INL/MIS-24-77144-Revision-0

BISON: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms

March 2024

Changing the World's Energy Future

Kyle A Gamble

Idaho National Laboratory

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Kyle A. Gamble, Ph. D.

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INL/MIS-24-77144

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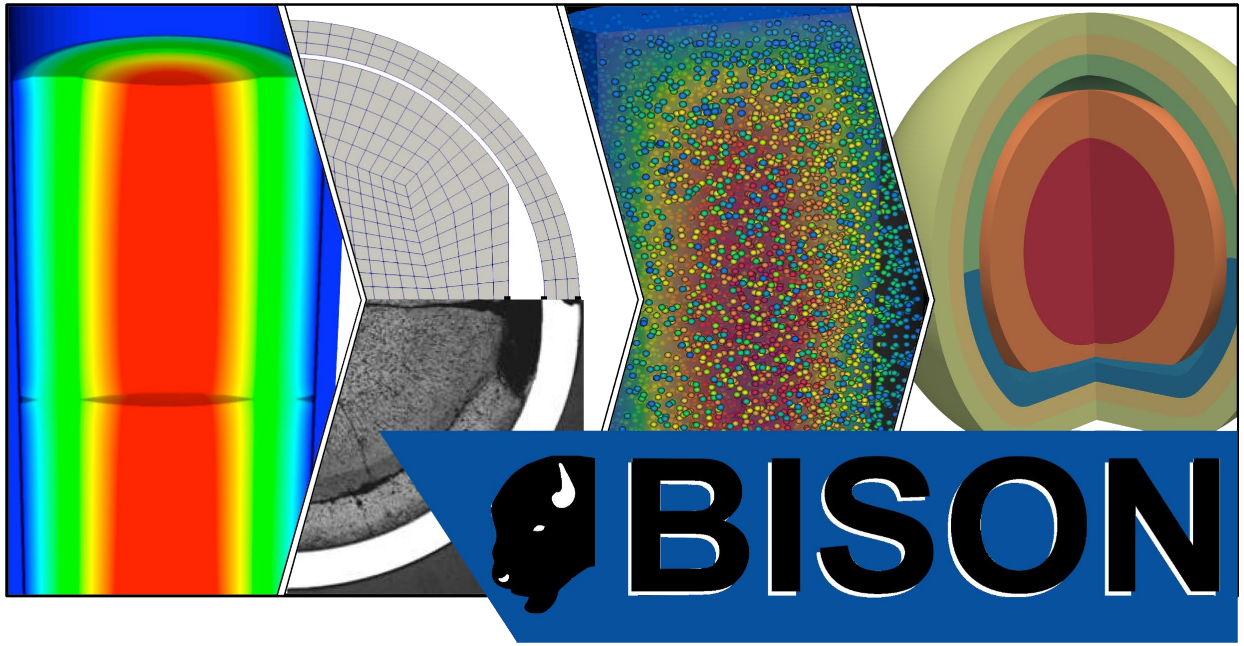
Outline

- Introduction
- History and Timeline
- Tributes to Key Contributors
- Applications to various Nuclear Fuel Forms
  - Light Water Reactor (LWR) Fuel
  - Accident Tolerant (Advanced Technology) (ATF) Fuel
  - Fast Reactor Mixed Oxide (MOX) Fuel
  - Metallic Fast Reactor Fuel
  - TRIstructural ISOtropic (TRISO) Fuel

What is BISON?

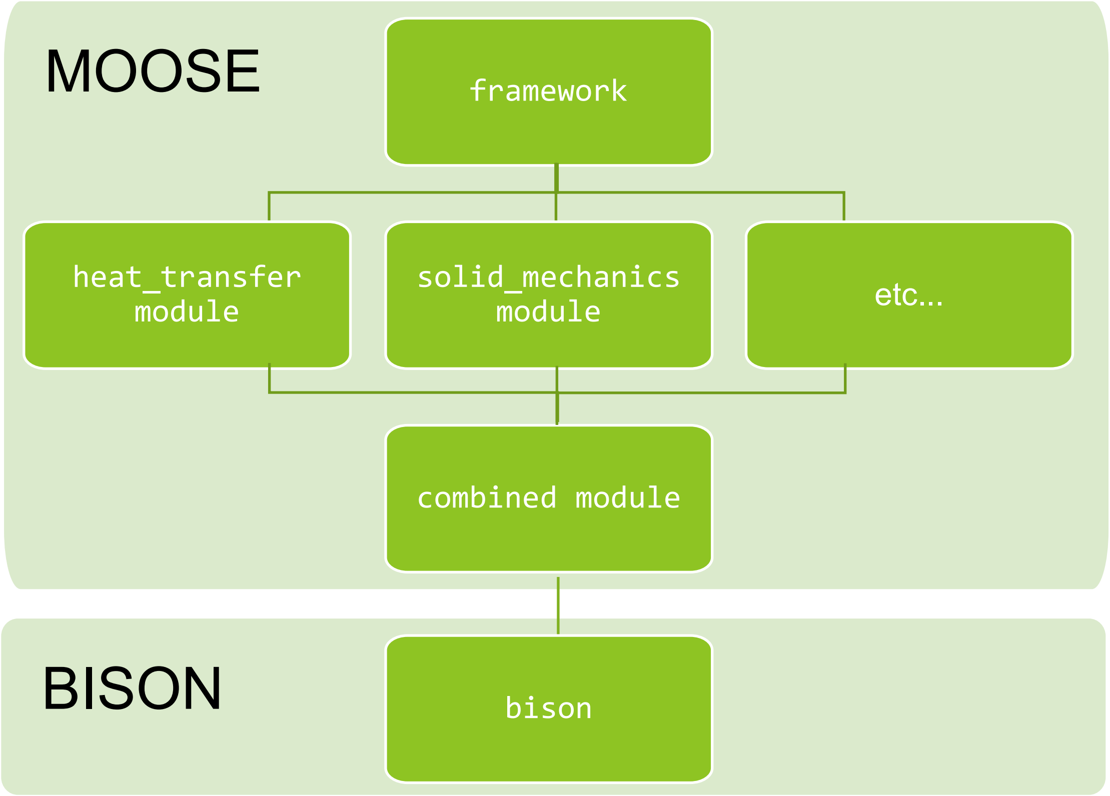
- BISON is a finite element-based nuclear fuel performance code
  - Evaluate the thermo-mechanical behavior of nuclear fuels under a wide variety of operational conditions
- Development primarily funded by a variety of sources within the Department of Energy Office of Nuclear Energy
- BISON is based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) Framework
- BISON
  - Is free to use
  - Attracts diverse users and developers
  - Is used for engineering and research
  - Inherently considers multiphysics
  - Can couple to multiscale codes
  - Scales well from laptops to clusters
  - Features a flexible, modular design
  - Is under continuous development
  - Follows rigorous SQA practices

2021 R&D 100 WINNER



MOOSE and BISON code structures and executables

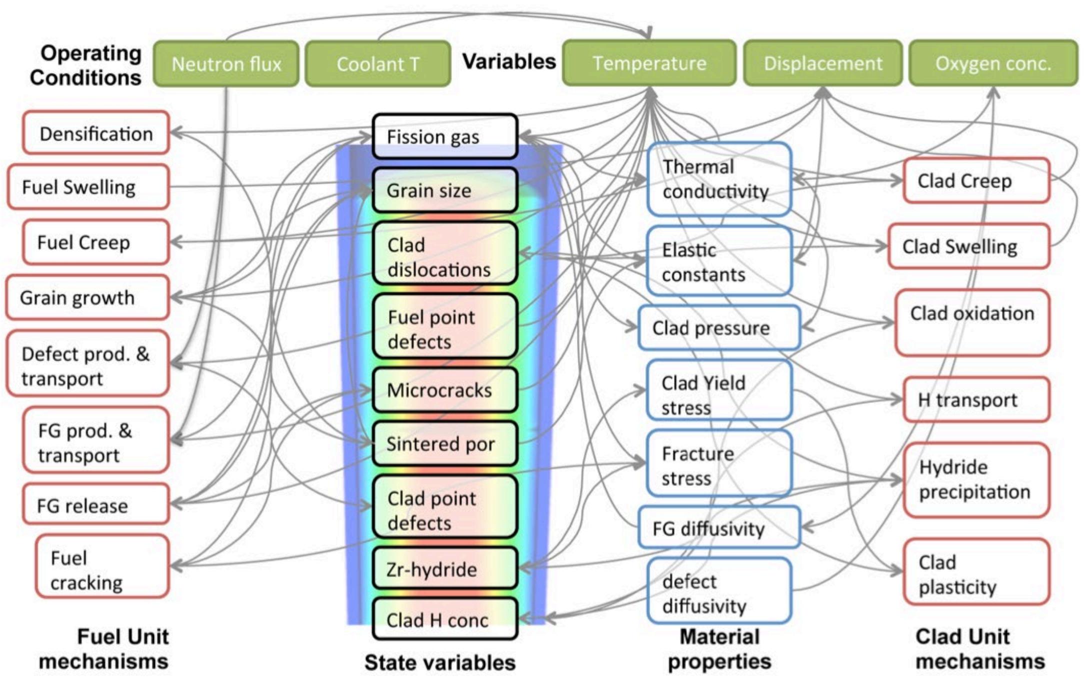
- Basic MOOSE functionality, such as solver and output options, is provided at the `framework` level
  - libMesh (numerical PDE solution framework out of UT Austin) depends on:
    - PETSc, Exodus II, MPI, etc.
- Physics modules such as the `heat_transfer` module, each with an executable, build on the framework level functionality to model individual "branches" of physics
- Other "branches" include `solid_mechanics`, `contact`, `thermal_hydraulics`, and more
- The combined physics module has access to all the others, enabling multiphysics functionality
- BISON captures the above functionality and provides additional fuel performance capabilities
  - Fission gas behavior, burnup, irradiation effects



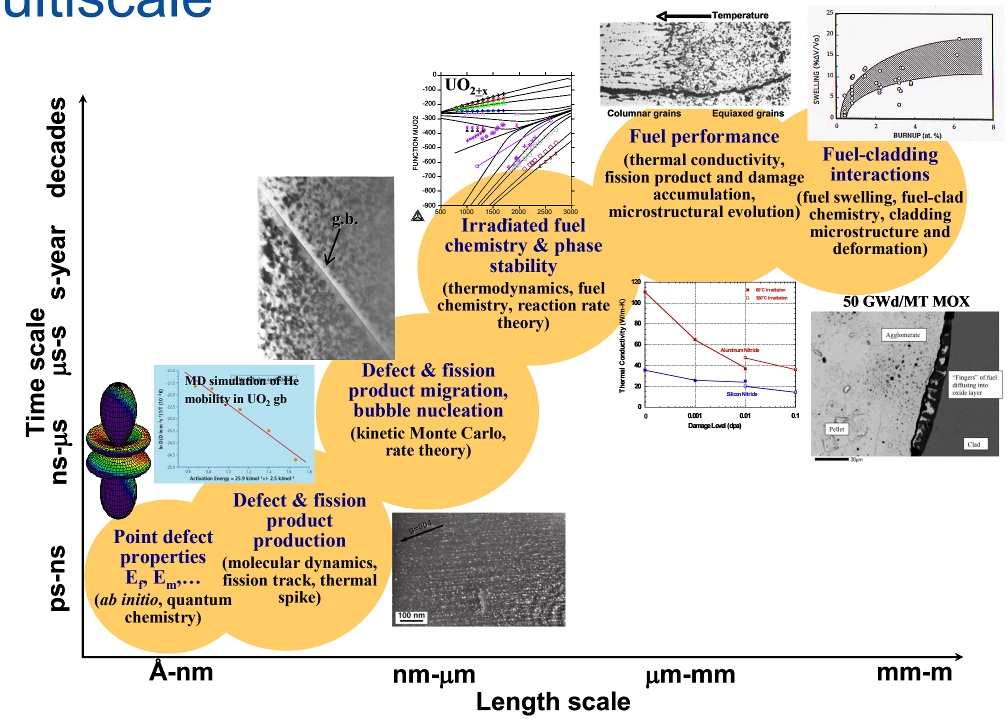
Adapted from R. T. Sweet

There are many reasons to study fuel performance

- To develop, deploy, and support nuclear reactor technology
- To conduct research and acquire fundamental knowledge
- Because it's interesting: multiphysics and multiscale



M.R. Tonks, et al., "Mechanistic materials modeling for nuclear fuel performance," Ann. Nucl. Energy, 105 (2017) 11–24.



Adapted from works by Brian Wirth (ORNL, University of Tennessee - Knoxville)

Courtesy of R. T. Sweet

BISON Timeline

2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 | 2016

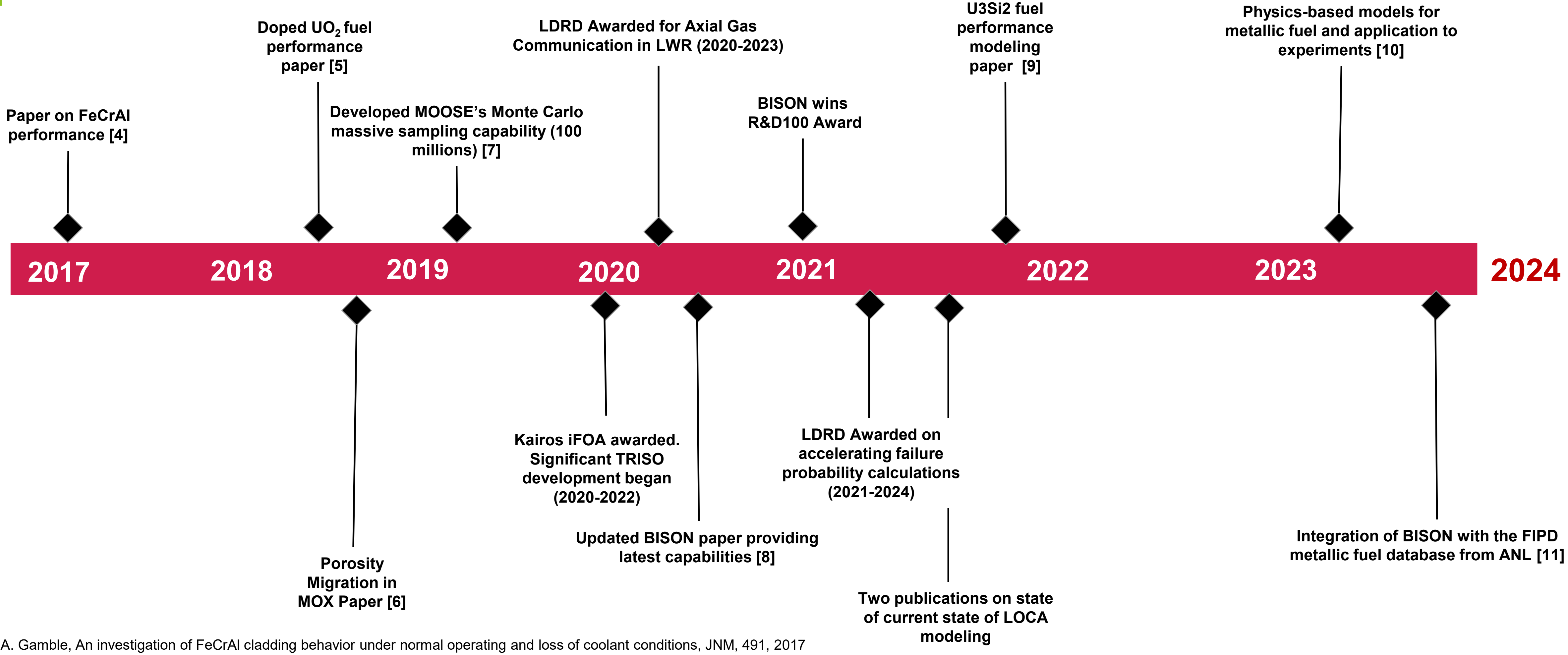
- **2012:** First major BISON paper was published. Paper focused on LWR fuel but also had a TRISO example [1].
- **2013:** The BISON team decided to add a baseline TRISO capability, including thermal, mass diffusion, and mechanical models. A first BISON TRISO paper was published.[2]
- **2013:** LDRD Awarded for implementation of advanced fracture models awarded (2013-2016)
- **2014:** ATF development began for priority fuel and cladding concepts.
- **2014:** LDRD Awarded for implementation of initial LOCA capabilities funded (2014-2017)
- **2016:** First validation paper assessing LWR capability performance during normal operation [3]

- **Several main papers, funding sources, and capability development start dates highlighted.**
- **BISON has been used in several publications by industry, university, and national laboratories.**

[1] R.L. Williamson et al, Multidimensional multiphysics simulation of nuclear fuel behavior, JNM, 2012
[2] J.D. Hales et al, Multidimensional multiphysics simulation of TRISO particle fuel, JNM, 2013
[3] R. L. Williamson, et al. Validating the BISON fuel performance code to integral LWR experiments, JNM, 2016

9 additional TRISO publications since [7] between 2019 and 2022

BISON Timeline: Continued



[4] K.A. Gamble, An investigation of FeCrAl cladding behavior under normal operating and loss of coolant conditions, JNM, 491, 2017

[5] Y. Che, Modeling of Cr2O3-doped UO2 as a near-term accident tolerant fuel for LWRs using the BISON code, NED, 337, 2018

[6] S. Novascone, "Modeling porosity migration in LWR and fast reactor MOX fuel using the finite element method, JNM, 508, 2018

[7] W. Jiang et al, TRISO particle fuel performance and failure analysis with BISON, JNM, 548, 152795, 2021

[8] R.L. Williamson, et al, BISON: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms, NT, 2020

[9] K. A. Gamble, et al., Improvement of the BISON U3Si2 modeling capabilities based on multiscale developments to modeling fission gas behavior, JNM, 555, 153097, 2021

[10] C. Matthews, et al., Development and formulation of physics based metallic fuel models and comparison to integral irradiation data, JNM, 578, 2023

[11] Y. Miao et al., BISON-FIPD integration enhanced low-burnup SFR metallic fuel swelling model evaluation framework, NED, 414, 112611, 2023.

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UNIVERSITY OF MICHIGAN

OntarioTech UNIVERSITY

WISCONSIN UNIVERSITY OF WISCONSIN–MADISON

Richard Williamson (Team lead 2009 to 2016)

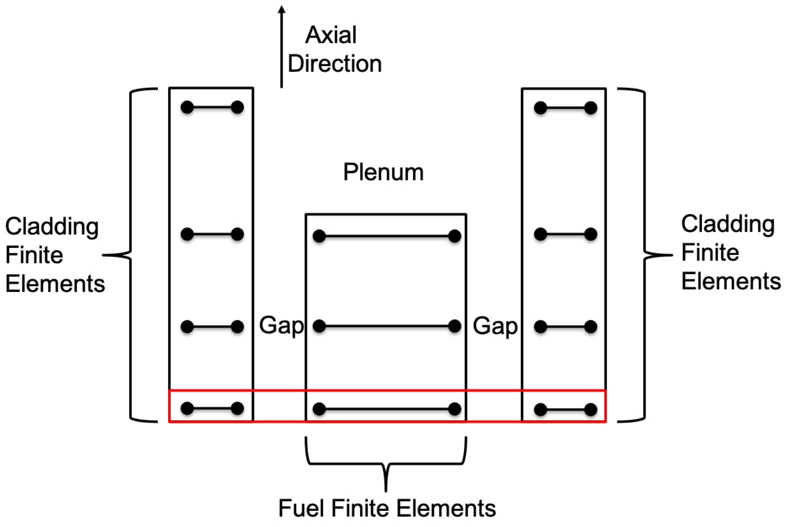
- Spent his entire career at INL, retired as a Laboratory Fellow
- Extensive experience in many key areas of computational modeling research including those important for fuel performance
  - Nonlinear thermo-mechanics
  - Fracture mechanics
- Held senior leadership roles in both NEAMS and CASL for several years.
- Secondee to Halden from 2016-2017
- INL Laboratory Director’s Award for Exceptional Scientific Achievement in 2014

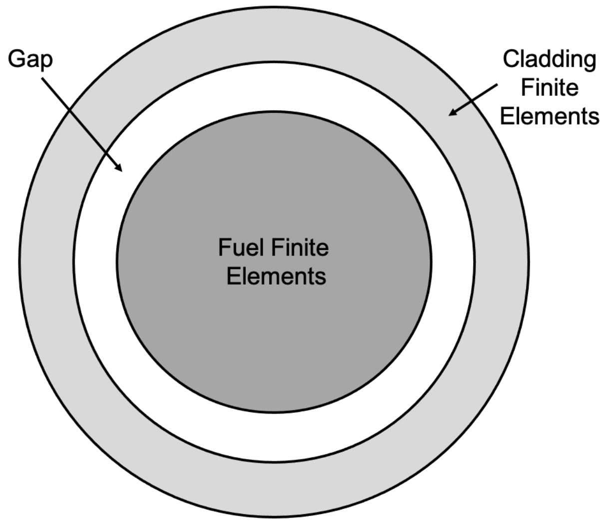
Giovanni Pastore (Team Lead 2017-2020)

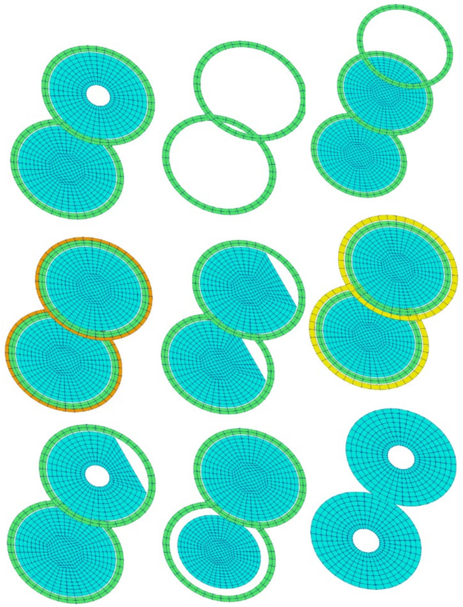
- Joined INL in 2012 as a postdoc, converted to staff in 2013.
- Significantly improved BISON's fission gas behavior modeling and predictions to fission gas release measurements.
- Initiated LOCA capability implementation into the code.
- Twice was a principal investigator for U.S. DOE Scientific Discovery through Advanced Computing (SciDac) projects.
- DOE chief investigator on an International Atomic Energy Agency Coordinated Research Project on accident tolerant fuels
- Secondee to Halden from 2015-2016
- Visiting scientist at MIT 2018

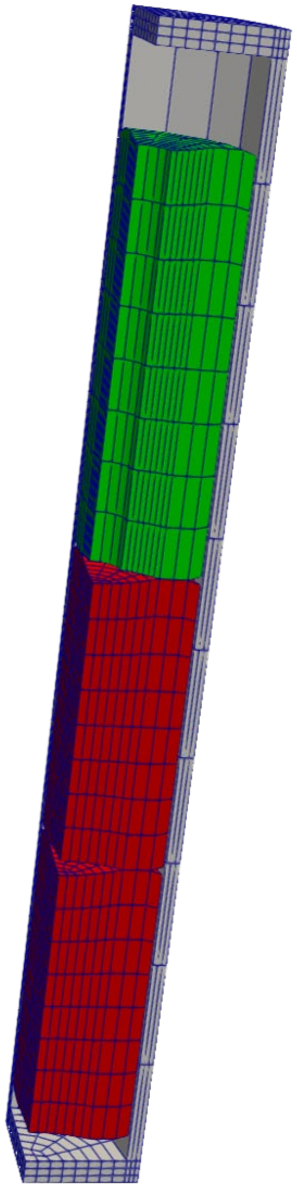
Available Geometric Representations

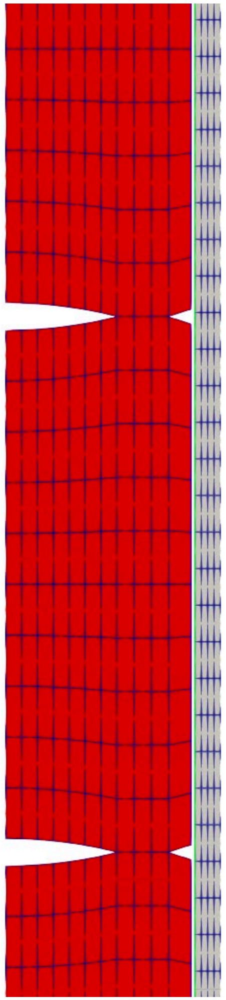
- Layered1D (1.5D)
- Layered2D (2.5D)
- 1D Spherical
- 1D, 2D, 3D Cartesian
- 2D-RZ axisymmetric





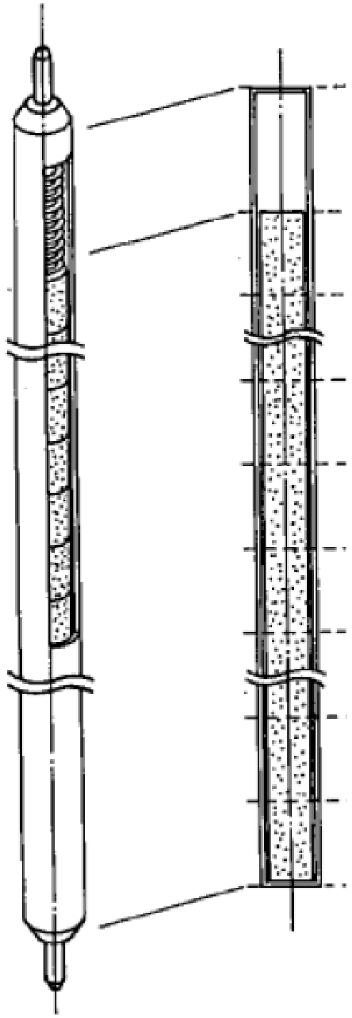


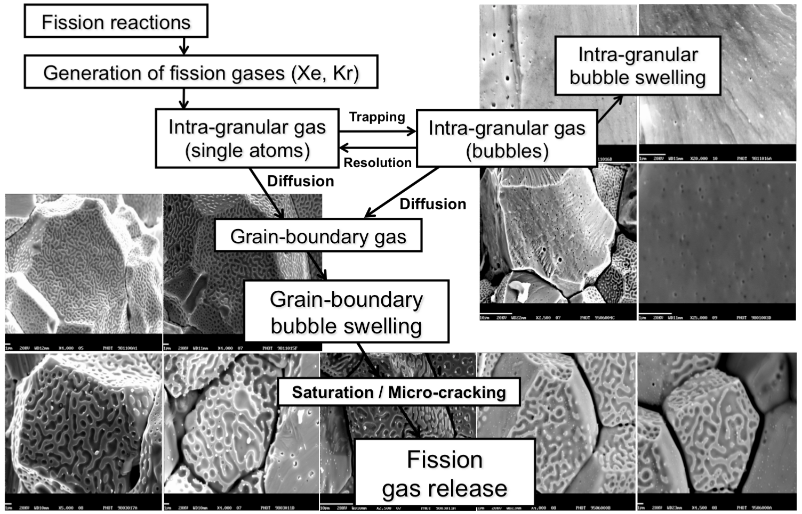




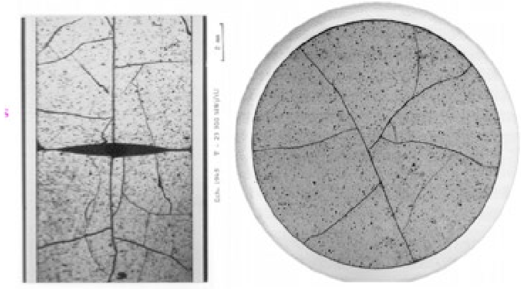
Light Water Reactor Fuel

- Consists of UO_2 fuel with Zirconium-based (Zircaloy) cladding.
- Most common reactor type in operation
- Comes in two flavors:
  - Pressurized Water Reactor
  - Boiling Water Reactor
- BISON historically developed primarily for PWR application.

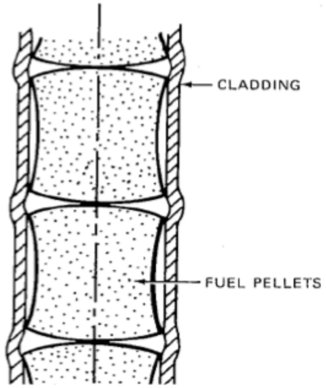




Fission Gas Behavior



Fuel Fracture

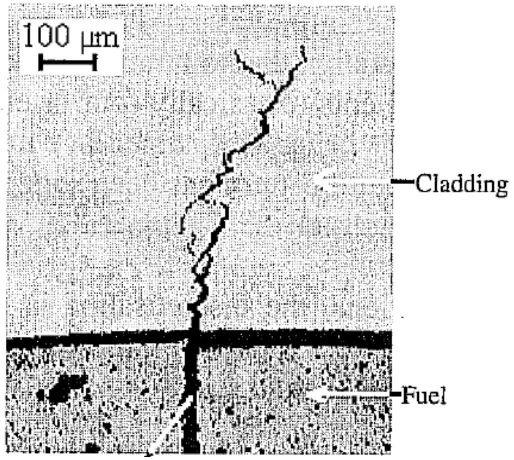


Multidimensional Contact

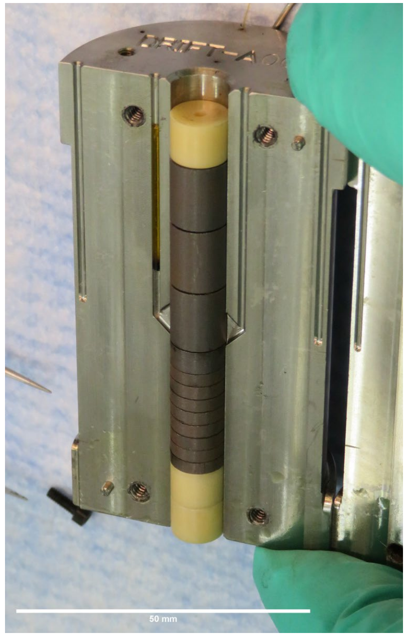
Nakajima et al., Nuc. Eng. Des, **148**, 41 (1994)
Michel et al., Eng. Frac. Mech., **75**, 3581 (2008)
Olander, p. 584 (1978)

Light Water Reactor Fuel: Fracture

- Fracture has multiple important effects on LWR fuel:
  - Affects the stress state in fuel
  - Causes fuel relocation (diameter increase), which influences conductance (due to gap size change)
  - Causes stress concentrations in cladding adjacent to the cracked fuel (see image on right)
  - Affects the thermal conductivity of fuel
  - Creates paths for release of trapped fission gas
  - Permits fuel dispersal in accident scenarios
- Two major efforts have improved and validated the capabilities of BISON for LWR fuel fracture:
  - **2013-2016 LDRD:** Implemented advanced fracture methods (XFEM, DEM, peridynamics) for fuel performance modeling
  - **2016-2021 IRP:** Laboratory and in-reactor experiments (including DRIFT experiments in TREAT reactor) provided validation data on fracture initiation and propagation.



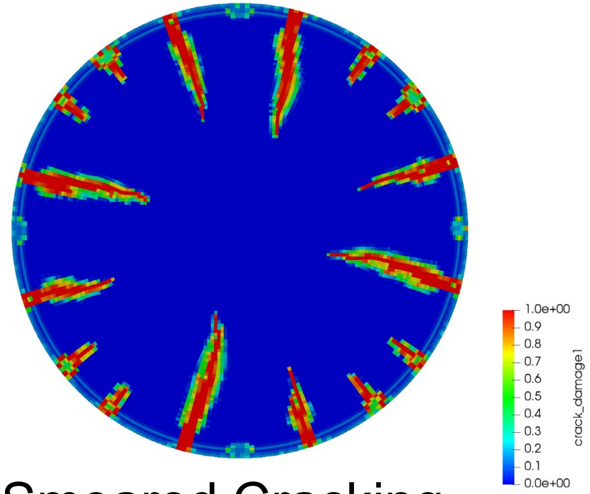
Cladding failure affected by fuel fracture
Bentejac et al., PCI Seminar (2004)



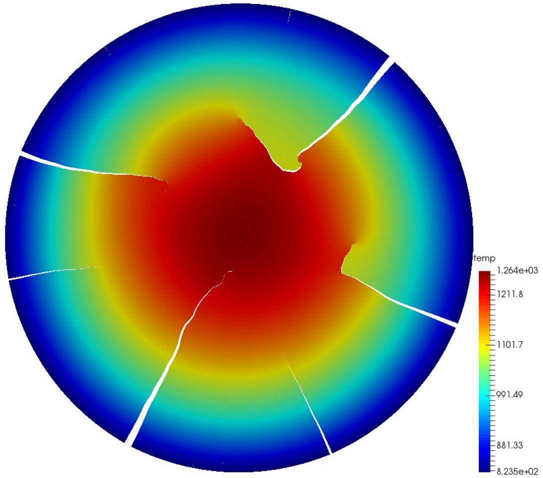
Fuel tested in DRIFT experiment

Light Water Reactor Fuel: Fracture Modeling

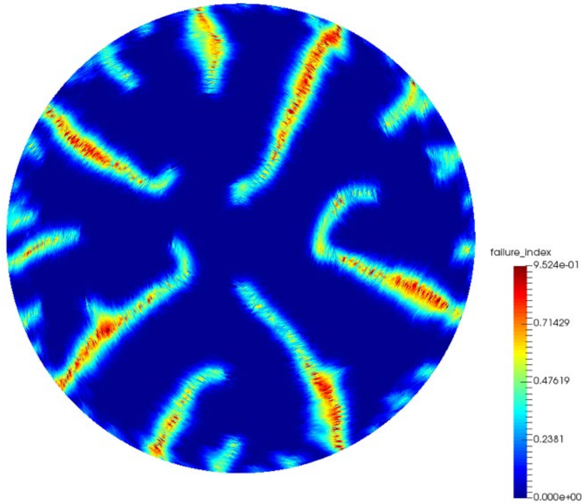
- Fracture modeling methods explored for LWR fuel fracture modeling



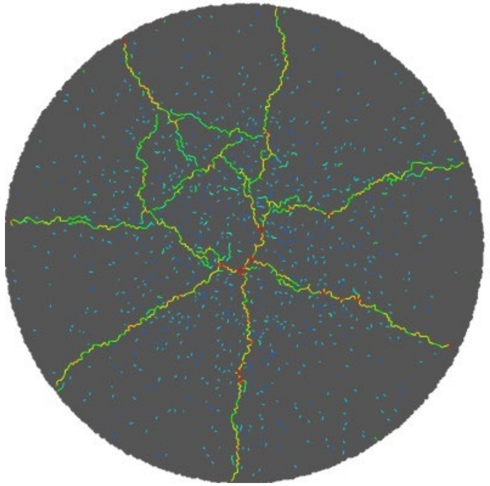
Smeared Cracking



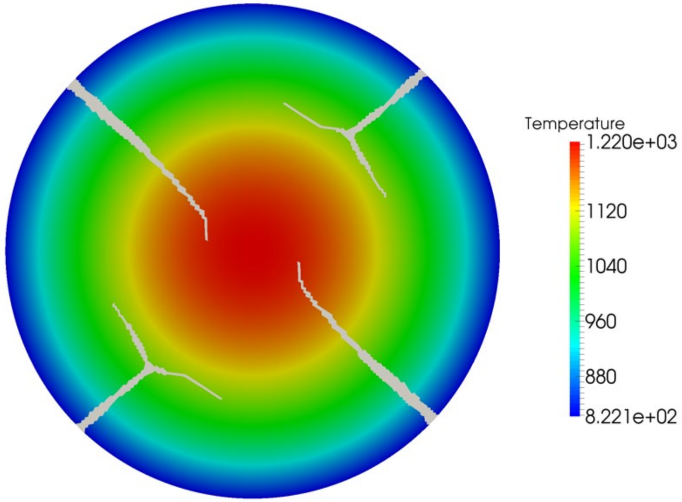
XFEM



Peridynamics



Discrete Element Method



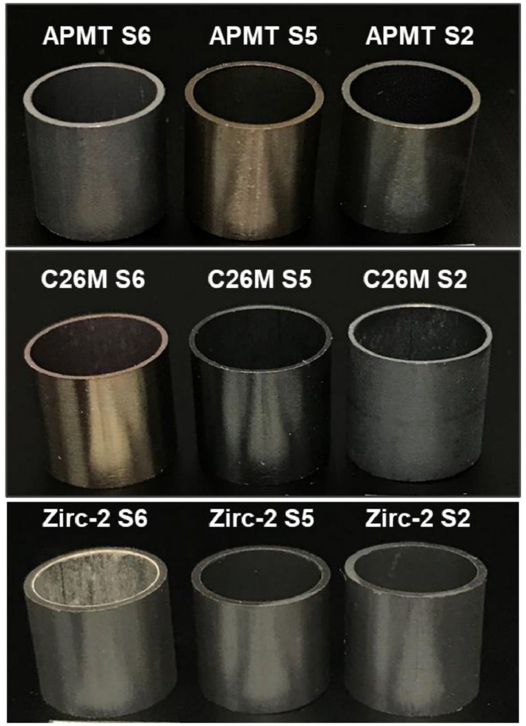
Phase Field

Jiang et al., Eng. Fract. Mech., 223:106713 (2020)
Huang et al., Nucl. Eng. Des., 278:515-528 (2014)
Hu et al., Eng. Fract. Mech., 197:92–113, (2018)

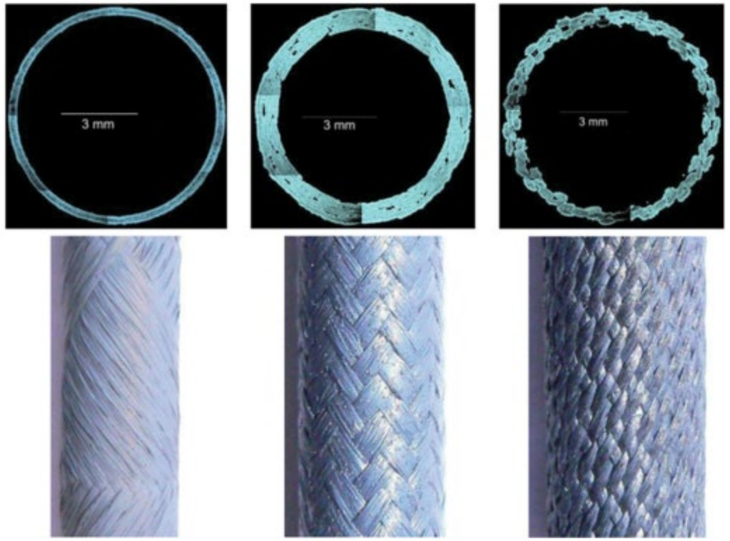
Light Water Reactor Fuel: LOCA Demonstration

Accident Tolerant (Advanced Technology) Fuel

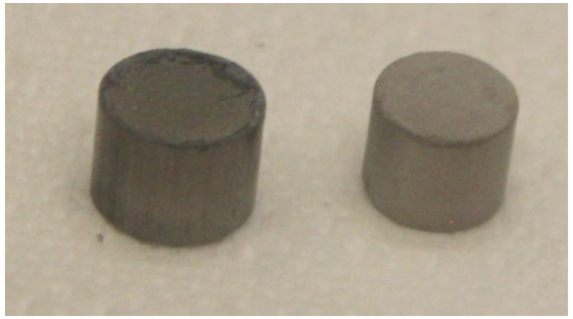
- ATF candidates are materials that can tolerate a loss of cooling for longer than the standard LWR system while maintaining or improving performance during normal operation.
- Utilize a multiscale modeling approach.
- Candidate materials investigated with BISON
  - U_3Si_2 fuel
  - Cr_2O_3-doped UO_2 fuel*
  - FeCrAl Cladding*
  - SiC/SiC Cladding*
  - Cr-coated Zircaloy Cladding*



L. Yin et al.. Journal of Nuclear Materials 554 (2021) 153090



T. Koyanagi, Y. Katoh, G. Singh, M. Snead, “SiC/SiC Cladding Materials Properties Handbook, Technical Report ORNL/TM-2017/385, ORNL, August 2017.



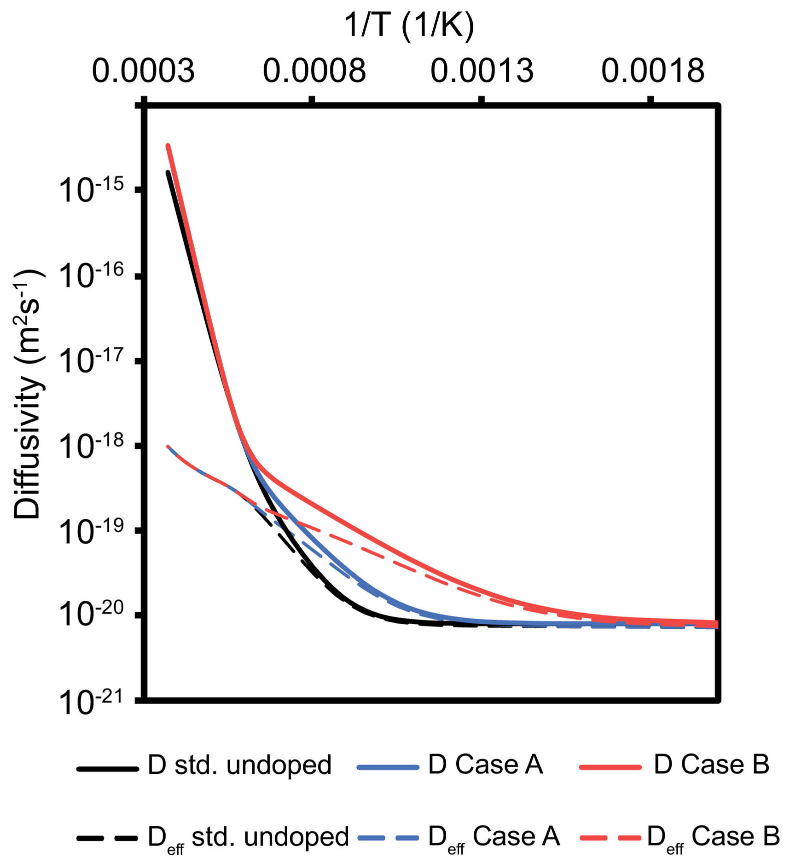
*Ongoing

Accident Tolerant (Advanced Technology) Fuel: Cr_2O_3-doped UO_2

- Fission gas behavior (FGR and gaseous swelling) are computed using BISON's physics-based model for UO_2
- A specific FG diffusivity correction for Cr_2O_3-doped UO_2 developed at LANL using atomistic modeling was applied
- Model can also naturally account for the larger grain size in doped UO_2 compared to standard UO_2

$$D^{doped} = \exp\left(-\frac{\Delta H_1}{k_B}\left[\frac{1}{T}-\frac{1}{T_1}\right]\right)D_1^{undoped} + \exp\left(-\frac{\Delta H_2}{k_B}\left[\frac{1}{T}-\frac{1}{T_2}\right]\right)D_2^{undoped} + D_3^{undoped}$$

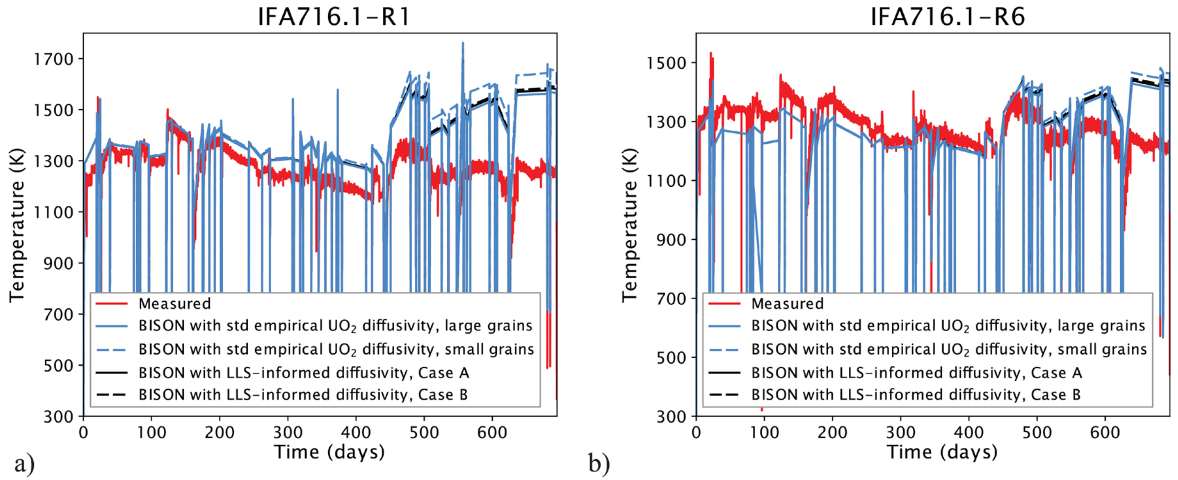
Parameter	Case A	Case B
$T_1 = T_2$ (K)	1773	1773
ΔH_1 (eV)	0.3198	0.3282
ΔH_2 (eV)	−0.3345	−0.6998

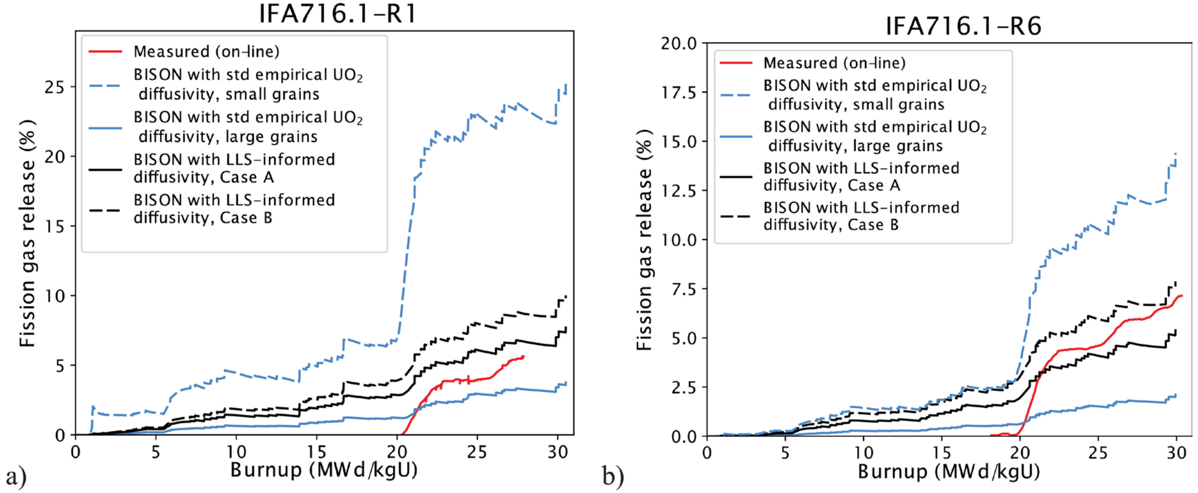


M. W. D. Cooper et al. Journal of Nuclear Materials 545 (2021) 152590

Accident Tolerant (Advanced Technology) Fuel: Cr_2O_3-doped UO_2

- Validation to Halden IFA-716.1 rods 1 and 6.
  - Upper centerline fuel temperature
  - Fission gas release
- Regardless of diffusivity model selected an over prediction in temperatures at the later cycles of irradiation.
- Improved fission gas release predictions when using the LLS-informed models for Xe diffusivity.





BISON Mixed Oxide Fuel Capabilities

- Developed fast spectrum oxide fuel performance capability via combined JAEA/INL efforts
- Requirement: run simulations with the following equations
  - Heat equation (T)
  - Pore migration (p)
  - Oxygen diffusion (o)
  - Actinide diffusion (Pu/Am)

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

$$\frac{\partial p}{\partial t} + \nabla \cdot [(1-p)p\vec{v} - \upsilon \nabla p] = 0$$

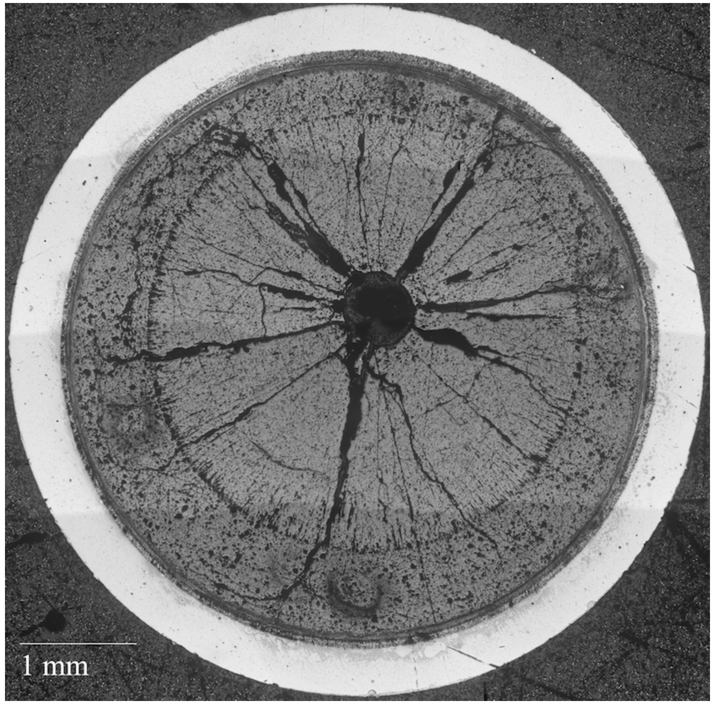
$$\frac{\partial o}{\partial t} + \nabla \cdot ND\left(\nabla o + o\frac{Q}{RT^2}\nabla T\right) = 0$$

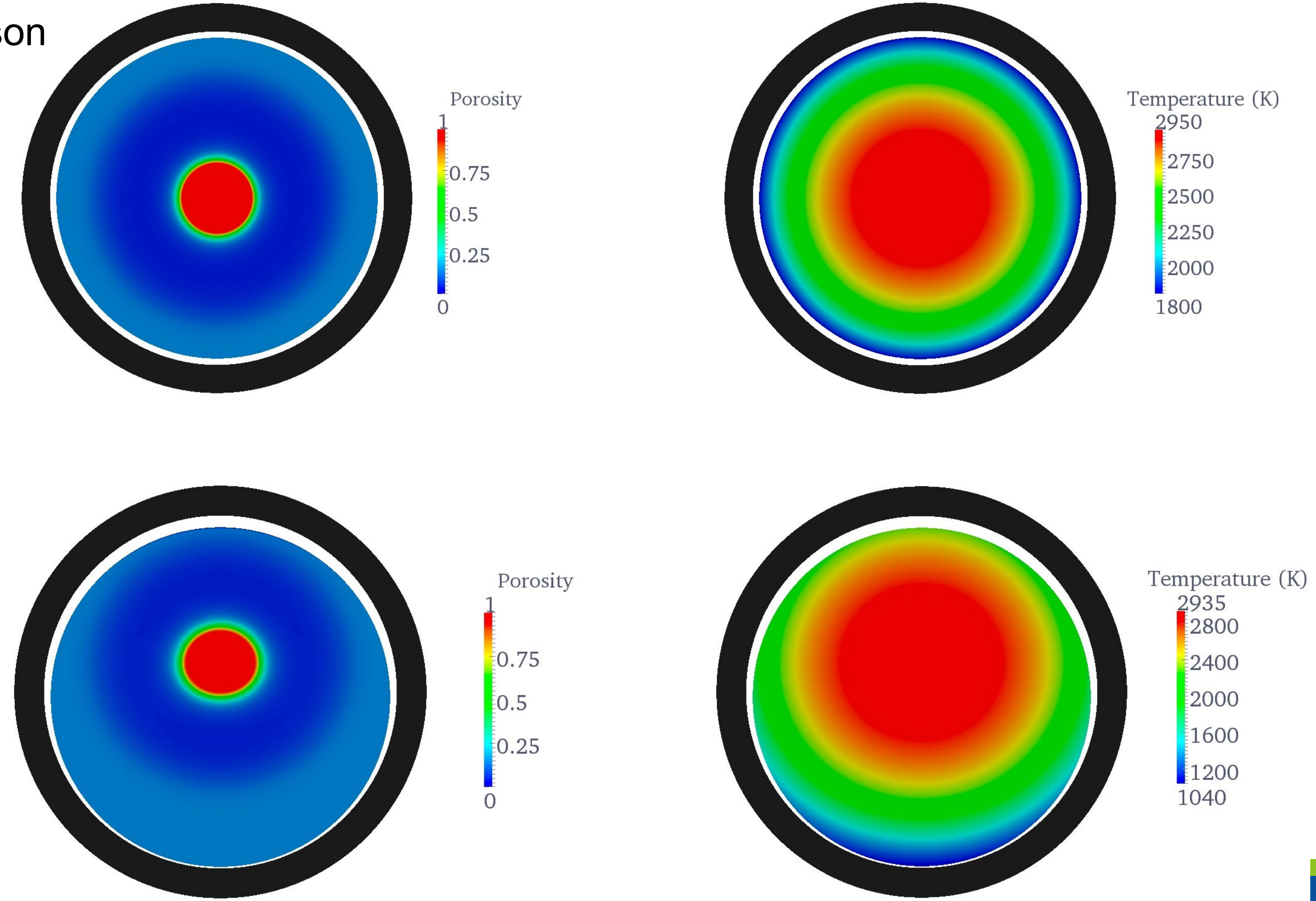
$$\frac{\partial c}{\partial t} - \nabla \cdot \left\{D\left[\nabla c + c(1-c)\frac{Q}{RT^2}\nabla T\right] - D\left[Apc\frac{l}{d}\nabla T \exp\left(-\frac{D}{l\vec{v}}\right)\right]\right\} = 0$$

S. Novascone, "Modeling porosity migration in LWR and fast reactor MOX fuel using the finite element method, JNM, 508, 2018

BISON Example: Pore migration in MOX

Concentric vs. offset: qualitative comparison

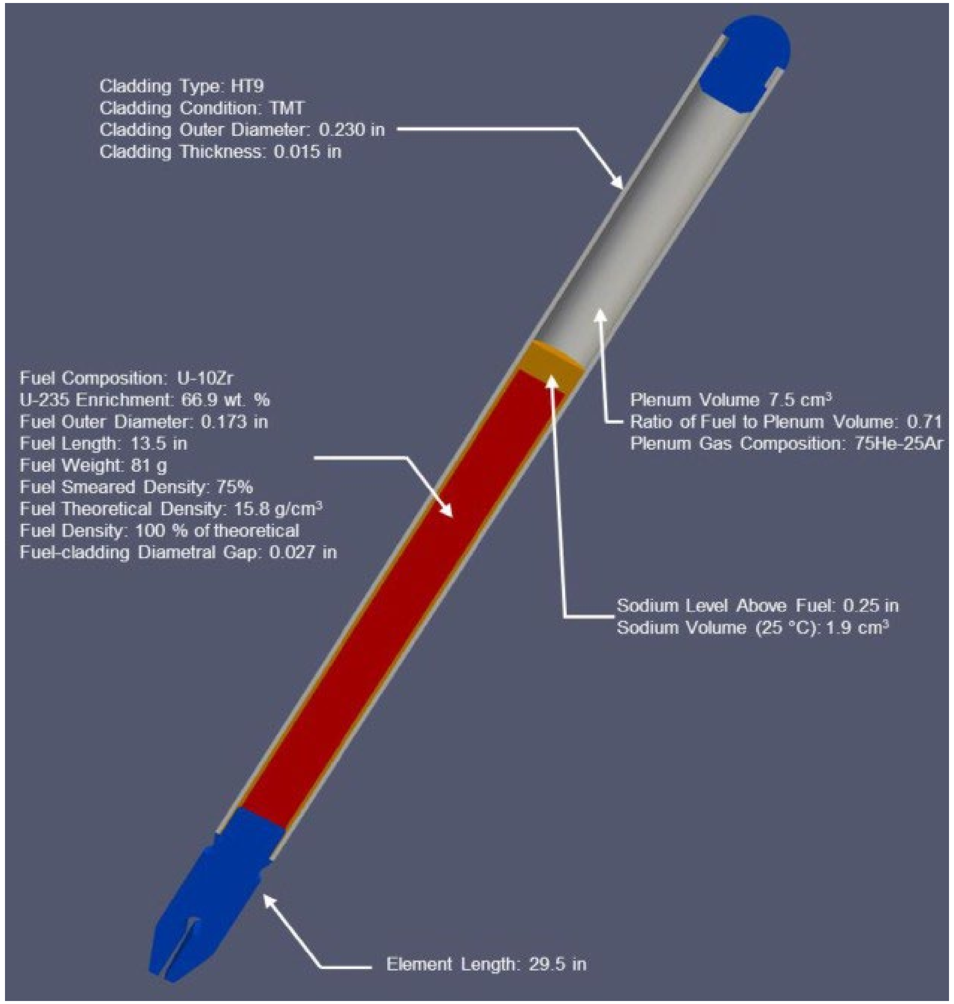




S. Novascone, "Modeling porosity migration in LWR and fast reactor MOX fuel using the finite element method, JNM, 508, 2018

Metallic Fast Reactor Fuel

- **Conventional Fuel Design**
  - Plain binary/ternary alloy injection cast fuel slug
  - Stainless steel cladding (HT9, CW D9 or CW 316SS)
  - Sodium bonded gap to provide ~75% smeared density
  - Large upper plenum to accommodate released fission gas
  - Hexagonal patterning in fuel assemblies with spacer wires
- **Advanced Fuel Design**
  - Annular alloy fuel co-extruded with stainless steel cladding
  - Helium filled gas for a sodium-free environment within cladding
  - Optional lower plenum configuration

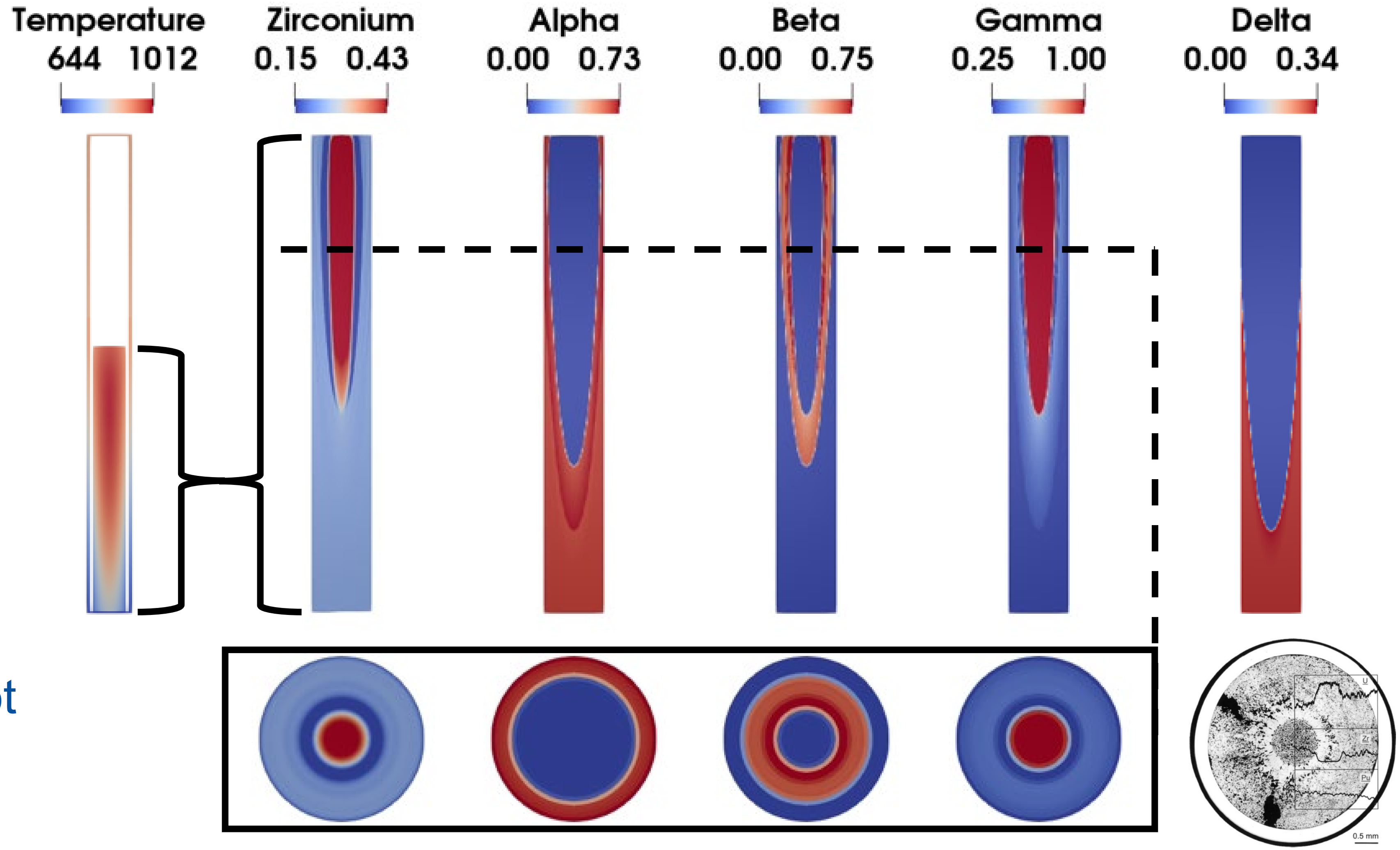


A typical SFR metallic fuel pin (IFR experiment pin irradiated in EBR-II)

A.M. Yacout et al., *Nucl. Eng. Des.* 280 (2021) 111225

Coupling thermo-mechanics to species evolution is possible

- 2D axisymmetric simulation conducted with actual geometry, temperature, and power history
- Radial dimension is exaggerated by 10 times for visualization
- Displacements are not shown

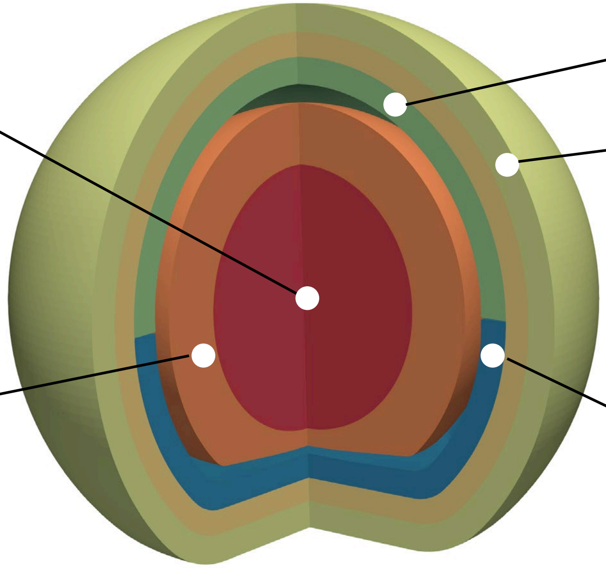


J. A. Hirschhorn, et al., Journal of Nuclear Materials 544 (2021) 152657
Kim, Y. S., et al., Journal of Nuclear Materials 327 (2004) 27–36.

TRISO Fuel Particle Modeling

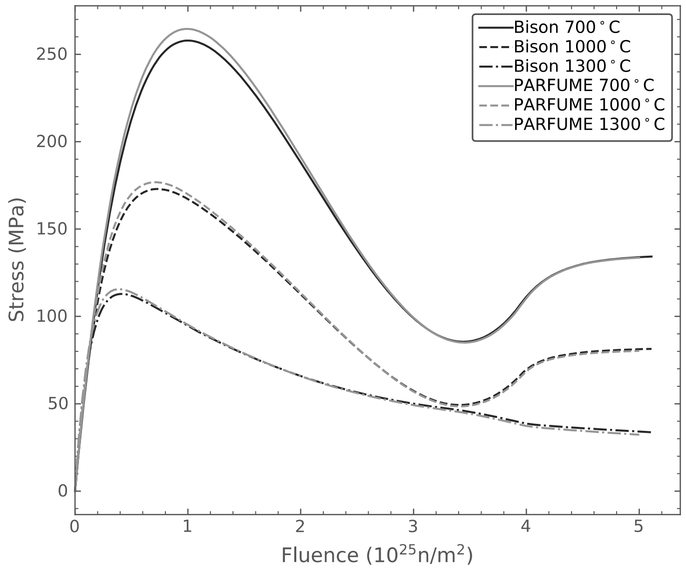
Kernel
Thermal
Burnup
Elasticity Tensor
Volumetric Swelling
Fission Gas Release

Buffer
Thermal
Elasticity Tensor
Creep
Thermal Expansion
IIDC

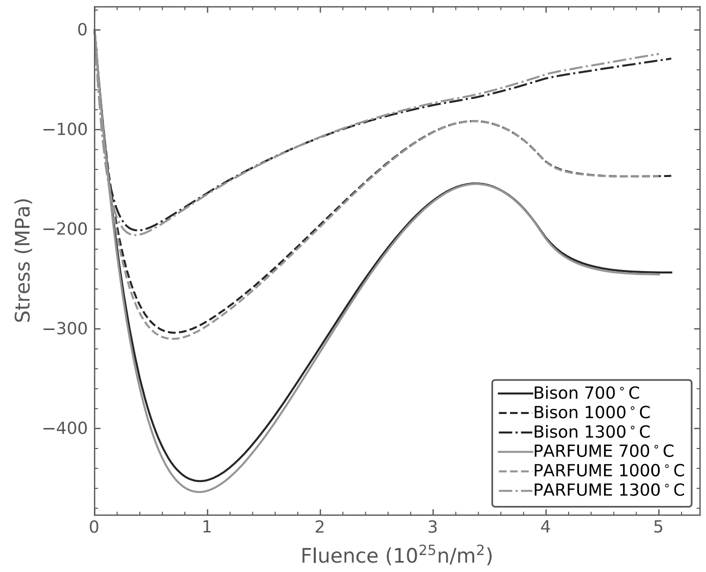


IPyC and OPyC
Thermal Expansion
Elasticity Tensor
Creep
IIDC

SiC
Elasticity Tensor
Thermal Expansion



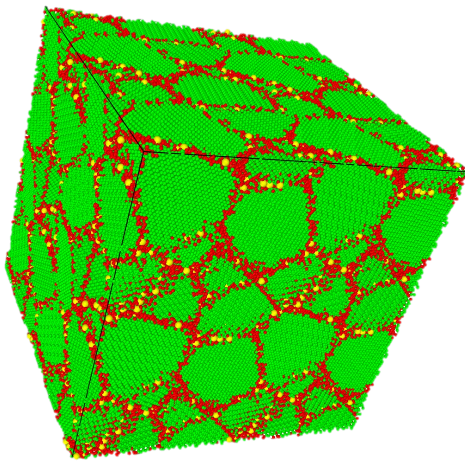
Tangential stress in IPyC

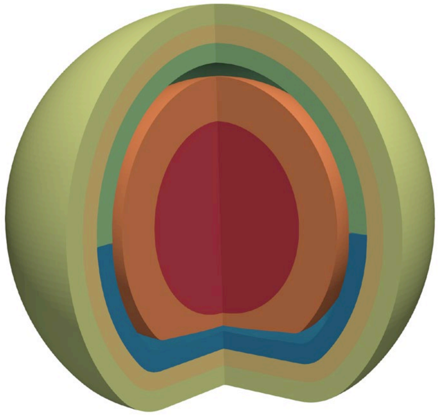


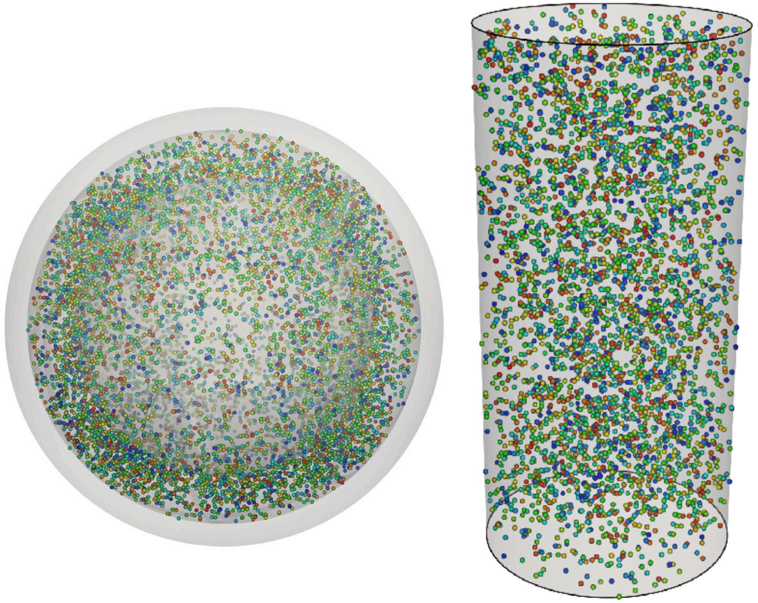
Tangential stress in SiC

Courtesy of W. Jiang

Multi-scale TRISO modeling







Lower-length scale modeling

- **Fission gas release model:** Xe, Kr diffusivity in UCO
- **Fission product diffusivity:** Silver diffusion in SiC, Pd Penetration

TRISO particle

- **Thermal-mechanical modeling**
  - **Failure analysis:** asphericity, IPyC cracking and debonding
- **Fission product diffusion through layers**

Pebble and Compact modeling

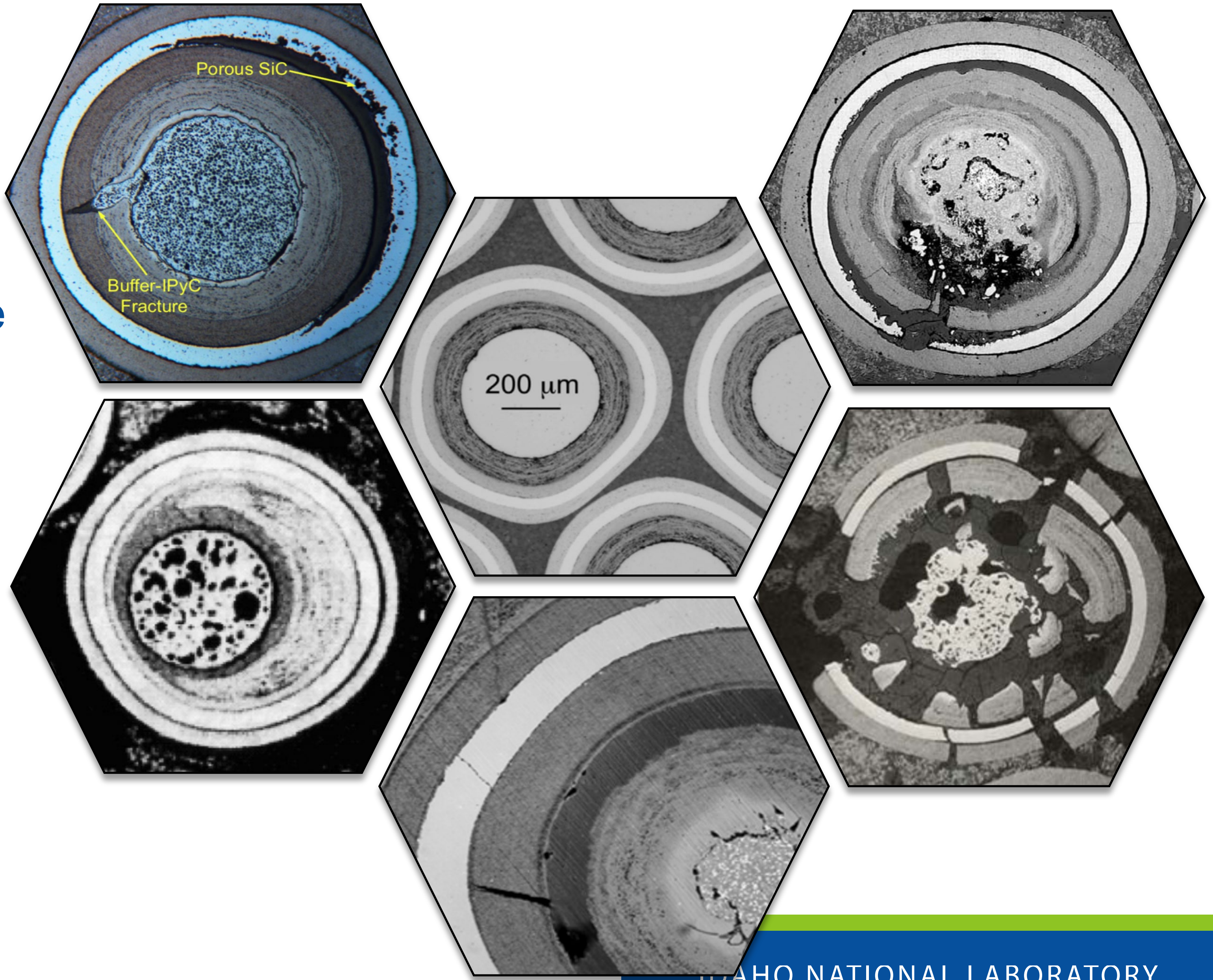
- **Failure probability calculation**: Monte Carlo and Fast Integration Approach
- **Fission product diffusion through matrix**
- **Particle-Matrix interaction**

Courtesy of W. Jiang

TRISO Failure Modes

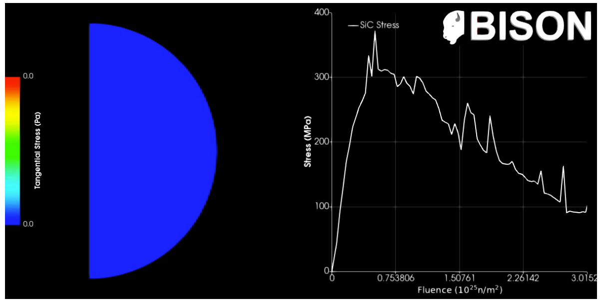
- **Mechanical**
  - Pressure vessel failure
  - Irradiation-induced PyC failure leading to SiC cracking
  - IPyC-SiC / Buffer-IPyC partial debonding

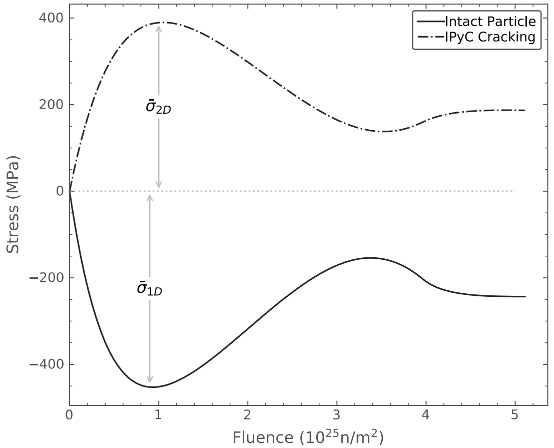
- **Thermochemical**
  - Kernel migration
  - SiC thermal decomposition
  - Fission product attack of SiC
  - Corrosion of SiC by CO



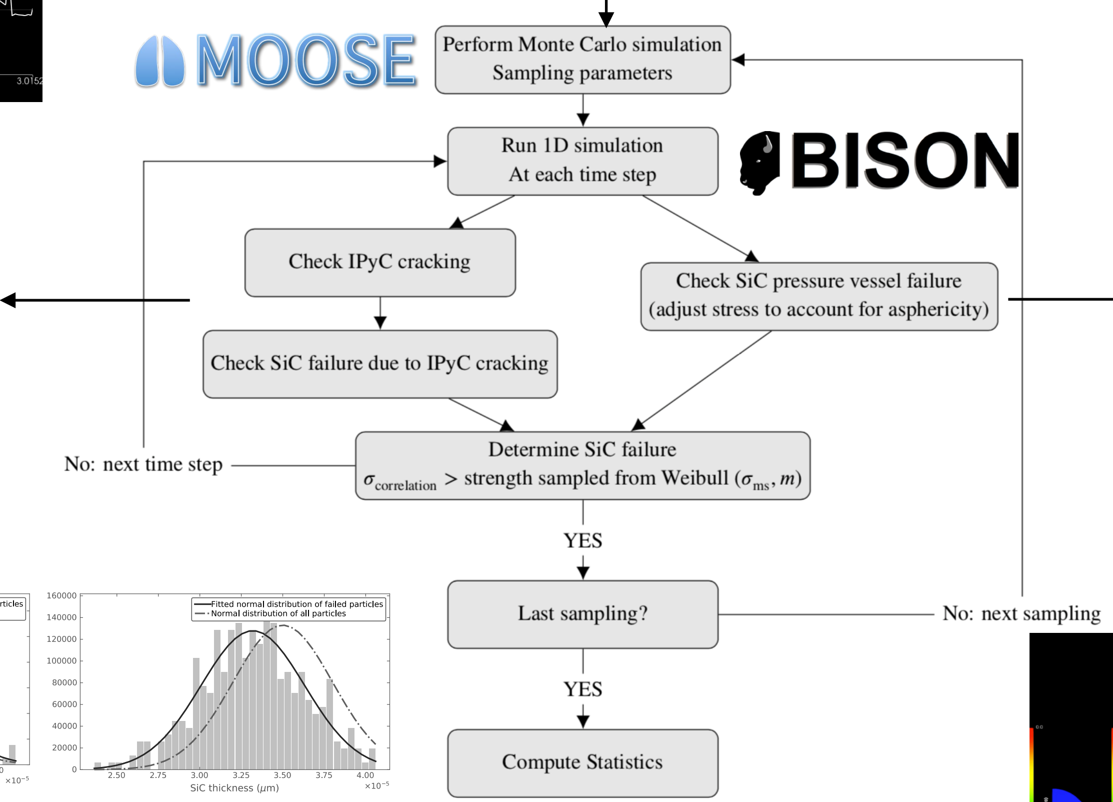
Courtesy of W. Jiang

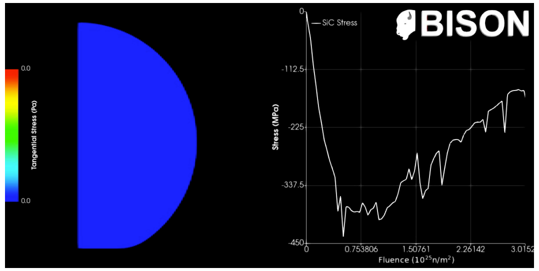
BISON Example: TRISO Failure Analysis

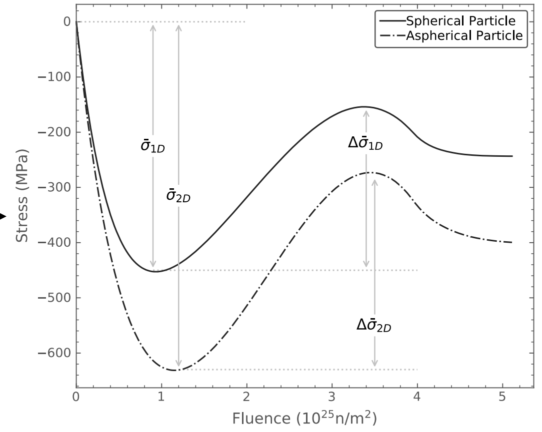


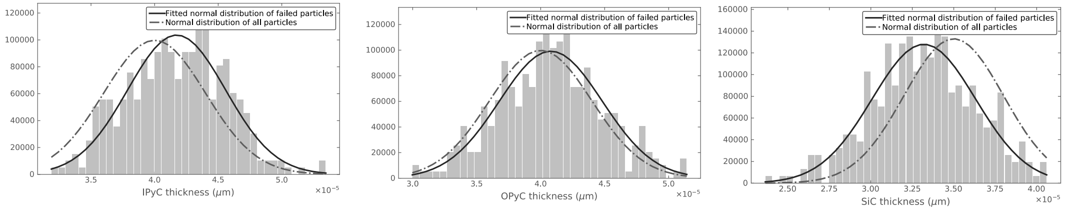


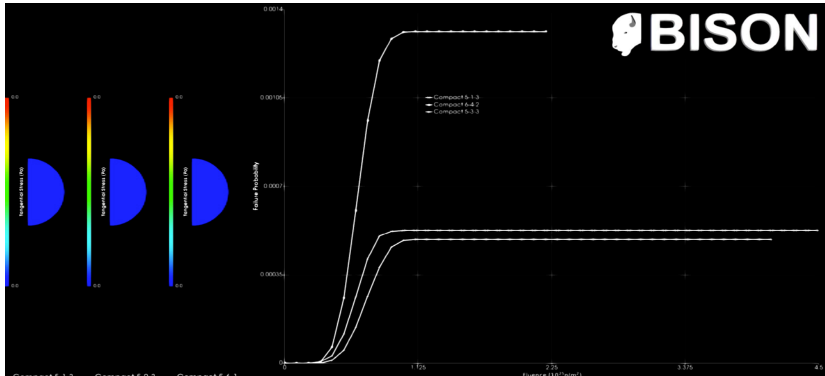
Category	Parameter	Nominal values ± Standard Deviation
Particle geometry	Kernel diameter (μm)	425±10
	Buffer thickness (μm)	100±10
	IPyC/OPyC thickness (μm)	40±3
	SiC thickness (μm)	35±2
	Particle asphericity (SiC aspect ratio)	1.04
Fuel properties	IPyC density (g/cm^3)	1.90±0.02
	OPyC density (g/cm^3)	1.90±0.02
	IPyC/OPyC BAF	1.05±0.005







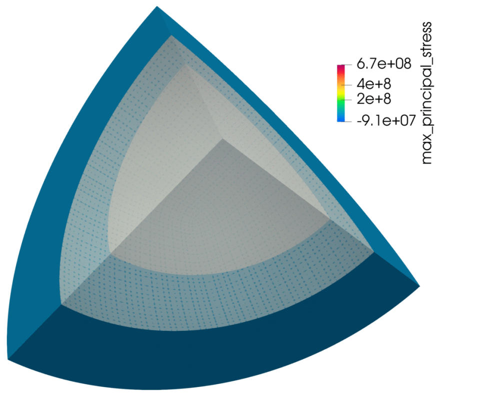




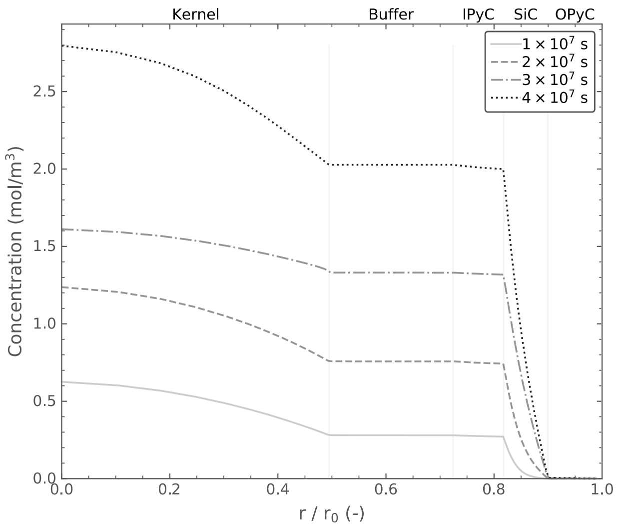
Courtesy of W. Jiang

Courtesy of W. Jiang

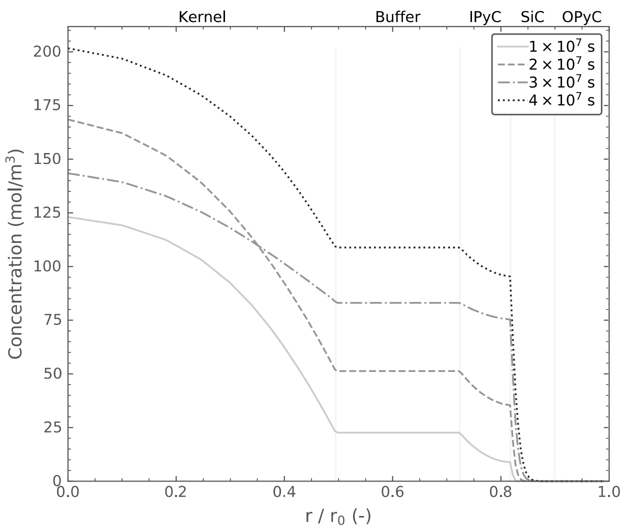
Fission product diffusion through intact and failed particle



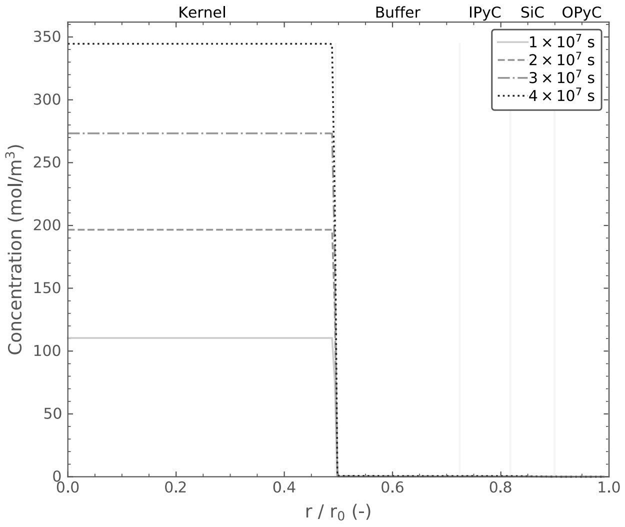
Intact Particle



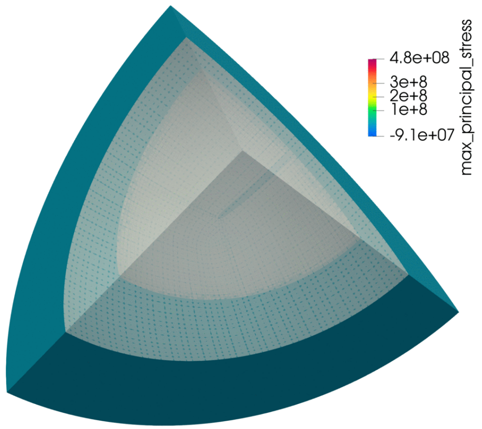
Silver



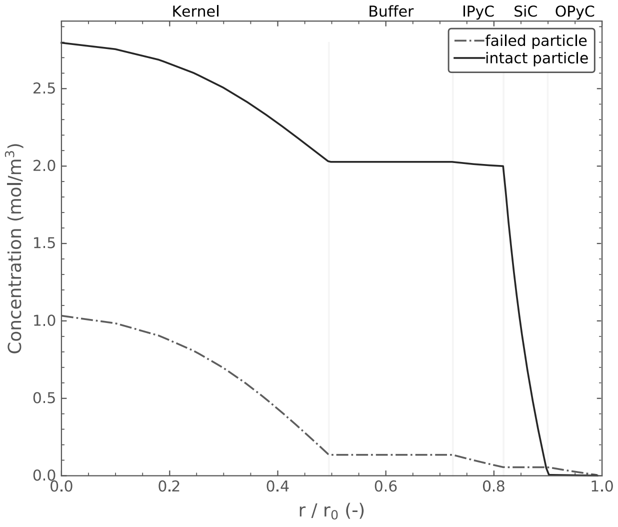
Cesium



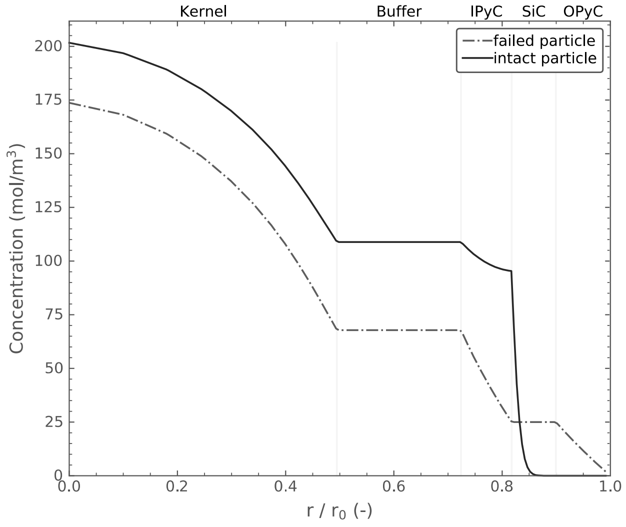
Strontium



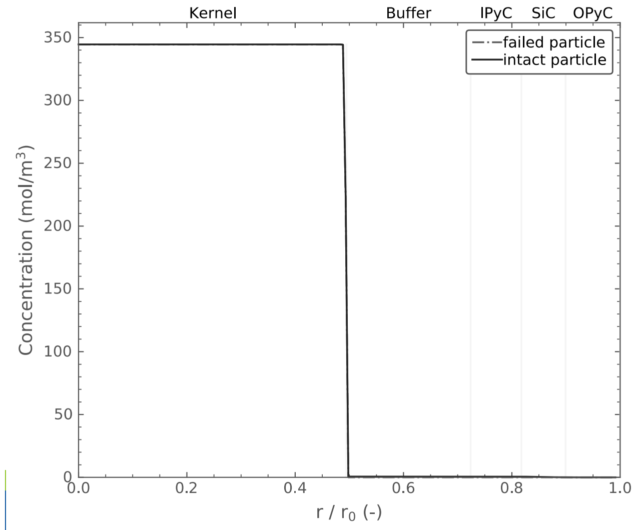
Failed Particle



Silver



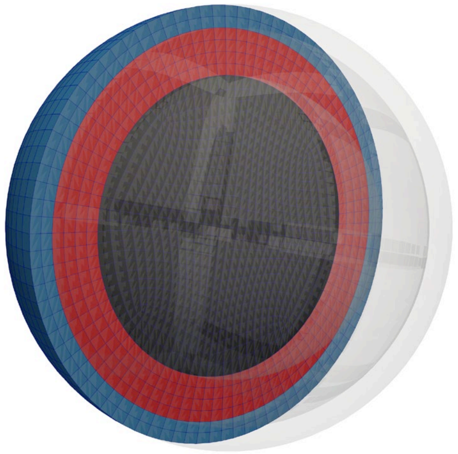
Cesium

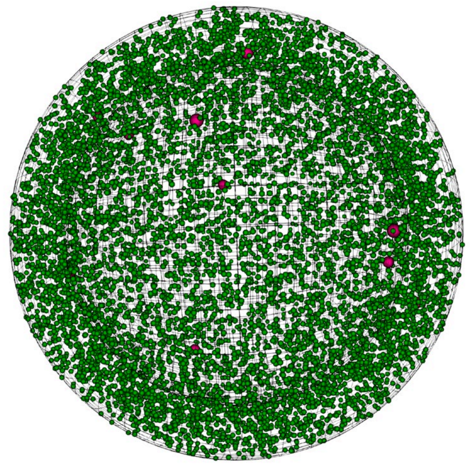


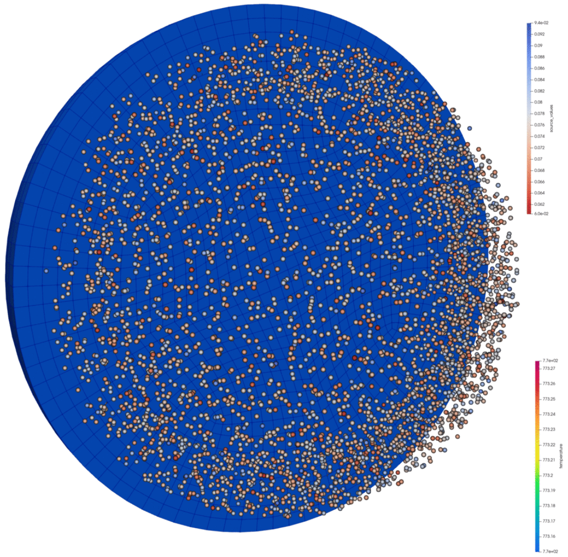
Strontium

Pebble modeling

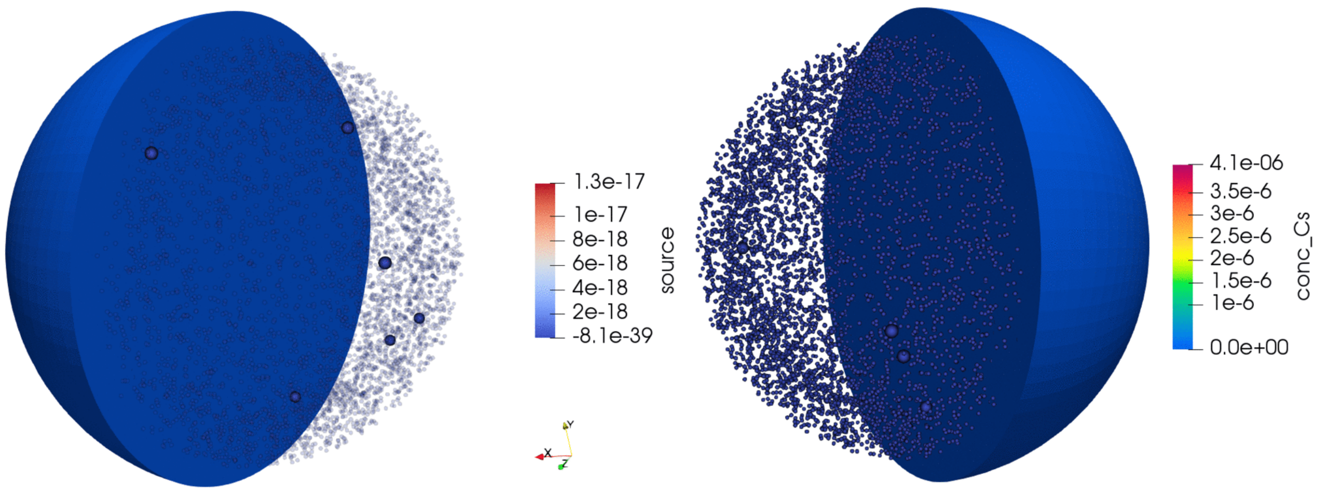
RADIUS (CM)	2.000
SHELL LAYER THICKNESS (CM)	0.200
FUEL LAYER THICKNESS (CM)	0.420
(AGR-5/6/7) TRISOS	9022
U-235 ENRICHMENT (% WT)	19.55

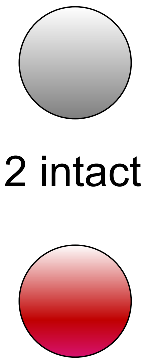






Heat point source



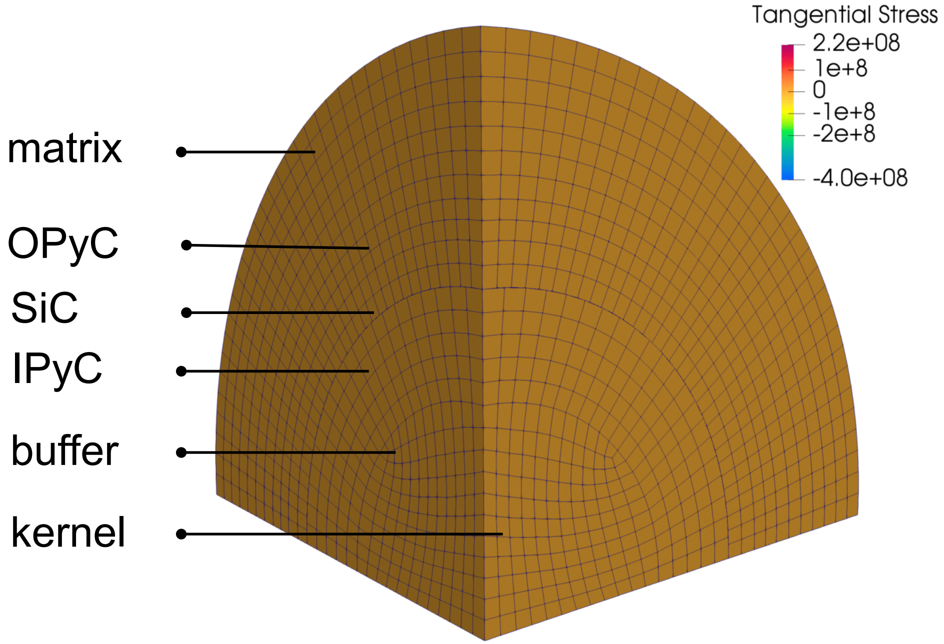


Cs point source

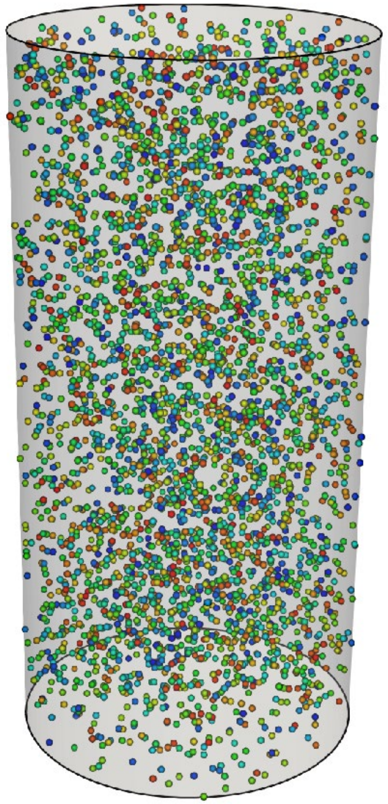
Courtesy of W. Jiang

Graphite Matrix Modeling

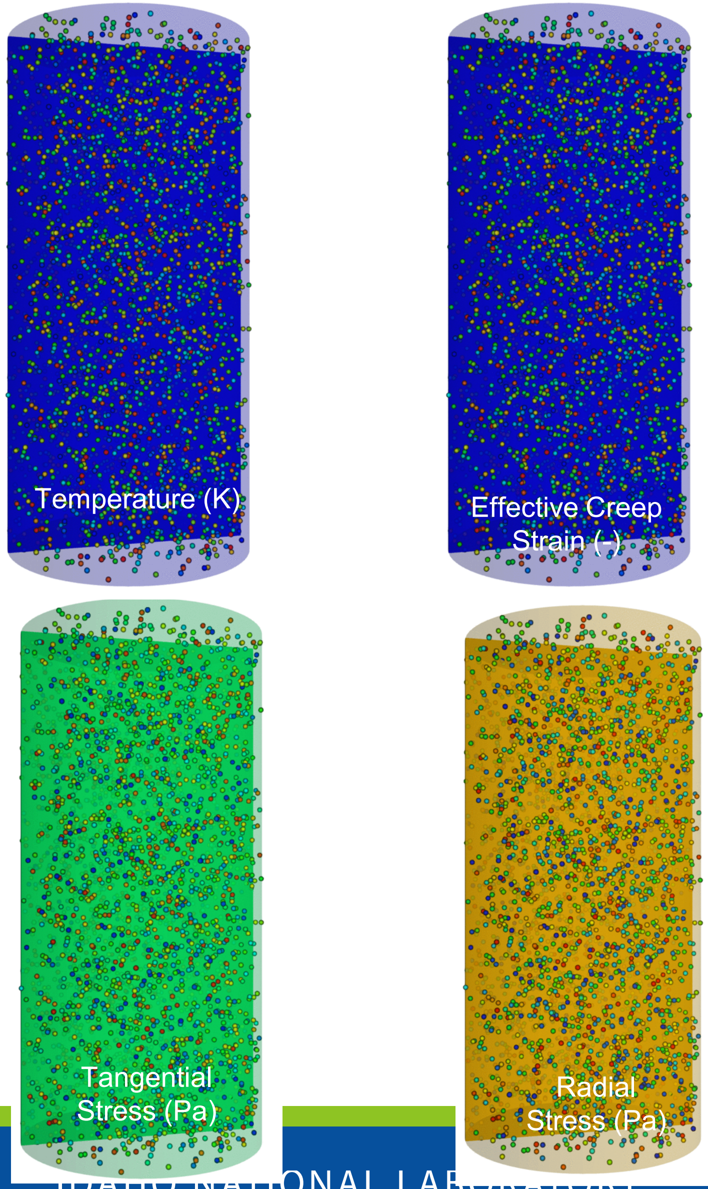
- **The cores and reflectors in HTGRs are made of graphite materials**
  - the graphite acts as a moderator, a fuel host matrix, a structural component to provide
    - channels for fuel, coolant gas, and control rods
    - a thermal/neutron shielding component
    - heat sink/conduction path during transients



Tangential stress during irradiation for the particle-matrix debonding example (displacements are magnified 2x)



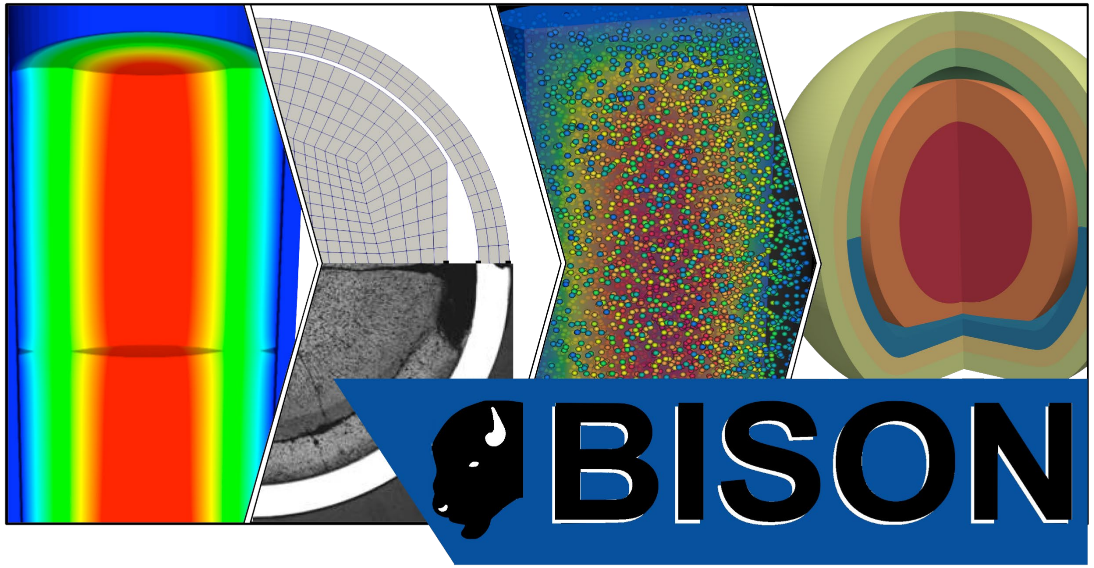
Fuel compact containing 4,000 TRISO particles randomly generated from an MC simulation.



Courtesy of W. Jiang

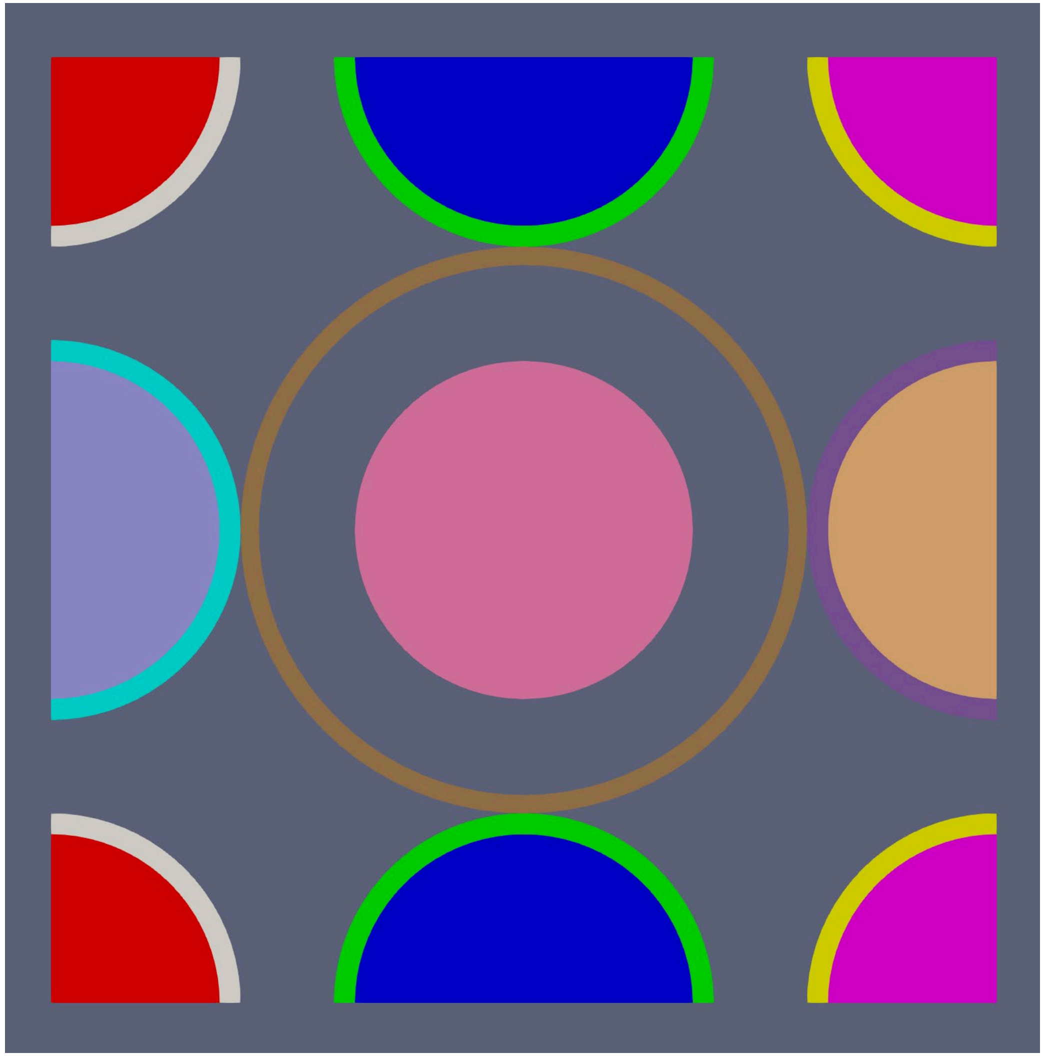
Summary

- An overview of the purpose of BISON and why it was created was provided.
- A brief history of major developments, publications, and awards was presented.
- A tribute to two personnel with instrumental contributions to the code was given.
- Several example applications covering different dimensionalities, geometric representations, and fuel designs were highlighted.
- Publications using BISON were provided.



Future Work

- Continued work in metallic fuel, TRISO, and high burnup/LOCA LWR behavior.
  - Multiscale model development including reduced order models
- Support of rod-to-rod interactions in a single simulation during LOCA transients.
- Ongoing effort to get BISON approved for use in safety calculations for experiments at INL.
- Incorporating machine learning for model optimization.
- Sensitivity analysis and uncertainty quantification.



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