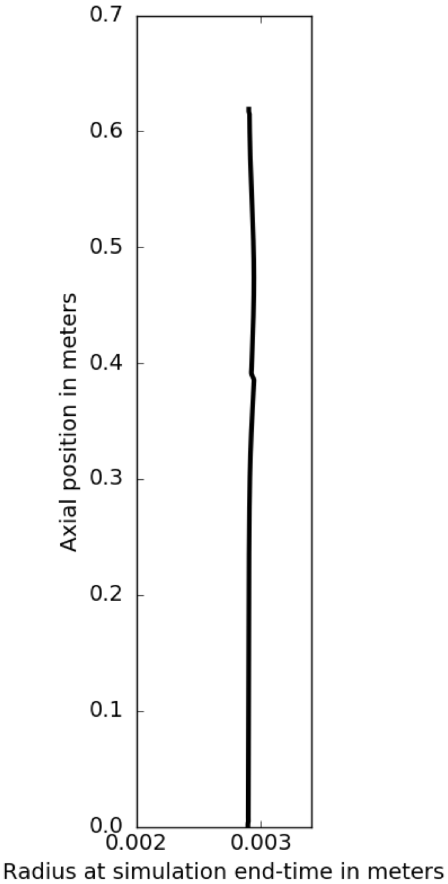


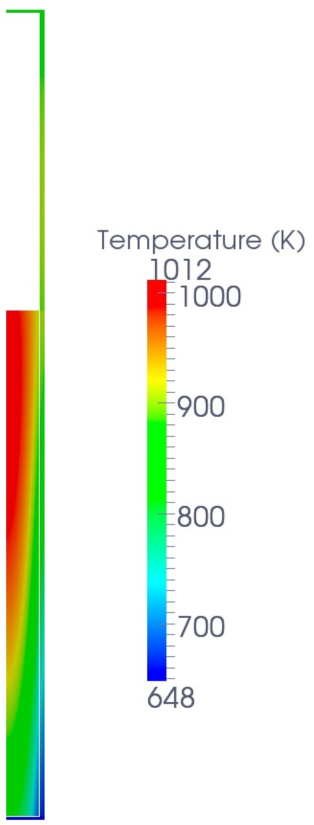


[Pavel Medvedev]

Bison Application: Metal Fuel

- **Sodium-filled gap**
- **Sodium coolant**
- **UPuZr models**
  - Thermal and irradiation creep
  - Thermal conductivity
  - Swelling
  - Fission Gas release
  - Zr distribution
- **HT9 Models**
  - Thermal and irradiation creep
  - Thermal conductivity
  - Damage accumulation





Recent Bison Work: Porosity Migration in MOX Fuel

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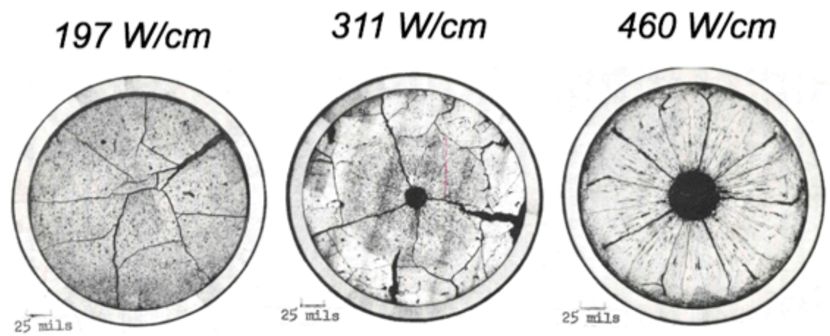
- **Solving the following equations, fully coupled in BISON**

$$\rho C \frac{\partial T}{\partial t} - \nabla \cdot k \nabla T - q = 0$$

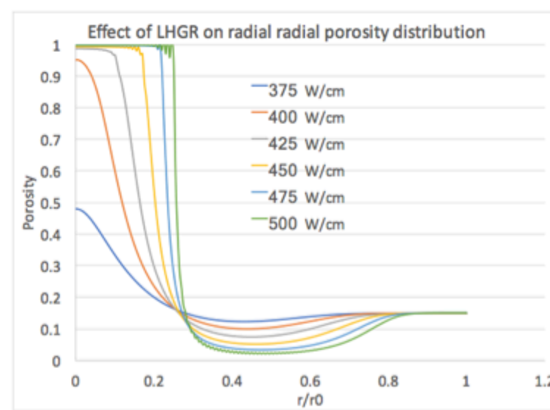
$$\frac{\partial p}{\partial t} + \nabla \cdot (\vec{v} p - \nu \nabla p) = 0$$

T is temperature
ρ is mass density
C is specific heat
k is thermal conductivity
q is power source
p is porosity (fraction per volume)
$\vec{v}$ is pore velocity (function of thermal gradient)
ν is pore Fickian diffusivity

Effect of LHGR on central void diameter experimental data



BISON result



Used to predict central void size in MOX fuel, or UO2 at high temperature. Shown at right are micrographs with central void size at different linear heat rates and corresponding porosity profile along the fuel radius.

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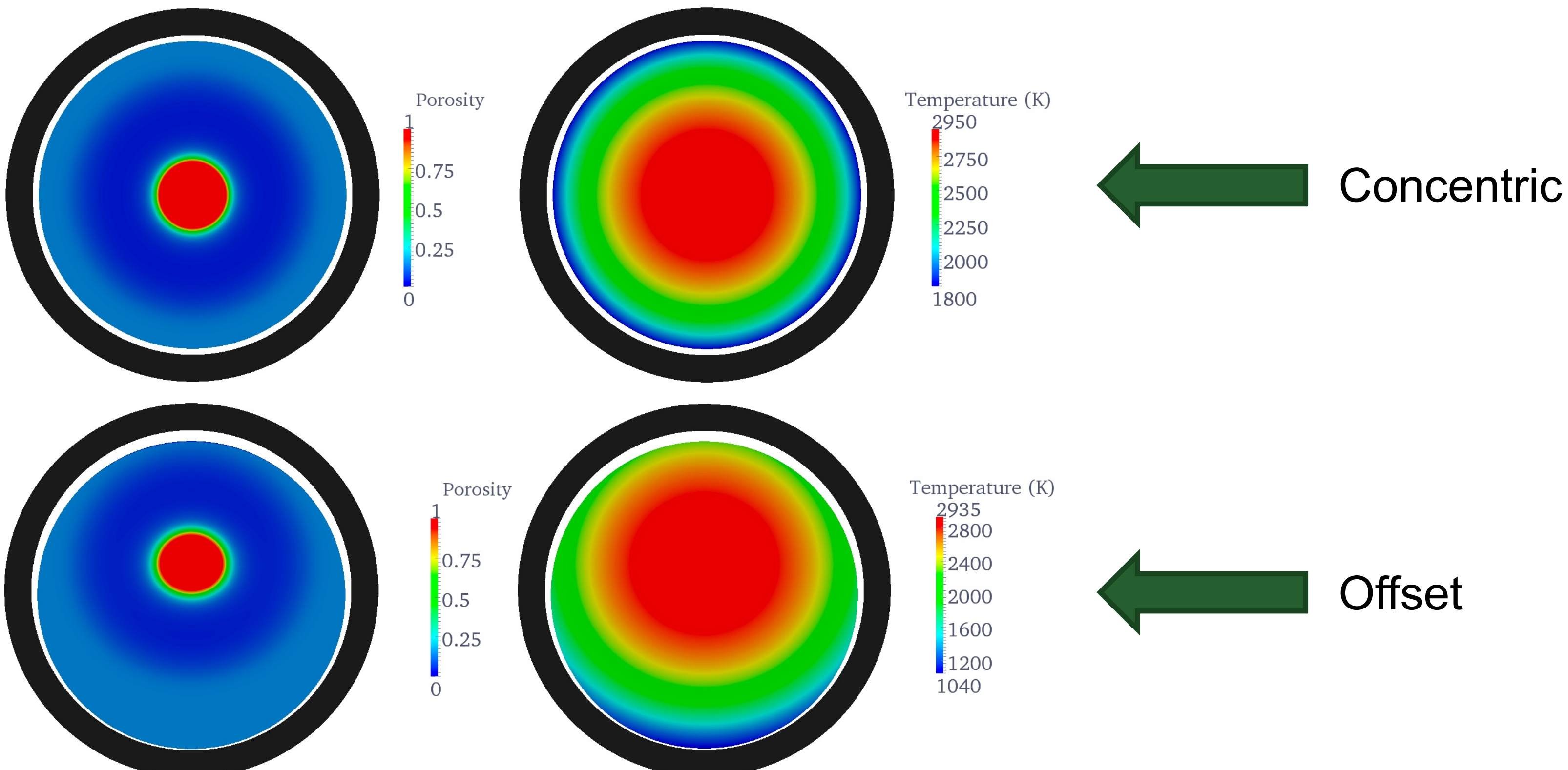
Porosity Multi-dimensional Effects

- **Offsetting fuel within the cladding affects porosity and temperature distribution, and therefore central void location.**



Recent Bison Work: Modeling LWR Fuel Relocation with XFEM

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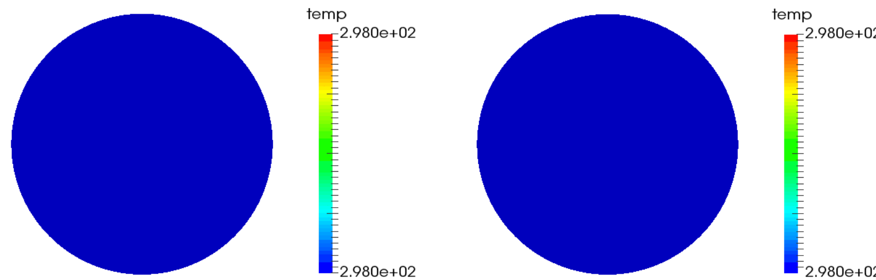
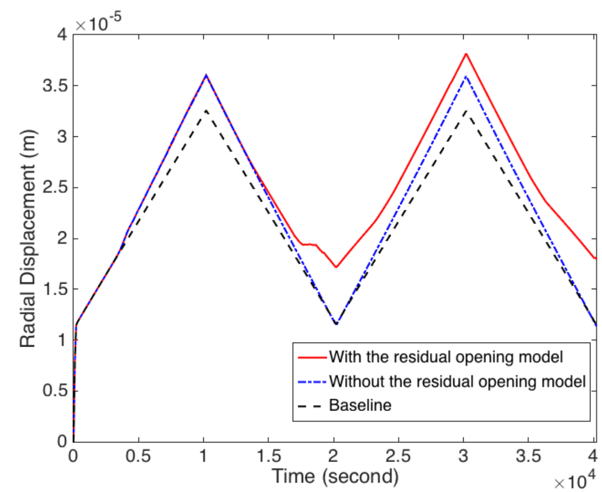
- Bison's XFEM capability is being used to better understand radial relocation in LWR fuel
- XFEM technique permits discrete cracks to dynamically propagate across a finite element mesh, independent of element boundaries
- A surface interaction model has recently been developed to represent residual opening across cracks due to the presence of asperities
- When this model is included, relocation is shown to increase over multiple power cycles due to a "ratcheting" effect

W. Jiang, B. W. Spencer, D. Schwen, K. A. Gamble, and L. Liu. Improved fracture models for relocation modeling. INL/EXT-18-44495, Idaho National Laboratory, January 2018.



Cracks shown on displaced mesh (magnified 10x) without (left) and with (right) residual opening model. Time history of radial displacement shown below for two power cycles.



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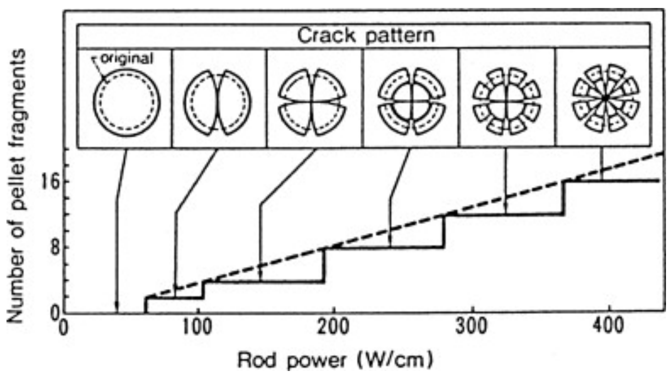
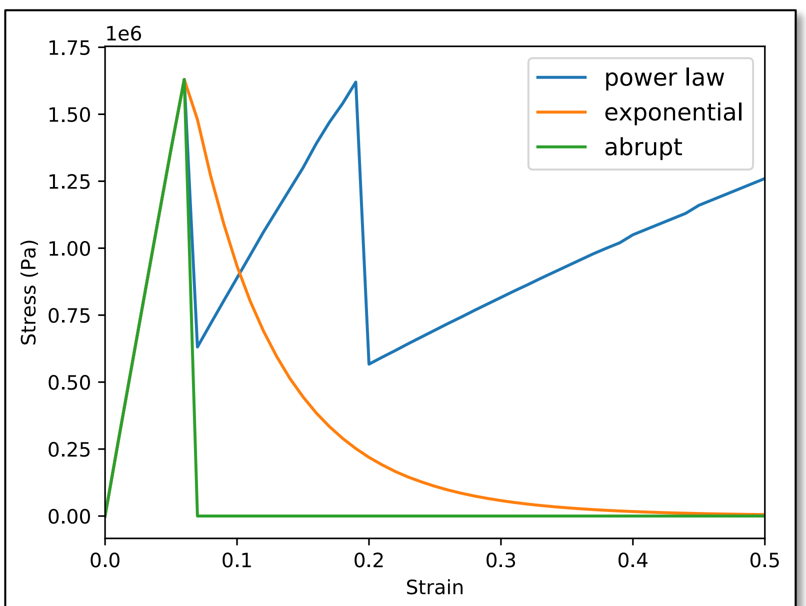
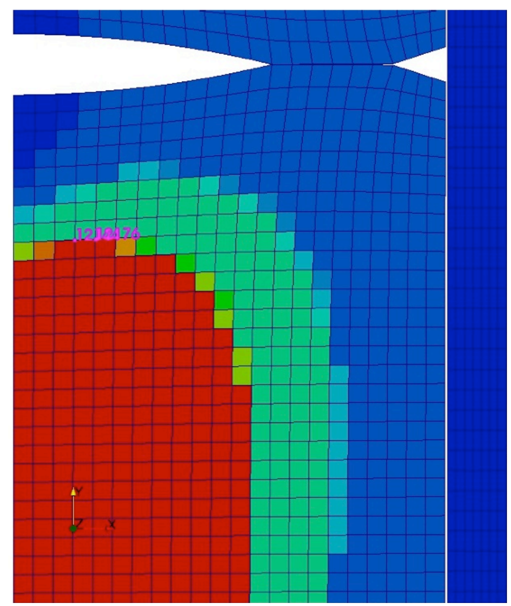
Recent Bison Work: Smeared Cracking



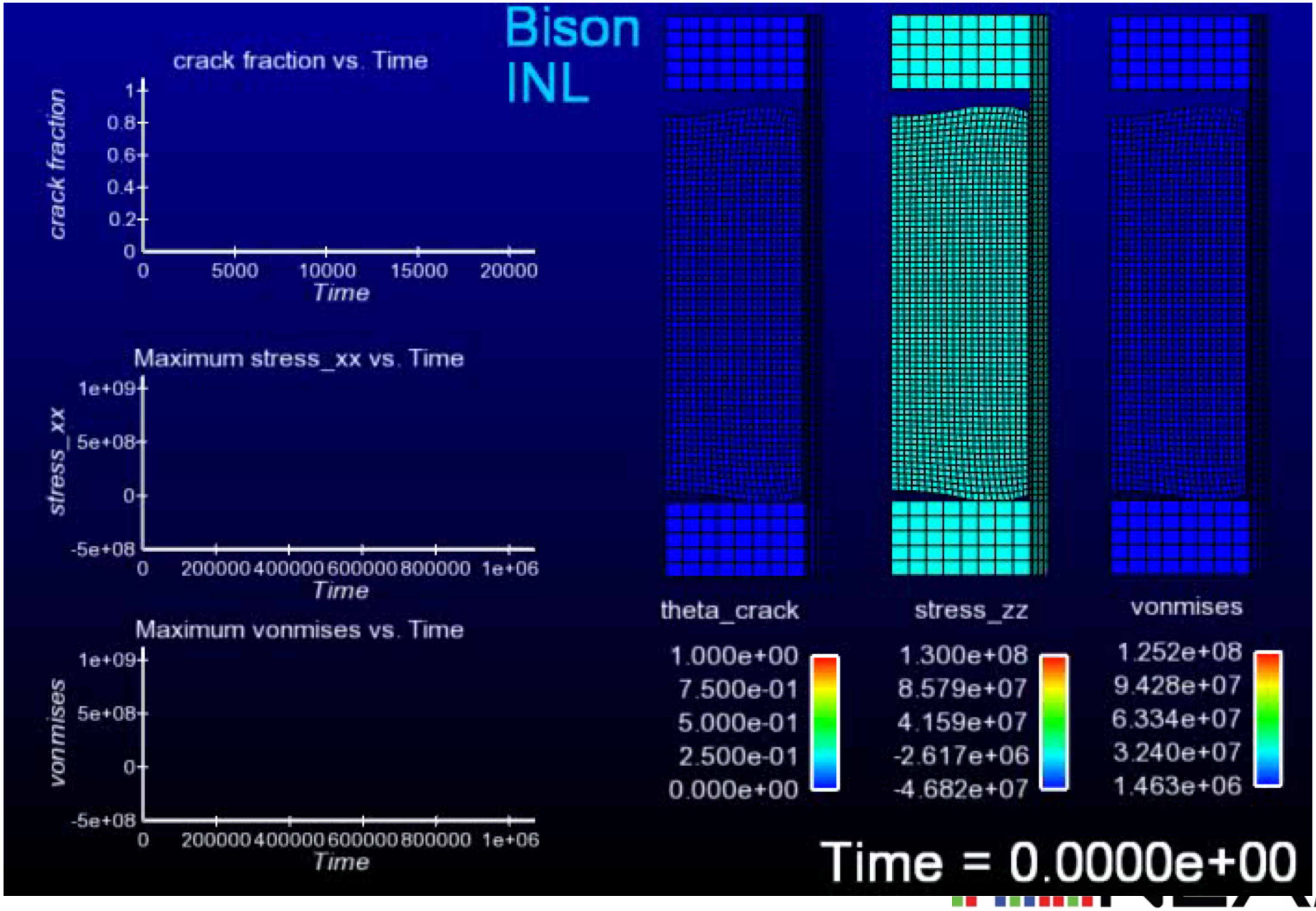
Oguma, 1983

- LWR fuel fractures during the first rise to power
- Fracture affects the mechanical and thermal behavior of the fuel and cladding
- Smeared cracking adjusts the material stiffness at individual integration points





Smeared Cracking Demonstration



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Recent Work on Smeared Cracking Models in Bison

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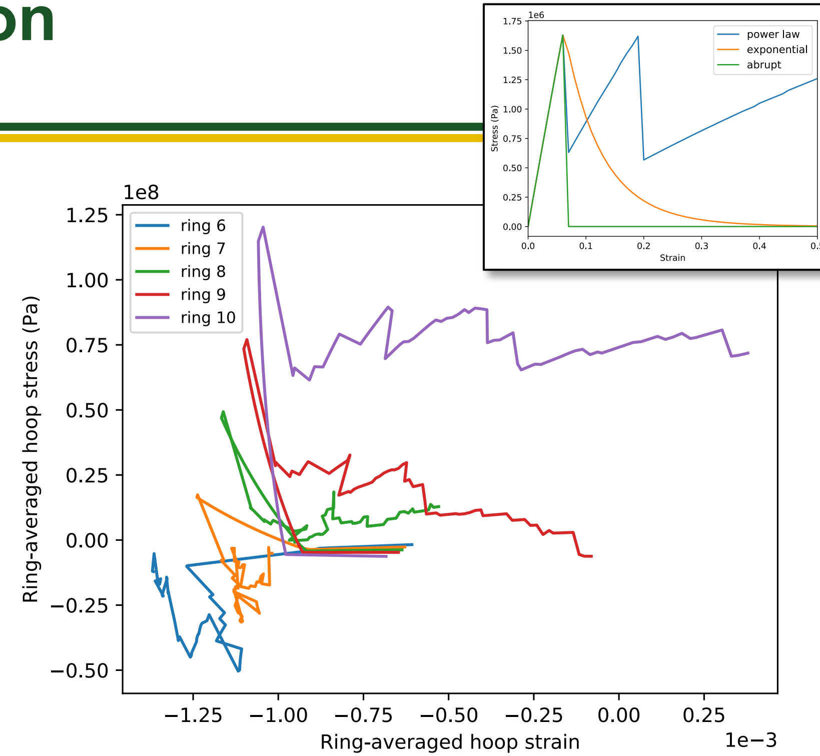
- Enhancements have been made that greatly improve robustness.
- A detailed model of a fuel rod cross-section using XFEM was used to assess appropriate softening models for radial cracking in axisymmetric simulations.
- An option added to select softening model by crack direction.
- A full-length rod in the Bison assessment test suite was converted to use fuel smeared cracking and creep models, and it runs robustly.



Ring-averaged stress-strain curves from 2D cross-section model. Bison's power law softening model more closely replicates this behavior than does the exponential model typically used, and can now be selectively applied only in the hoop direction in axisymmetric simulations.

B. W. Spencer and R. J. Gardner. Improved LWR fuel rod mechanics models. INL/EXT-18- 44749, Idaho National Laboratory, February 2018.

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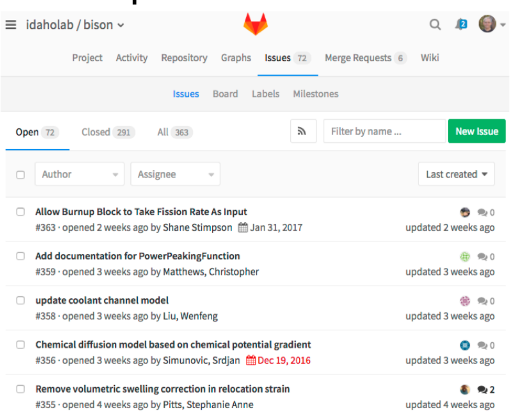
Software Quality Assurance

- Software quality is tightly controlled using issue tracking, merge requests and collaborative code review (via GitLab)

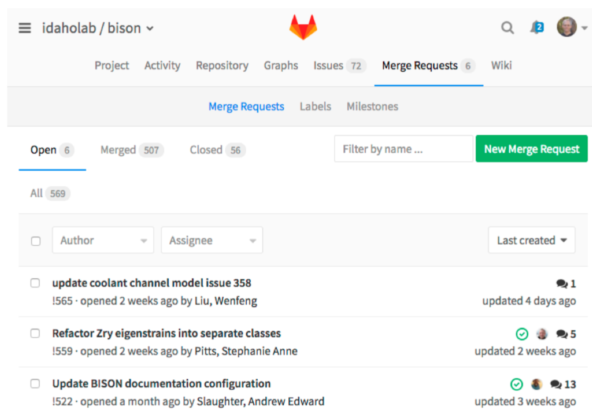
Issue Tracking

- Users can submit issues or request improvements
- Each issue is recorded and tracked to completion



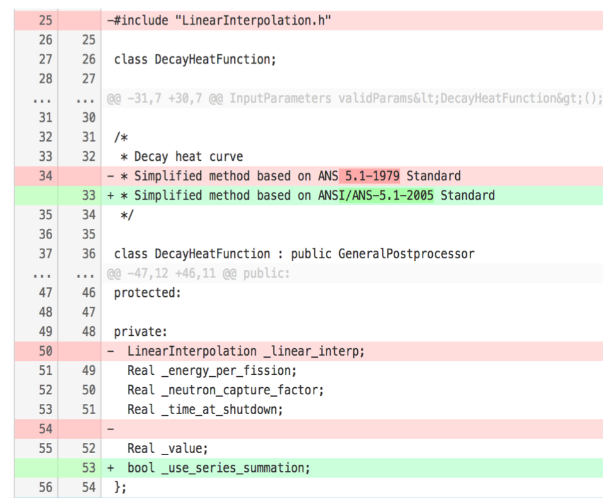
Merge requests and testing

- Code changes are submitted for review
- Review starts once the code updates pass all tests



Collaborative Code Review

- Code changes are posted on the GitLab site
- Users can comment and make suggestions on code
- Once satisfied with the changes, they are merged into the code



- In Nov 2015 underwent detailed software quality assessment. Deemed NQA-1 compliant for R&D software.

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Code Testing and Verification

- Bison thru MOOSE is supported by 1000's of unit and regression tests (>900 in Bison)
- All new code must be supported by regression testing
- All tests are run and must pass prior to acceptance of any code modification
- Current line coverage is at 87.5%

LCOV - code coverage report

Current view: top level
Test: BISON Test Coverage
Date: 2018-03-06 10:17:37
Legend: Rating: low: < 70 % medium: >= 70 % high: >= 80 %

	Hit	Total	Coverage
Lines:	18188	20797	87.5 %
Functions:	1515	1655	91.5 %

Directory	Line Coverage		Functions	
src	91.7 %	11 / 12	100.0 %	3 / 3
src/actions	88.2 %	911 / 1033	96.9 %	62 / 64
src/auxkernels	82.8 %	961 / 1160	91.4 %	96 / 105
src/auxkernels/tensor_mechanics	87.0 %	40 / 46	100.0 %	5 / 5
src/base	89.8 %	283 / 315	45.0 %	9 / 20
src/bcs	78.1 %	484 / 620	81.0 %	51 / 63
src/bcs/coolant	84.6 %	721 / 852	84.4 %	65 / 77
src/functions	91.8 %	811 / 883	98.0 %	50 / 51
src/ics	99.2 %	130 / 131	100.0 %	5 / 5
src/kernels	79.8 %	612 / 767	82.3 %	93 / 113
src/materials	87.7 %	8274 / 9434	95.1 %	559 / 588
src/materials/tensor_mechanics	91.7 %	2795 / 3049	94.8 %	290 / 306
src/mesh	84.9 %	568 / 669	68.6 %	24 / 35
src/parser	100.0 %	61 / 61	100.0 %	3 / 3
src/postprocessors	90.9 %	646 / 711	92.1 %	105 / 114
src/userobject	82.6 %	818 / 990	91.5 %	86 / 94
src/utils	100.0 %	21 / 21	100.0 %	3 / 3
src/vectorpostprocessors	95.3 %	41 / 43	100.0 %	6 / 6

Annals of Nuclear Energy 71 (2014) 81–90

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ELSEVIER

Verification of the BISON fuel performance code

CrossMark

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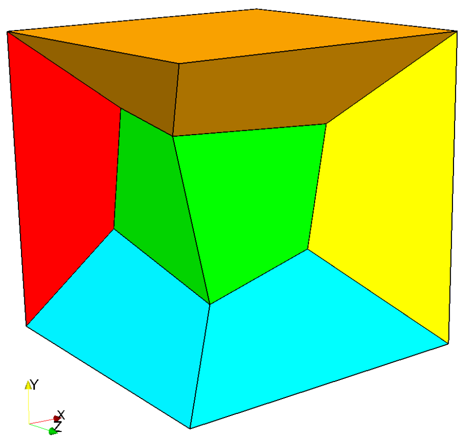
ABSTRACT

Complex multiphysics simulations such as those used in nuclear fuel performance analysis are composed of many submodels used to describe specific phenomena. These phenomena include, for example, mechanical material constitutive behavior, heat transfer across a gas gap, and mechanical contact. These submodels work in concert to simulate real-world events, like the behavior of a fuel rod in a reactor. If a simulation tool is able to represent real-world behavior, the tool is said to be validated. While much emphasis is rightly placed on validation, model verification is equally important. Verification involves showing that a submodel computes results consistent with its mathematical description. This paper reviews the differences between verification, validation, and calibration as well as their dependencies on one another. Verification problems specific to nuclear fuel analysis are presented. Other verification problems suitable to assess the correctness of a finite element-based nuclear fuel application such as

Two Verification Examples

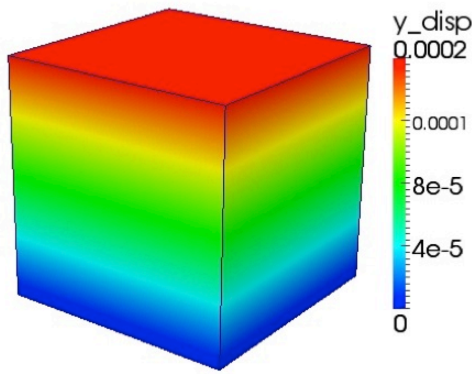
3D FEM Patch Test



Outer nodes displaced:
$u_x = 1\times10^{-6}$, $u_y = 2\times10^{-6}$, $u_z = 3\times10^{-6}$
Outer faces sheared:
1×10^{-6}, 2×10^{-6}, 3×10^{-6} for xy, yz, zx

Analytical solution is a spatially uniform stress/strain state:
$\sigma_{xx} = 1$, $\sigma_{yy} = 2$, $\sigma_{zz} = 3$
$\sigma_{xy} = 0.5$, $\sigma_{yz} = 1$, $\sigma_{zx} = 1.5$

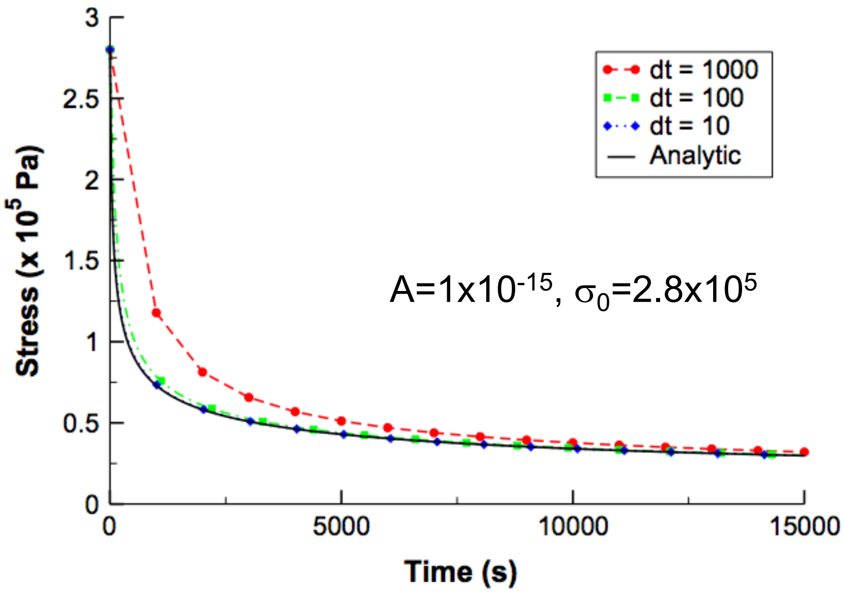
Power Law Creep



$$\dot{\epsilon}_{cr} = A\sigma^n e^{-Q/RT} t^m$$

For constant strain and
n = 4, Q = 0, m = 0

$$\sigma(t) = \frac{\sigma_0}{(3AE\sigma_0^3 t + 1)^{1/3}}$$



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Validation for LWR Fuel

- Validation of Bison is a continuing area of emphasis
- Our strong preference is comparison to experimental data versus comparison to other codes

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ELSEVIER

Validating the BISON fuel performance code to integral LWR experiments

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HIGHLIGHTS

- The BISON multidimensional fuel performance code is being validated to integral LWR experiments.
- Code and solution verification are necessary prerequisites to validation.
- Fuel centerline temperature comparisons through all phases of fuel life are very reasonable.
- Accuracy in predicting fission gas release is consistent with state-of-the-art modeling and the involved uncertainties.
- Rod diameter comparisons are not satisfactory and further investigation is underway.

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ABSTRACT

BISON is a modern finite element-based nuclear fuel performance code that has been under development at Idaho National Laboratory (INL) since 2009. The code is applicable to both steady and transient fuel behavior and has been used to analyze a variety of fuel forms in 1D spherical, 2D axisymmetric, or 3D geometries. Code validation is underway and is the subject of this study. A brief overview of BISON's computational framework, governing equations, and general material and behavioral models is provided. BISON code and solution verification procedures are described, followed by a summary of the experimental data used to date for validation of Light Water Reactor (LWR) fuel. Validation comparisons focus on fuel centerline temperature, fission gas release, and rod diameter both before and following fuel-clad mechanical contact. Comparisons for 35 LWR rods are consolidated to provide an overall view of how the code is predicting physical behavior, with a few select validation cases discussed in greater detail. Results demonstrate that (1) fuel centerline temperature comparisons through all phases of fuel life are very reasonable with deviations between predictions and experimental data within ±10% for early life through high burnup fuel and only slightly out of these bounds for power ramp experiments, (2) accuracy in predicting fission gas release appears to be consistent with state-of-the-art modeling and with the involved uncertainties and (3) comparison of rod diameter results indicates a tendency to overpredict clad diameter reduction early in life, when clad creepdown dominates, and more significantly overpredict the diameter increase late in life, when fuel expansion controls the mechanical response. Initial rod diameter comparisons are not satisfactory and have led to consideration of additional separate effects experiments to better understand and predict clad and fuel mechanical behavior. Results from this study are being used to define priorities for ongoing code development and validation activities.

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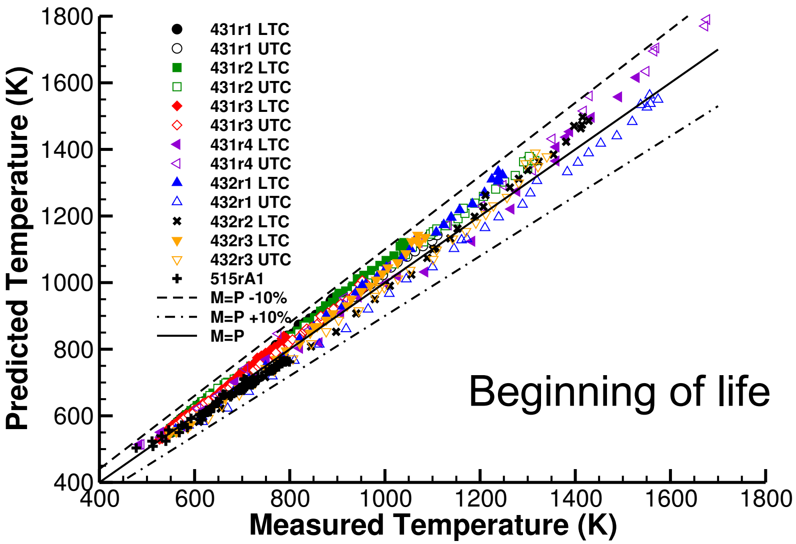
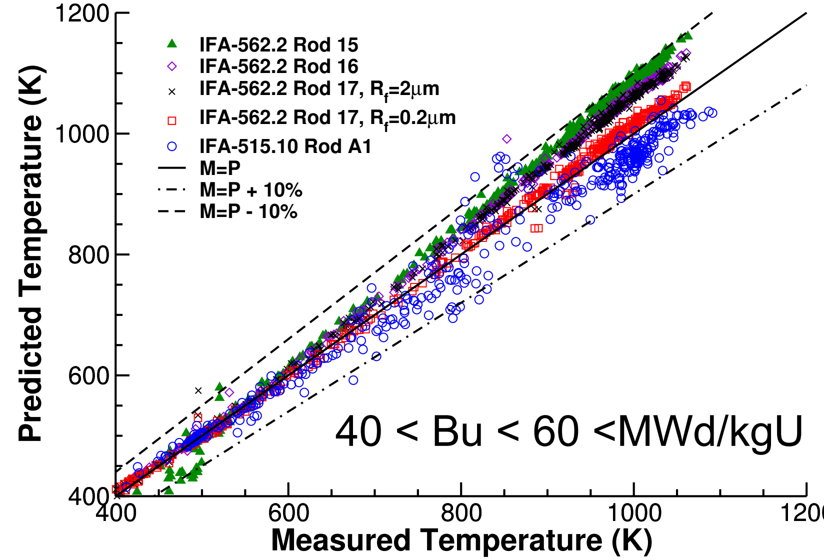
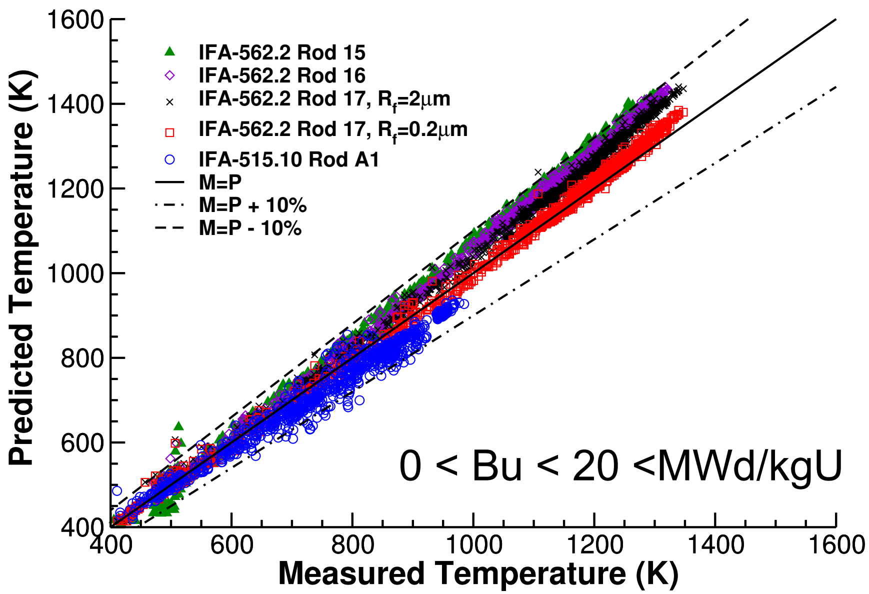
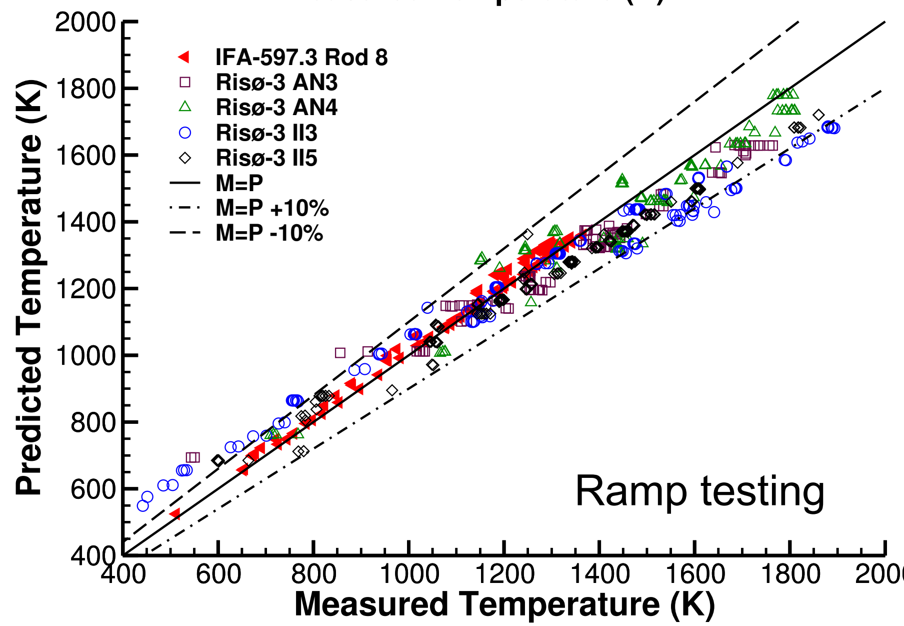
LWR Validation – Fuel Centerline Temperature









Bison Summary

- **Bison is an engineering-scale, finite element code for nuclear fuel performance analysis**
- **Bison is flexible**
  - Accepts user-defined meshes/geometries
    - 1D, 2D, or 3D
  - Runs on one processor or many
  - Analyzes a variety of fuel types
    - LWR, TRISO, plate, metal, etc.
  - Couples to other analysis codes
- **More information is at https://bison.inl.gov**
- **Or, contact me, jason.hales@inl.gov**

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- Russell Gardner
- Wen Jiang
- Steve Novascone
- Giovanni Pastore
- Danielle Perez
- Stephanie Pitts
- Ben Spencer
- Mudasar Zahoor

- The MOOSE Team

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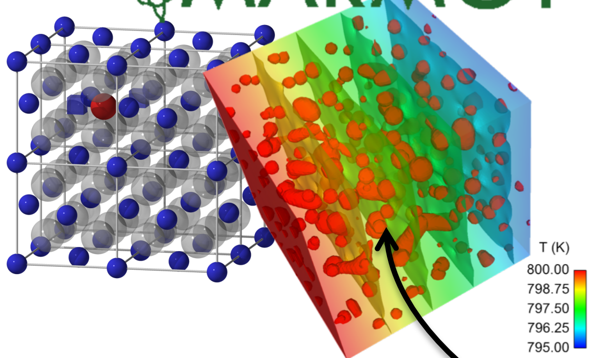
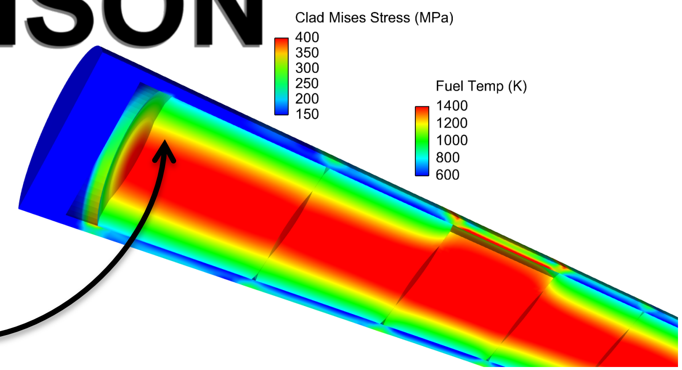
MOOSE-Bison-Marmot

- **The MOOSE-Bison-Marmot codes provide an advanced multiphysics multiscale fuel performance capability**

MARMOT



BISON



Atomistic/Mesoscale Material Model Development

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

Advanced 3D Fuel Performance Code

- Models LWR, TRISO and metal fuels in 1D, 2D and 3D
- Steady and transient reactor operations

MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework allowing rapid development of FEM-based applications

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What Marmot does