U.S. DEPARTMENT OF ENERGY | Office of Nuclear Energy

OVERVIEW of FUEL PERFORMANCE MODELING (BISON):

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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NRC-DOE Third Workshop on Advanced Reactors

Bethesda, MD

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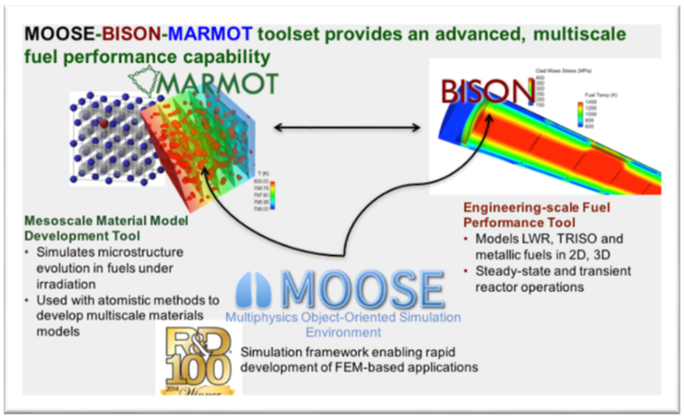
NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

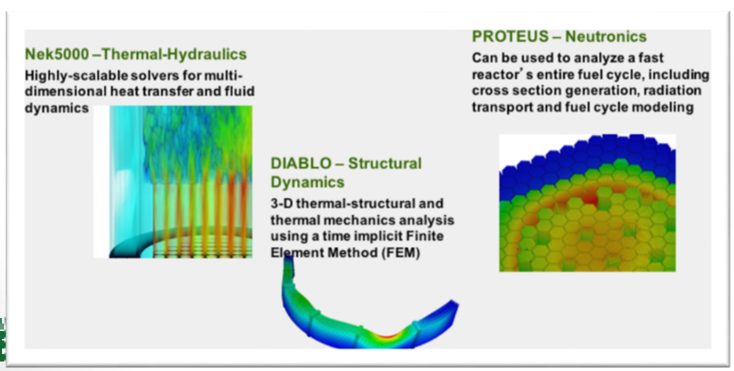
NEAMS (Nuclear Energy Advanced Modeling and Simulation) Program

Aim: Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

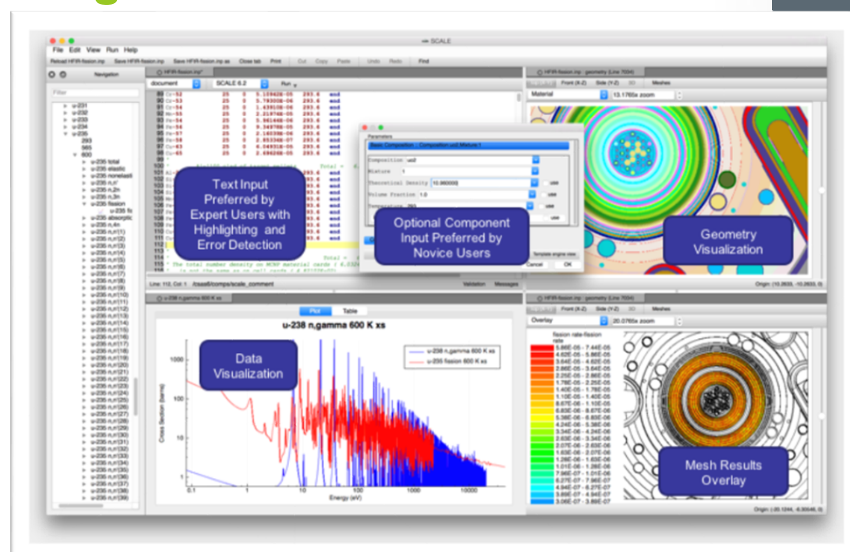
Fuels Product Line



Reactor Product Line



Integration Product Line



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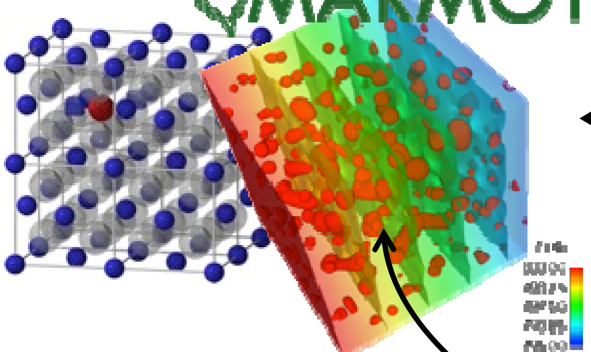
NEAMS Fuels Tools:

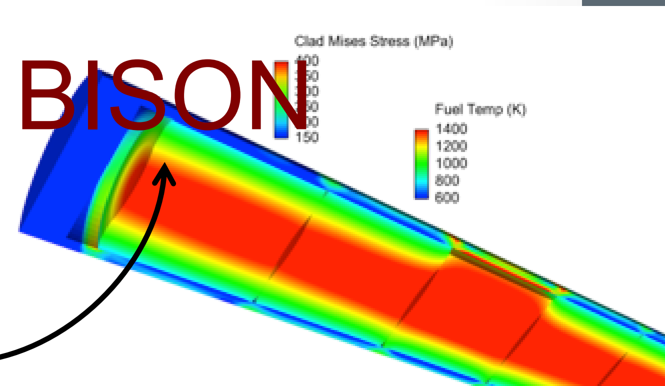
MBM: MOOSE-BISON-MARMOT

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

MARMOT



BISON



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

R&D 100 2014 Winner

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Hierarchical Multiscale Fuel Modeling

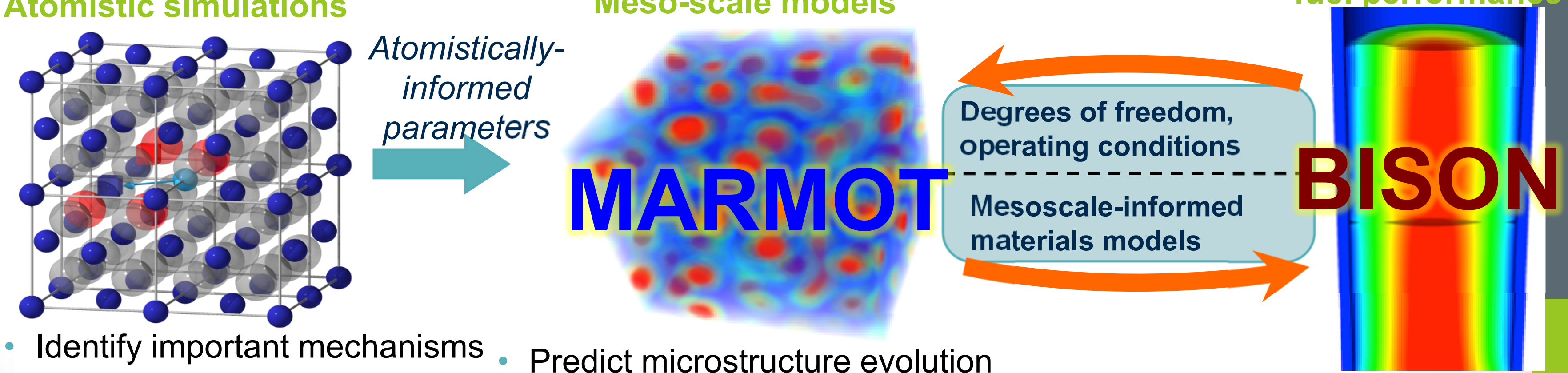
- Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds

- **Goal:** Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling - applied to existing, advanced (including accident tolerant) and used fuel.

Atomistic simulations

Meso-scale models

Engineering scale fuel performance



- Identify important mechanisms
- Determine material parameter values

- Predict microstructure evolution
- Determine effect of evolution on material properties

- Predict fuel performance and failure probability

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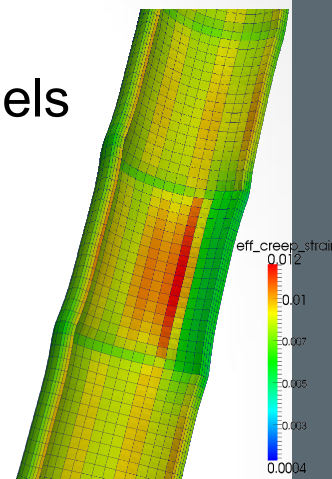
BISON Features



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

Potential Role for BISON in Licensing

- **For LWRs:**
  - Relatively limited use by NRC or vendors for UO_2/Zr designs
  - However, collaboration with NRC/Frap on materials/behavioral models worth pursuing
  - Potential for more expanded role for advanced LWR fuel, e.g. ATF

- **For advanced reactors:**
  - Different use case may exist for BISON than for LWRs
  - Potentially utilized by NRC for confirmatory analysis
  - Also, perhaps possible for code to maintain independence and thus also be used by vendors
  - Use as an R&D tool also remains important

NEAMS "High Impact Problems"

- High impact program concept introduced as a mechanism by which to direct NEAMS tools to address problem of applied relevance.
  - Core program is the "chassis" upon which HIP is built
- 3-year, ~$3M projects with a defined customer.
- Two HIPs initiated in FY15:
  - *Evaluation of Representative Accident Tolerant Fuel (ATF) Candidates for the Advanced Fuels Campaign*
    - Customer = DOE Advanced Fuels Campaign (and by extension, ATF vendors)
  - *Numerical Evaluation of Advanced Steam Generators for SMRs*
    - Customer = NuScale

NEAMS is currently designing FY18 HIP program to center around GAIN-relevant topics.

GAIN Gateway for Accelerated Innovation in Nuclear

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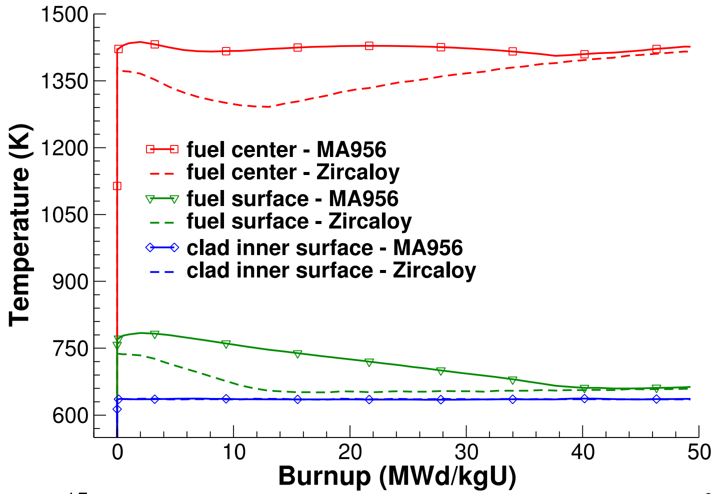
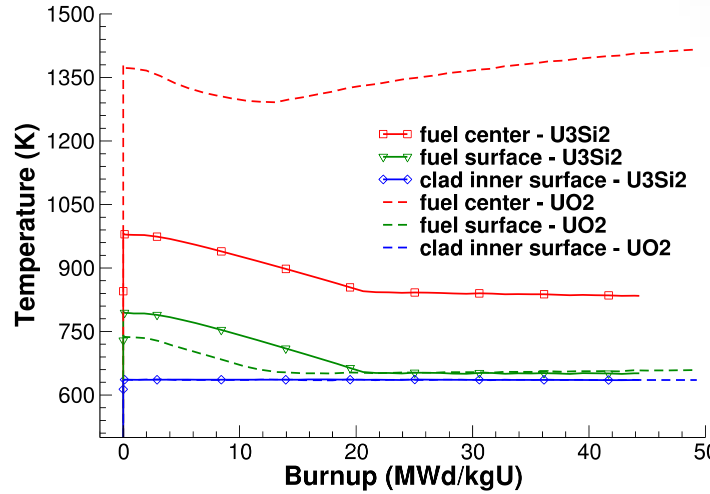
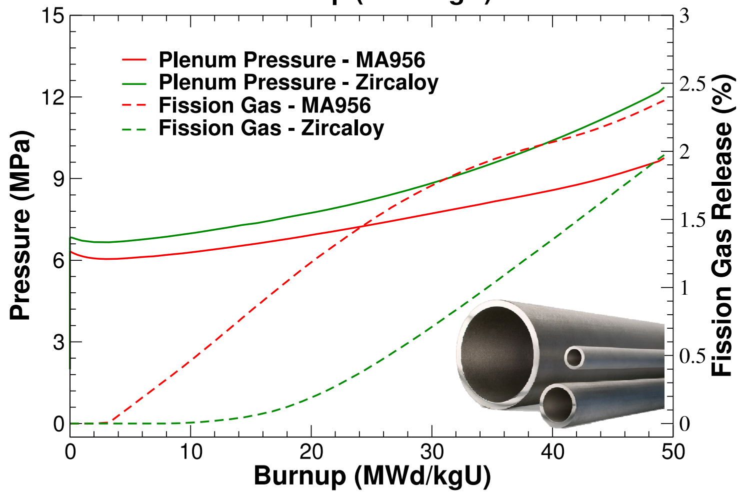
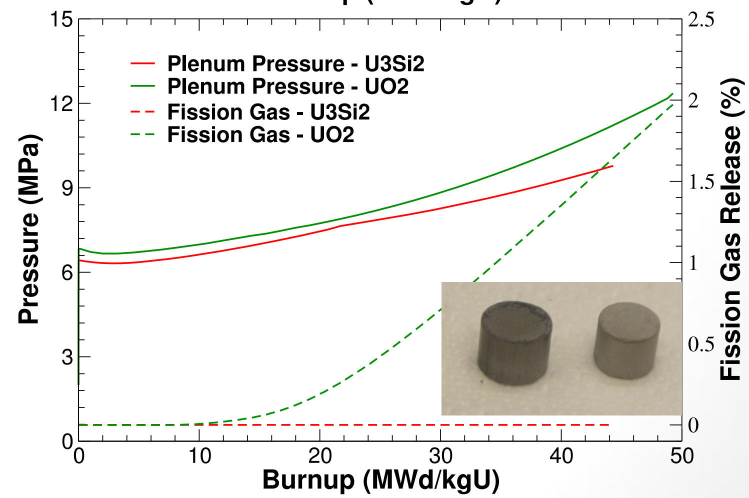
Application of BISON to ATF









Atomistic Simulations of Cr-doped UO_2

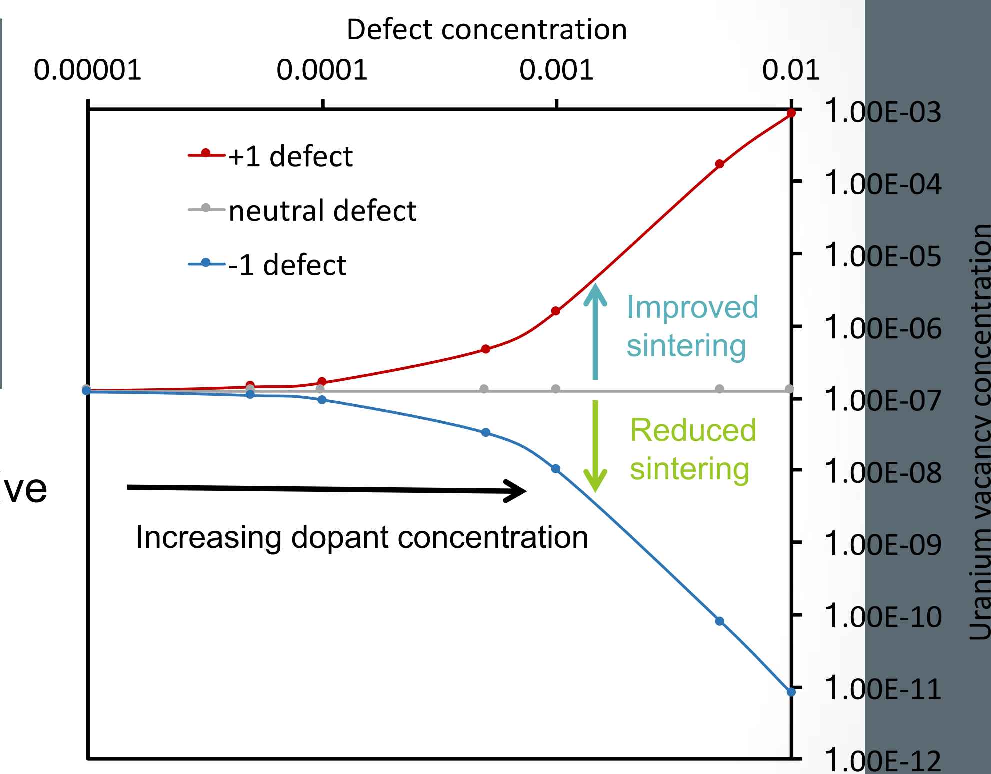
Use of first principles modeling to explain the detailed role of Cr.

Understanding of Cr solution required, e.g. to develop accurate Cr-UO_2 fission gas release model.

Modeling of intrinsic defects shows that positive defects would increase the uranium vacancy concentration, and thus sintering kinetics.

$\boxed{Cr_U''}$ vs $\boxed{Cr_I^{\bullet\bullet}}$

$$Cr_U'' \rightarrow Cr_I^{\bullet\bullet} + V_U''''$$



Preliminary DFT modeling that includes both enthalpy and entropy indicates that $\boxed{Cr_I^{\bullet\bullet}}$ is important

This points towards $\boxed{Cr_I^{\bullet\bullet}}$ in solution as mechanism for enhanced sintering

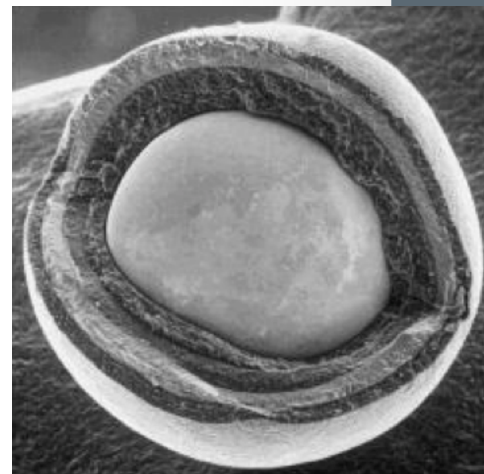
Extension of BISON for Particle Fuel

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

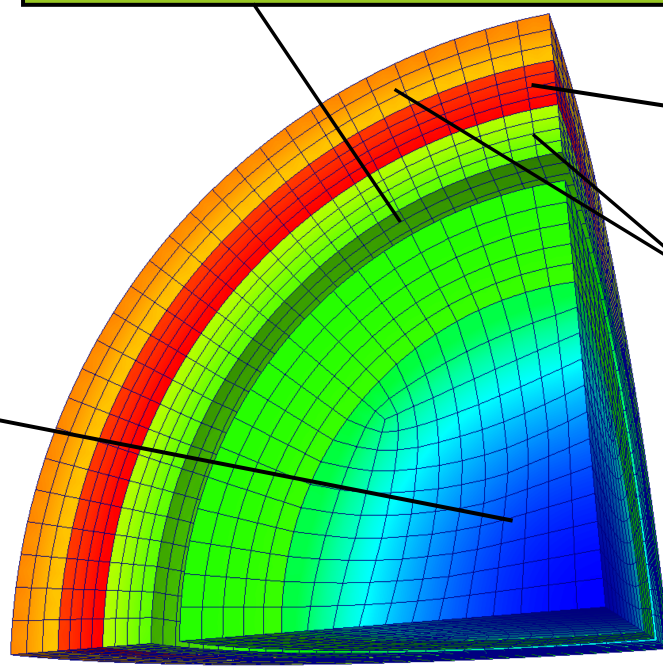
Gap Behavior

- 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

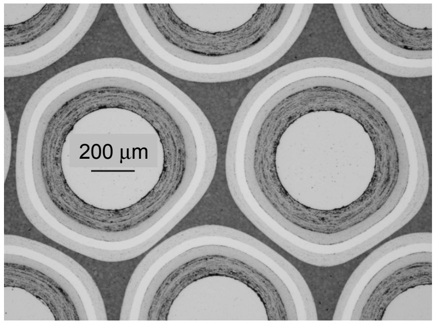
- irradiation creep

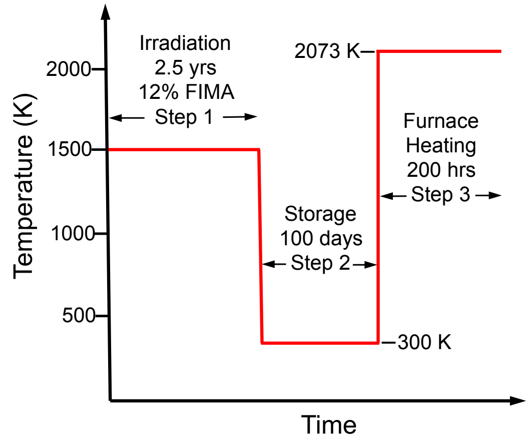
Pyrolytic Carbon

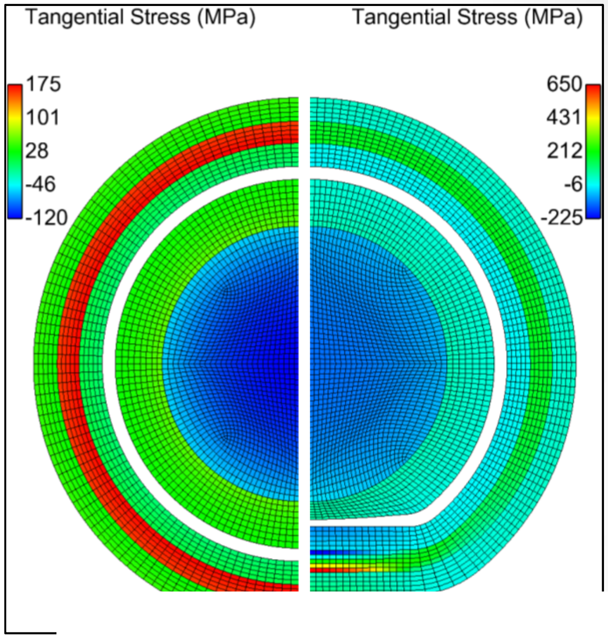
- Anisotropic irradiation-induced strain
- Irradiation creep

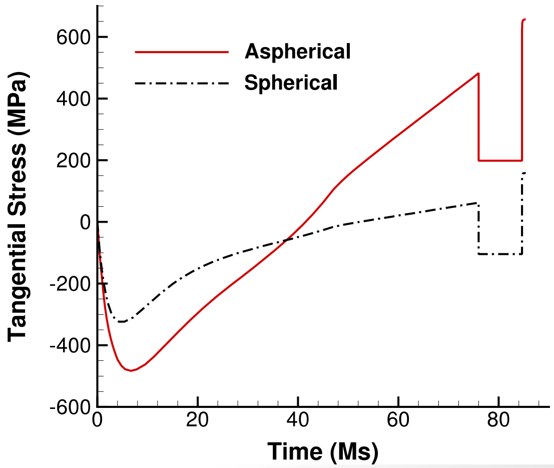
BISON Analysis of Aspherical Particles

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





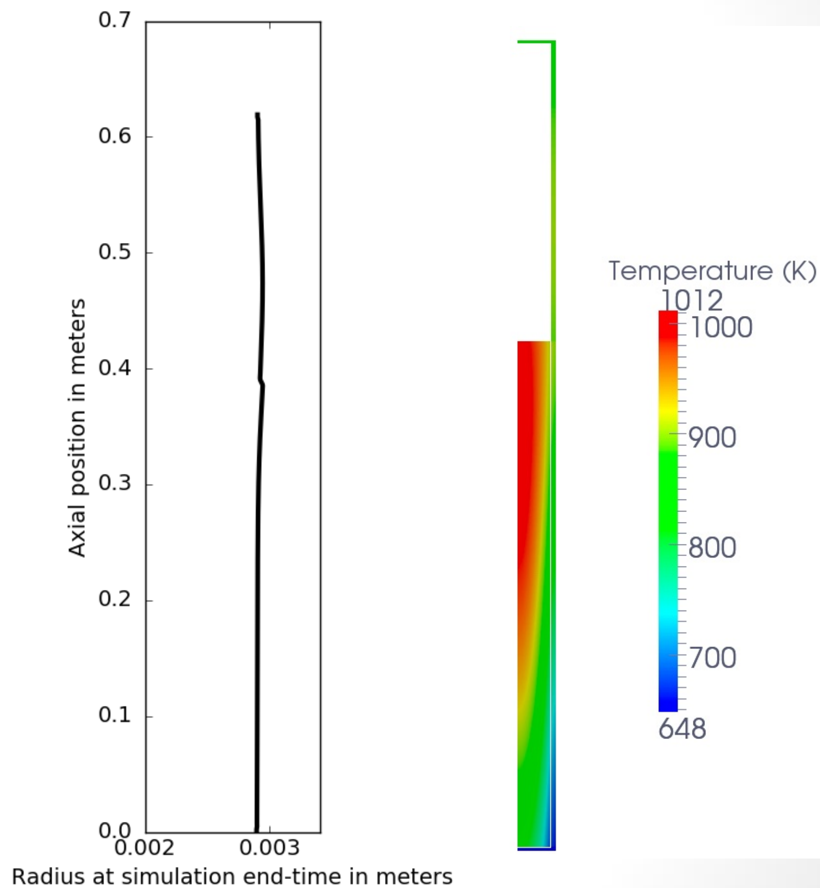




- During accident testing, asphericity raises peak tensile stress in SiC containment layer by almost 4x
- Typical run times of a few minutes on 8 processors

Example of BISON Analysis for Metallic 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



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Emphasis on SQA:

Code testing and verification

- BISON thru MOOSE is supported by >2000 unit and regression tests
- All new code must be supported by regression testing
- All tests are run and must pass prior to any code modification
- Current line coverage is at 85%
- Paper in *Ann. Nucl. Energy* provides detailed description.

LCOV - code coverage report

			Hit	Total	Coverage
Current view:	top level				
Test:	BISON Test Coverage	Lines:	14070	16450	85.5 %
Date:	2017-01-10 14:48:50	Functions:	1736	2020	85.9 %
Legend:	Rating: low: < 70 % medium: >= 70 % high: >= 80 %				

Directory	Line Coverage		Functions	
include/actions	93.3 %	14 / 15	63.3 %	19 / 30
include/auxkernels	89.7 %	26 / 29	46.6 %	27 / 58
include/auxkernels/tensor_mechanics	100.0 %	1 / 1	50.0 %	1 / 2
include/base	100.0 %	2 / 2	-	0 / 0
include/bcs	69.2 %	9 / 13	36.4 %	8 / 22
include/bcs/coolant	100.0 %	4 / 4	50.0 %	1 / 2
include/functions	61.0 %	111 / 182	78.6 %	11 / 14
include/ics	100.0 %	1 / 1	100.0 %	2 / 2
include/kernels	80.0 %	12 / 15	43.3 %	13 / 30
include/materials	78.6 %	121 / 154	58.2 %	96 / 165
include/materials/tensor_mechanics	92.9 %	39 / 42	56.8 %	21 / 37
include/postprocessors	100.0 %	19 / 19	60.6 %	20 / 33
include/userobject	91.7 %	11 / 12	82.4 %	14 / 17
src	92.3 %	12 / 13	100.0 %	3 / 3
src/actions	85.4 %	634 / 742	97.3 %	72 / 74

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ELSEVIER

Verification of the BISON fuel performance code

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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

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Emphasis on Validation

- Recent (2016) paper in *Nuclear Engineering and Design* describes status of BISON validation
- 72 steady state LWR cases, 21 ramp, 5 accident + >10 TRISO
- Validation areas
  - Fuel centerline temperature through all phases of fuel life
  - Fission gas release
  - Clad diameter (PCMI)

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Validating the BISON fuel performance code to integral LWR experiments

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H I G H L I G H T S

- 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.

A R T I C L E I N F O

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A B S T R A C T

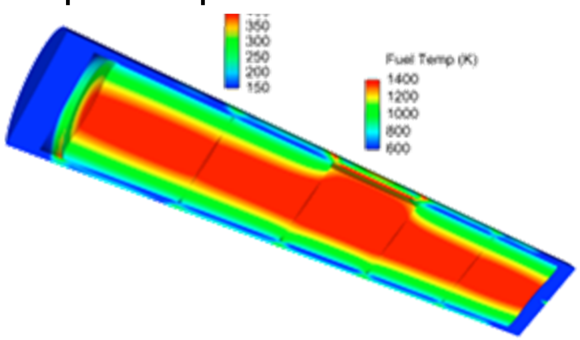
BISON is a modern finite element-based nuclear fuel performance code that has been under development at Idaho National Laboratory (INL) since 2009. The code is applicable to both steady and transient fuel behavior and has been used to analyze a variety of fuel forms in 1D spherical, 2D axisymmetric, 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.

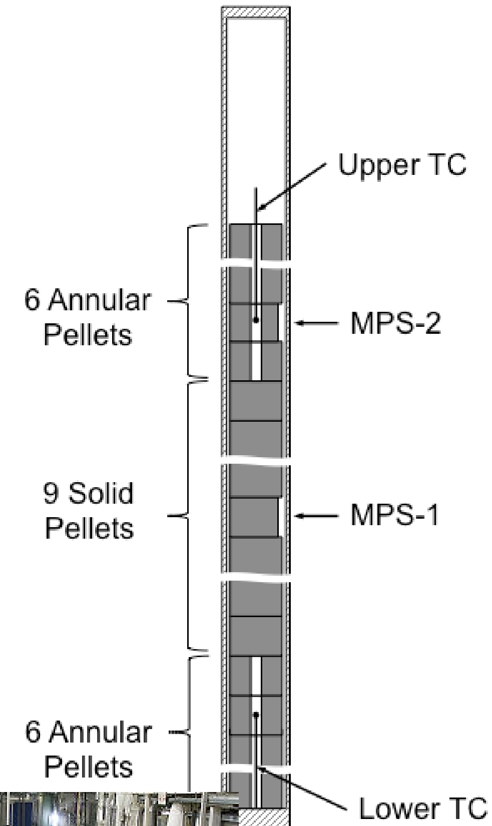
Advanced Validation:
Halden Missing Pellet Surface Experiment

Manufacturing flaws ("missing pellet surface" defects) in fuel pellets have been root cause of fuel failures. Pellet-cladding interaction (PCI) is a CASL challenge problem.

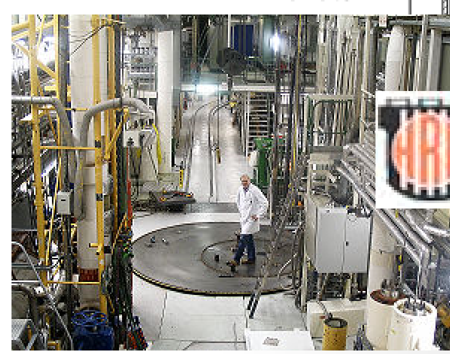
Validation experiments being planned for the Halden reactor later this year.

Example of a 3D fuel performance code addressing a 3D applied problem – which requires specific validation





Once validated, further analysis using BISON to define an MPS geometry threshold could used to inform fuel manufacturing tolerances.



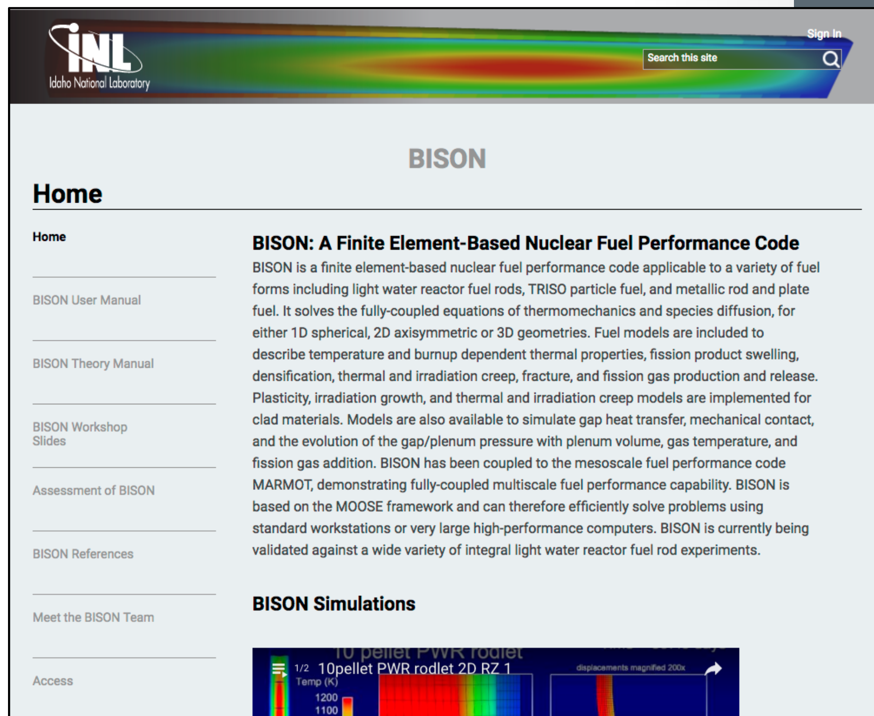
The OECD Halden Reactor Project

Obtaining BISON, Training, Hardware Requirements

BISON is obtained via INL license.
Export controlled (2D290).

Training held several times per year.
Materials @ https://bison.inl.gov

Computer requirements: laptop to supercomputer



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Summary

- Relative maturity of DOE-NE advanced mod-sim tools is coinciding with surge in advanced reactor start ups.

- A particular "critical path" issue (though there are many, e.g. validation) of immediate interest relevant to advanced mod-sim: *connecting mod-sim capability with industrial (advanced reactor) need.*

- GAIN initiative is catalyzing necessary interactions between NEAMS (and other DOE-NE programs) and advanced reactor industry community that will enable productive use of advanced mod-sim tools.

- Future may include use of some DOE-NE advanced mod-sim tools for NRC confirmatory calculations. If those codes maintain independence, potential exists for their use also in license application.

- Apart from licensing, many R&D issues exist where advanced mod-sim can assist, by e.g. revealing governing phenomena, targeting experiments, etc.