Nuclear Reactor Sustainment and Expanded Deployment

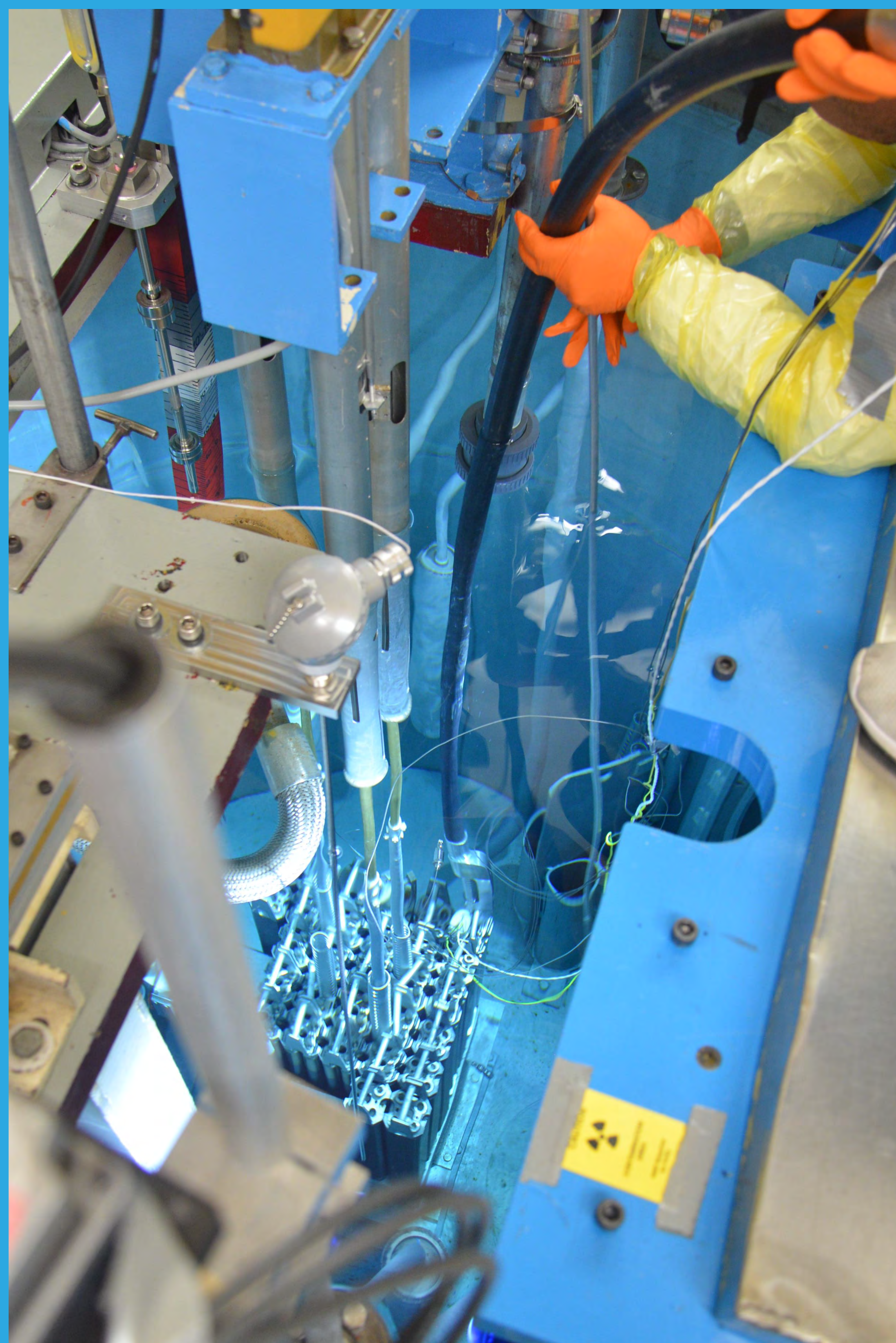
Abdalla Jaoude	Demonstrating Fueled-Salt Irradiation Capability to Support Reactor Deployment
Boone Beausoleil	Passive Strain Measurements for Experiments in Radiation Environments
Brelon May	Accelerating pathways to actinide materials discovery through combinatorial deposition
Chao Jiang	Machine Learning Interatomic Potentials for Radiation Damage and Physical Properties in Model Fluorite Systems
Cheng Sun	An Innovative Approach for Accelerated Irradiation Studies of Materials
Chuting Tsai	In situ positron annihilation spectroscopy for characterizing irradiation induced defects
David Frazer	An accelerated assessment of the creep mechanisms in uranium zirconium model alloys
Fidelma Di Lemma	A combinatorial Modeling and Simulation and Separate Effect Test approach to investigate unknown microstructural evolution in metallic fuel pin
Jeren Browning	Unattended Operation through Digital Twin Innovations
Kyle Gamble	Modeling and Measurement of Gas Transport in Nuclear Fuels
Kyle Gamble	High-fidelity multiscale model development for accelerated fuel qualification using finite element-informed discrete element modeling
Mauricio Tano Retamales	Thermochemical modeling of flow-accelerated corrosion in Molten Salt Reactors
Mohammad Abdo	Accelerated technology development through new extrapolation and validation methods
Nedim Cinbiz	Informative Design of High-Temperature Metal Hydride Moderators in Microreactors
Som Dhulipala	Accelerating and Improving the Reliability of Low Failure Probability Computations to Support the Efficient Safety Evaluation and Deployment of Advanced Reactor Technologies
Stefano Terlizzi	Development of Multiphysics Object Oriented Simulation Environment based capabilities to model hydrogen migration in hydrides-moderated microreactors
Steven Prescott	Quantitative Reliability Analysis for Unattended Operation of Fission Batteries
Trishelle Copeland-Johnson	Characterizing corrosion mechanisms of structural alloys in actinide-based molten chloride salt
Vivek Agarwal	Scalable Framework of Hybrid Modeling with Anticipatory Control Strategy for Autonomous Operation of Modular and Microreactors
Yifeng Che	Accelerating Utilization of Fuel Performance Modeling using Artificial Intelligence

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

First Ever Enriched Uranium Fueled Chloride Salt Irradiation



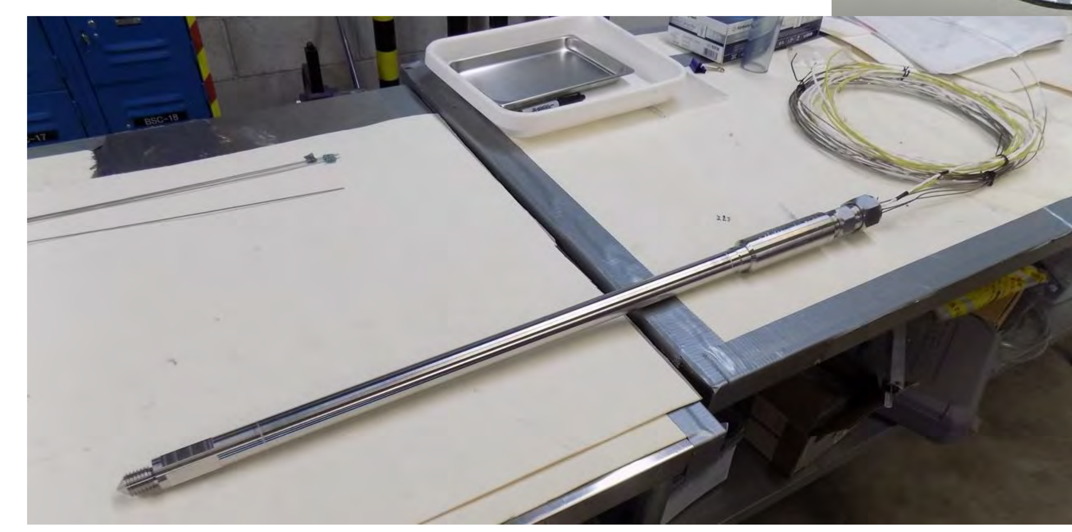
Abdalla Abou-Jaoude, William Phillips, Gregory Core, Chuting Tsai

Why?

- Interest is **surging** in Molten Salt Reactors
- **Need** to establish US-based salt irradiation capability
- Irradiating salt will help us understand:
  - **Source term**: where do radionuclides go?
  - **Properties**: do salt properties change with burnup?
  - **Corrosion**: does irradiation affect wall material corrosion rate

What?

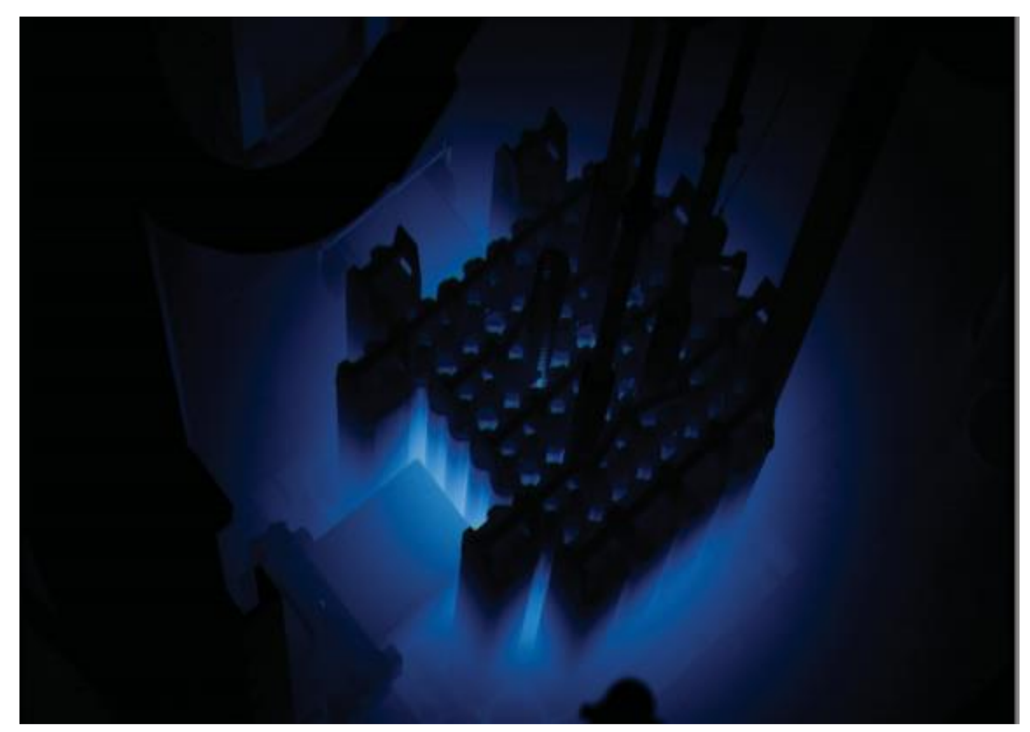
0.33 UCl_3 – NaCl at **93wt%** ^{235}U



Double-encapsulated temperature-controlled experiment vehicle

Where?

INL's Neutron Radiography Reactor **(NRAD)**



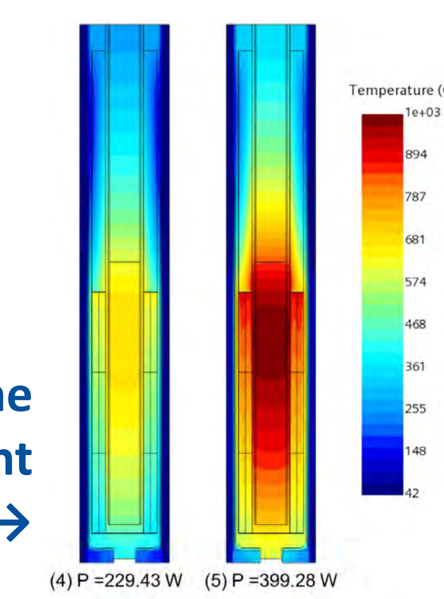
How?

Under irradiation:

- **Fission Heat** = 20 W/cm^3
- **Neutron Flux** = 3.5×10^{12} n/cm^2-s
- **Gamma Flux** = 1.4×10^{13} γ/cm^2-s
- **Salt Temperature** = 525-900°C

← Inserting the experiment in the reactor

Simulation of the experiment performance →



Project Number: 21A1050-016FP LRS Number: INL/MIS-23-74314

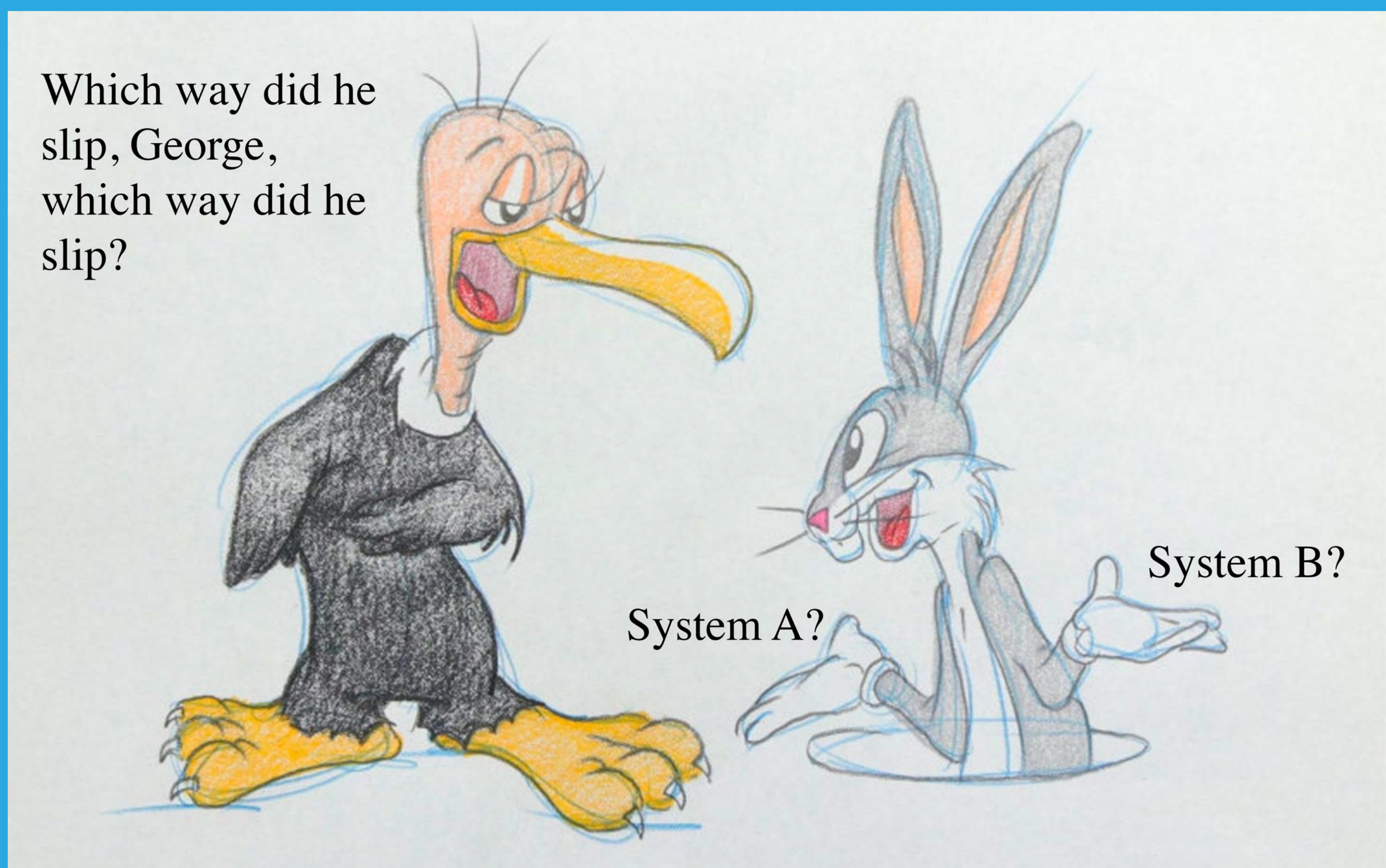
www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Plasticity is harder to catch than you might think…

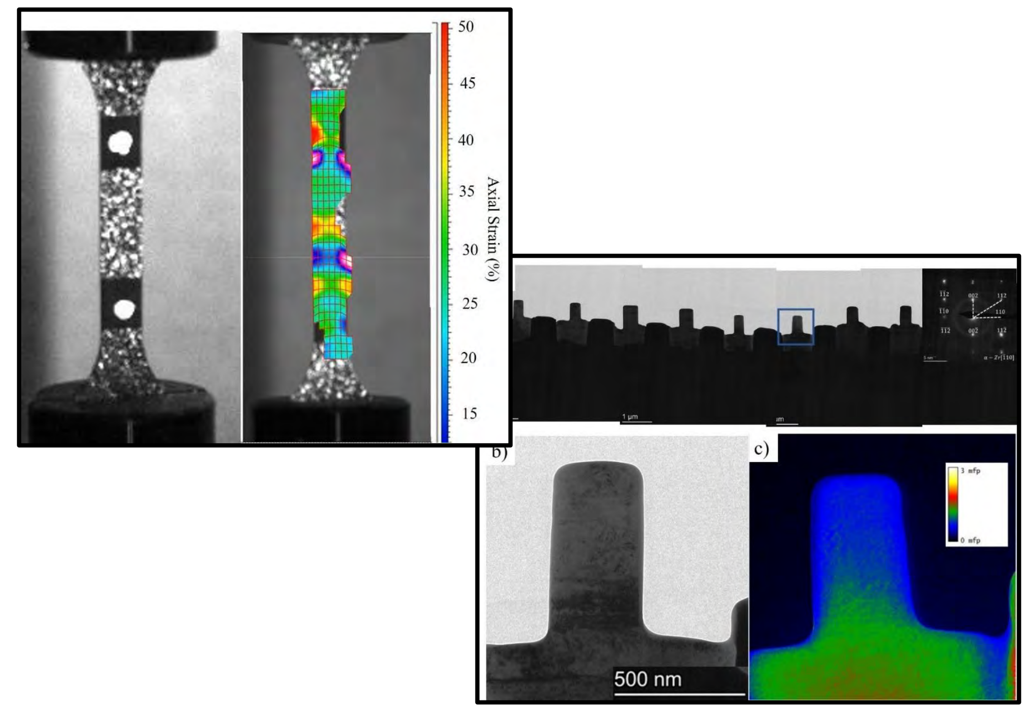


Single crystal testing helps clarify the confusion

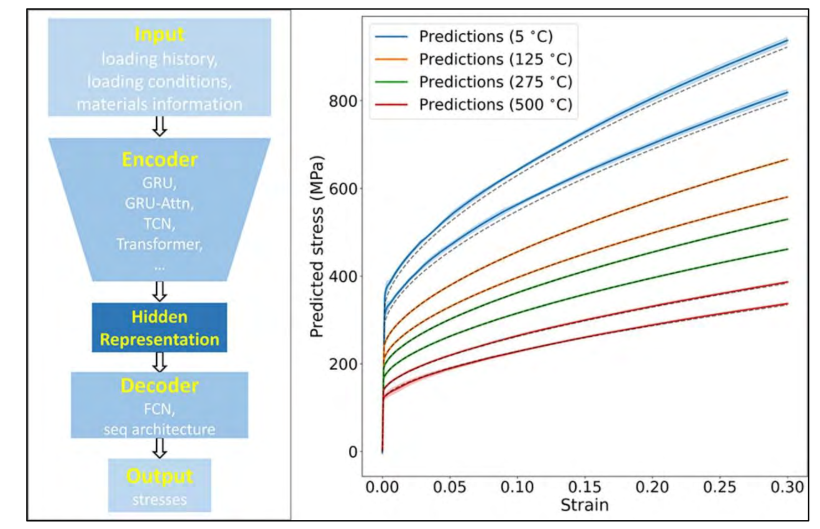
Boone Beausoleil, NS&T
INL Co-PIs: N. Cinbiz, Y. Wang, S. Pitts
NCSU Co-PIs: D. Kaoumi, M. DeJong, Philip Alarcón-Furman
MIT Co-PIs: J. Li, Q. Li

Conceptual Goal of the Project

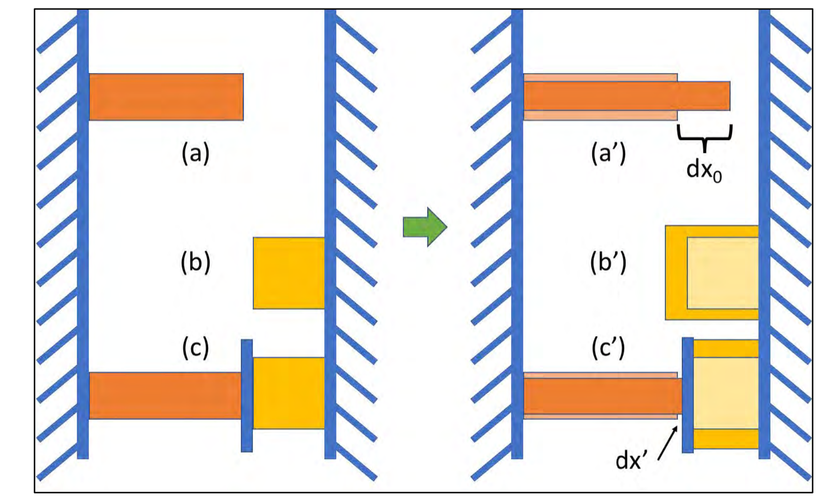
1. Use full scale and small-scale tests of wrought and single-crystal anisotropic materials



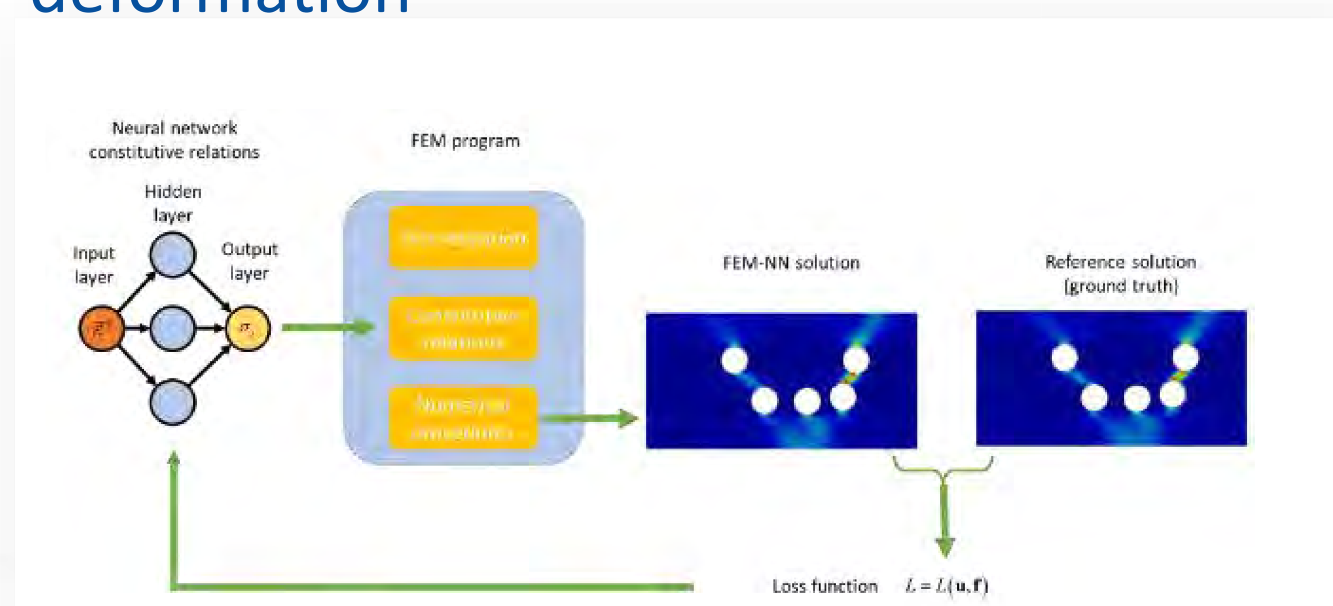
2. Utilize computational tools to understand constitutive relationships and uncertainties



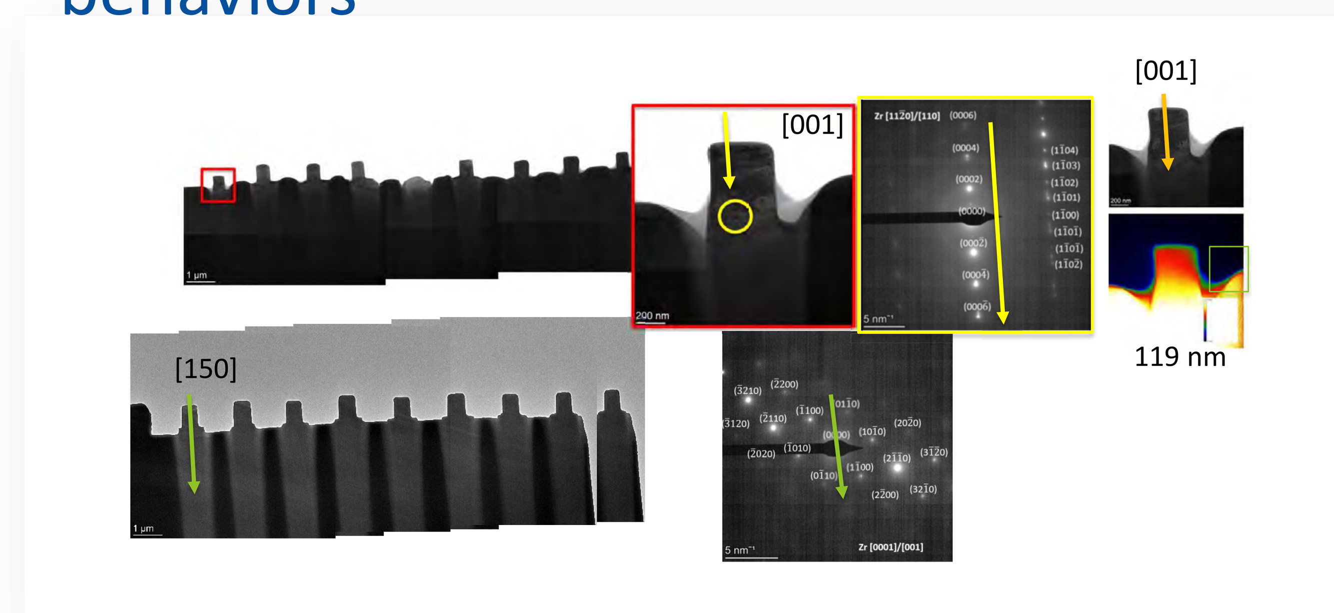
3. Use the results to design tests that could infer adjacent material properties



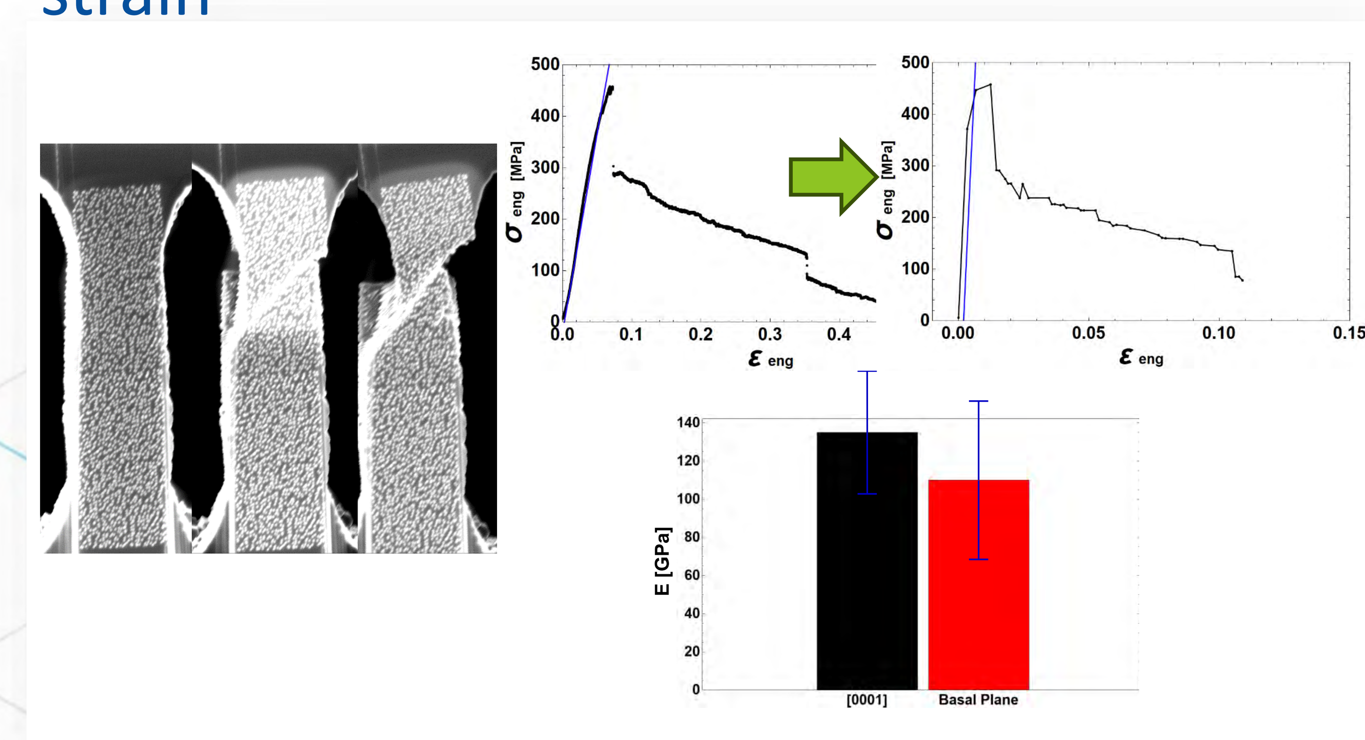
Machine learning with complex stress states better enable prediction of material deformation



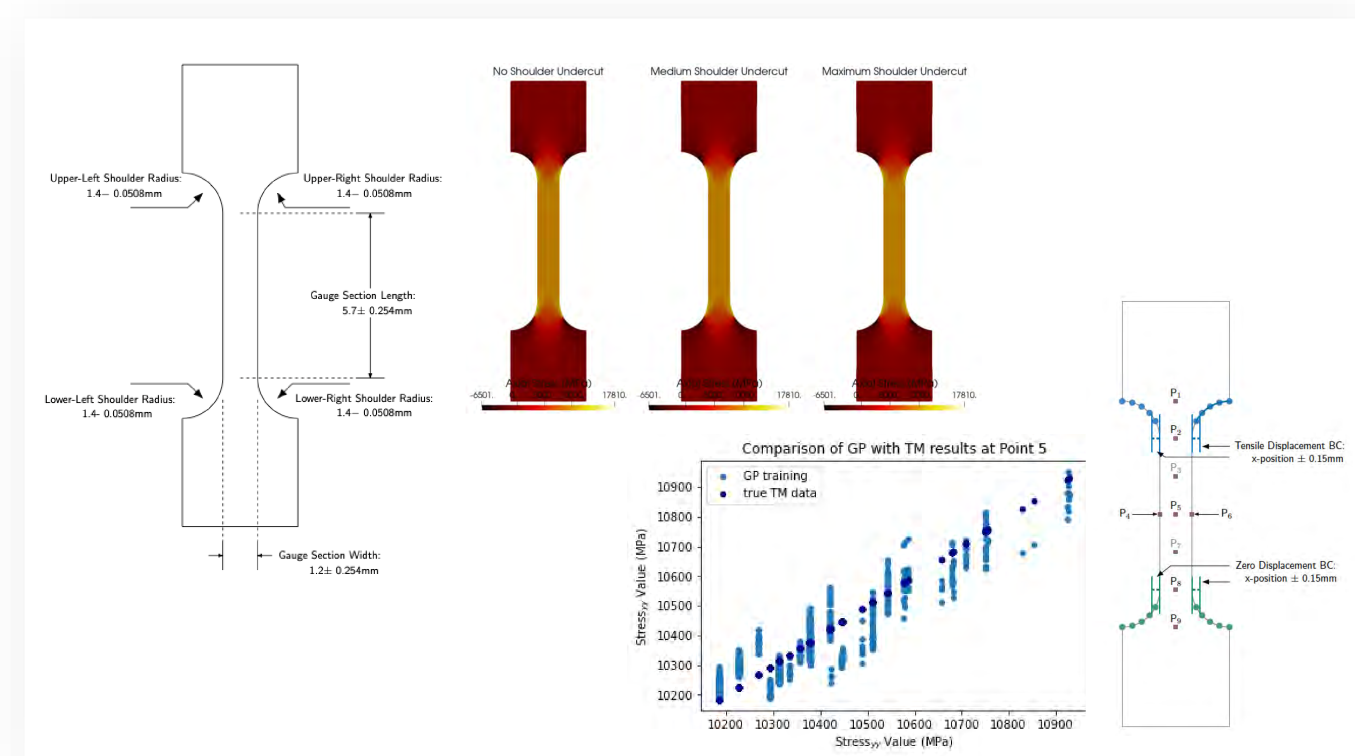
TEM compression micro-pillars generated a better understanding of anisotropic behaviors



Focused electron beam speckling for SEM-DIC correction of raw strain to engineering strain



Stochastic tools help understand dimensional sensitivities to testing

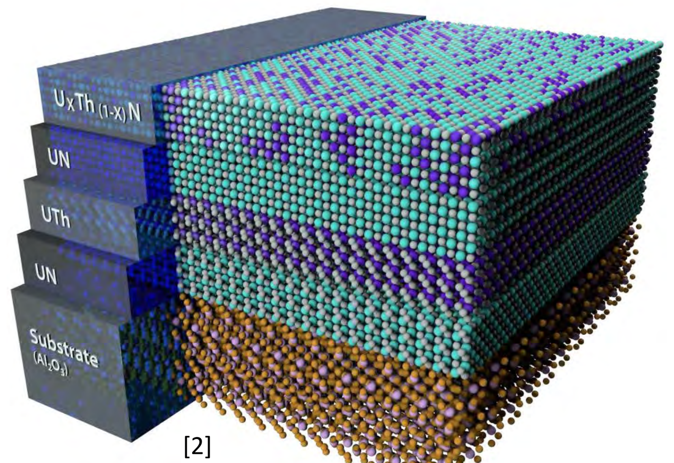


Project Number: 21A1050-060FP
LRS Number: INL/MIS-23-74130
www.inl.gov
Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."
Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

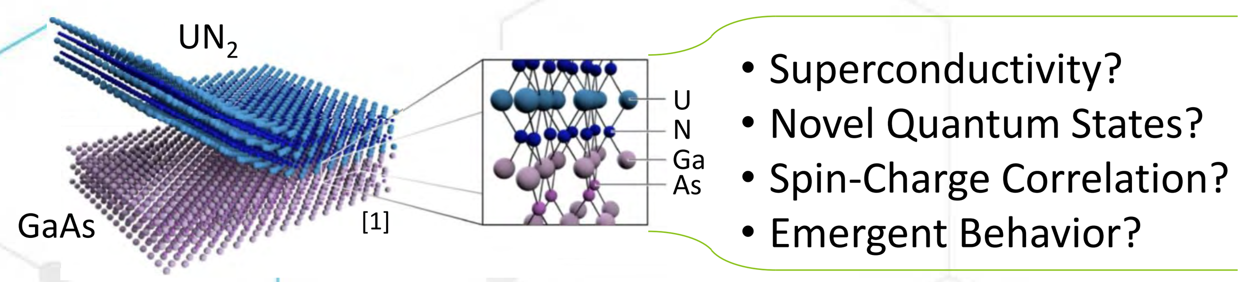
Massachusetts Institute of Technology
NC STATE UNIVERSITY Department of Nuclear Engineering
Idaho National Laboratory

Accelerating Pathways to Actinide Materials Discovery
Through Combinatorial Deposition

PRESENTER:
Brelon May

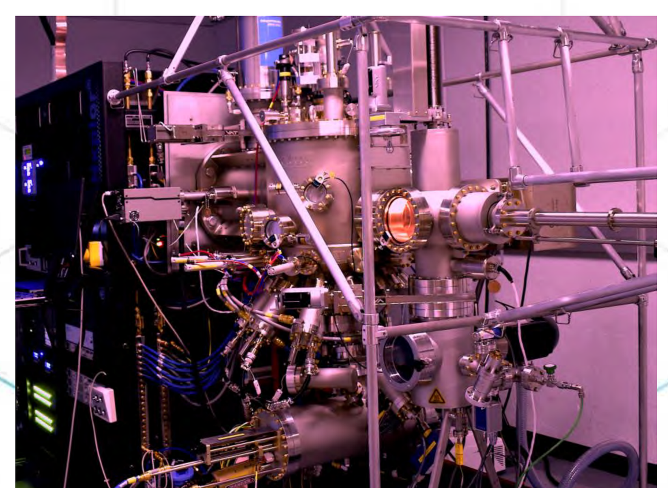


BACKGROUND
- Global lack of capabilities to fabricate, test, and screen actinides stifle research
- *Transport by design*: What pathways enable key transport properties?
  - Mass and energy
  - Need detailed understanding of correlation between the lattice, phonon, and electrons

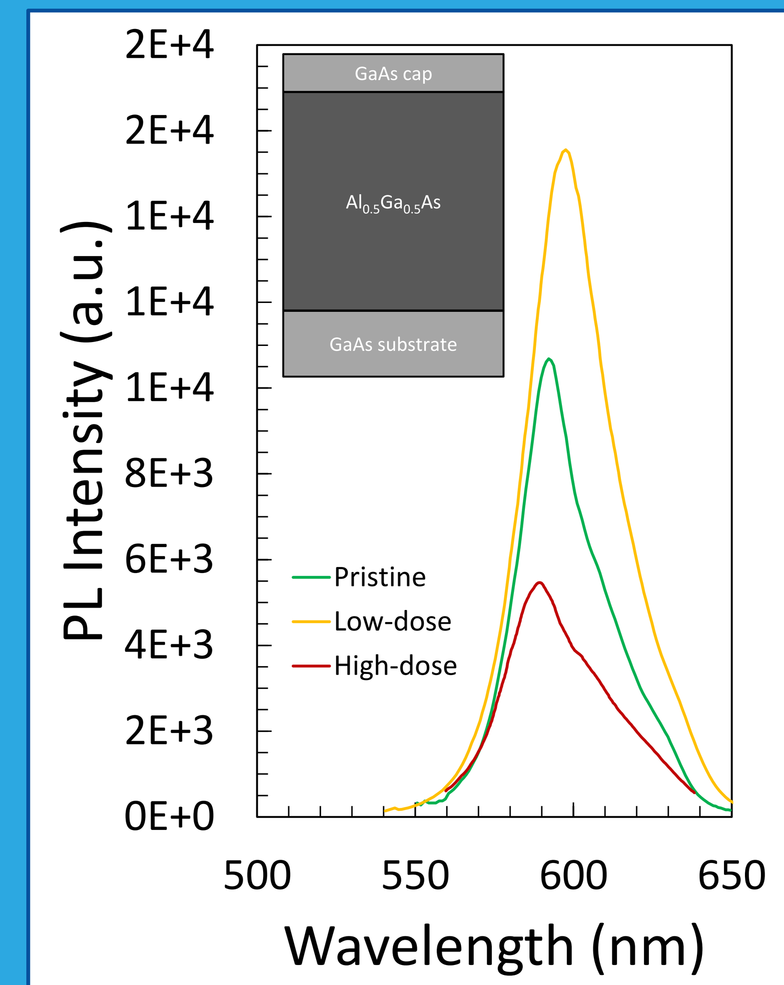


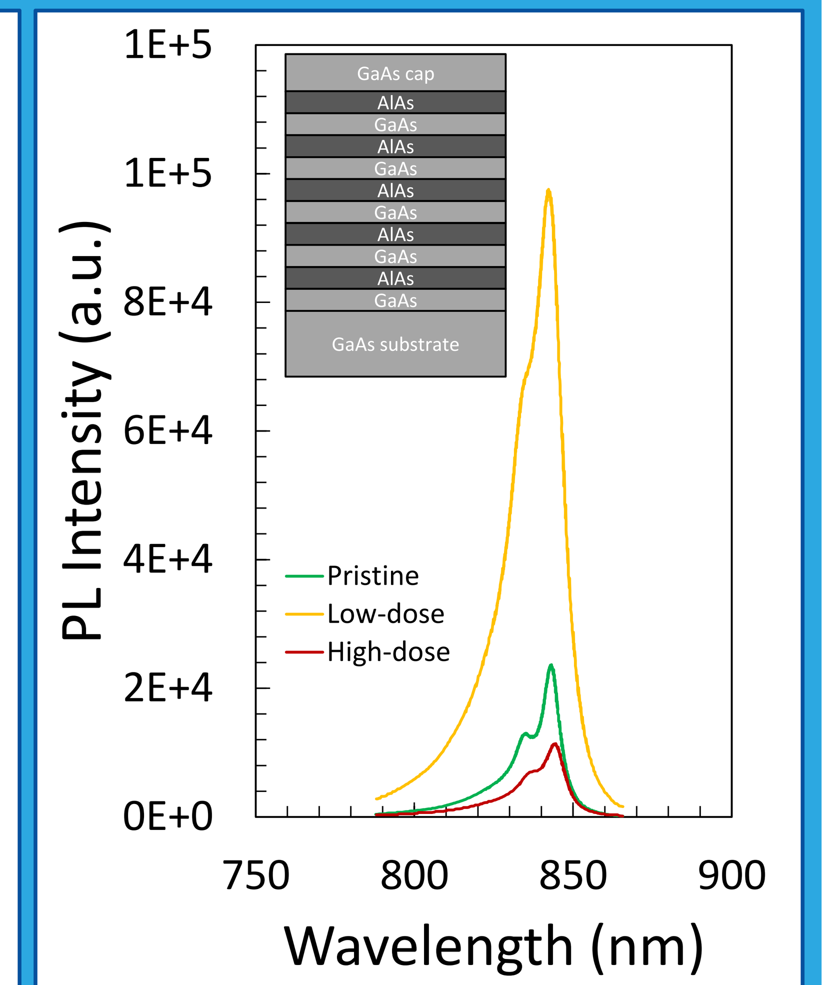
- Building foundational knowledge of thin film deposition for actinides at INL

METHODS
- **Molecular Beam Epitaxy** (MBE)
  - Nitrides at INL
  - III-Vs at Boise State University
- **Pulsed Laser Deposition** (PLD)
  - Ln-oxides at University of Utah
- **Computational modeling**
  - Phonon transport of various materials, INL & University of California-Riverside

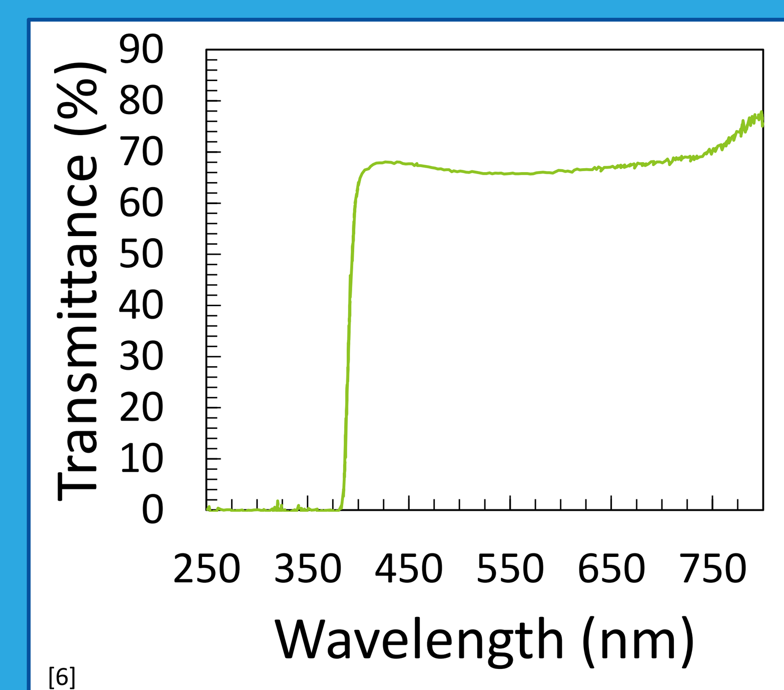


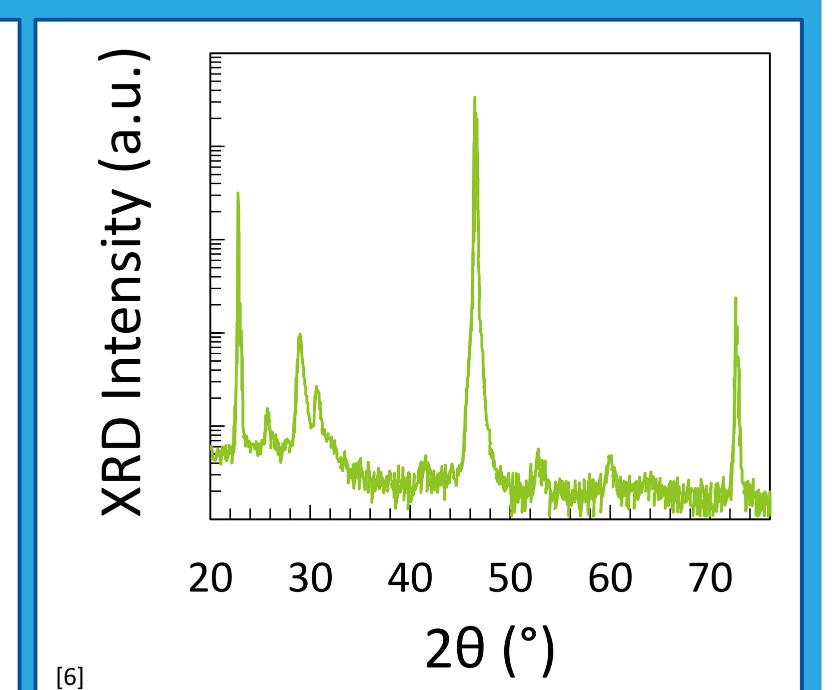
Interfaces change radiation damage
- MBE-grown
- Bulk material behaves differently compared to superlattices



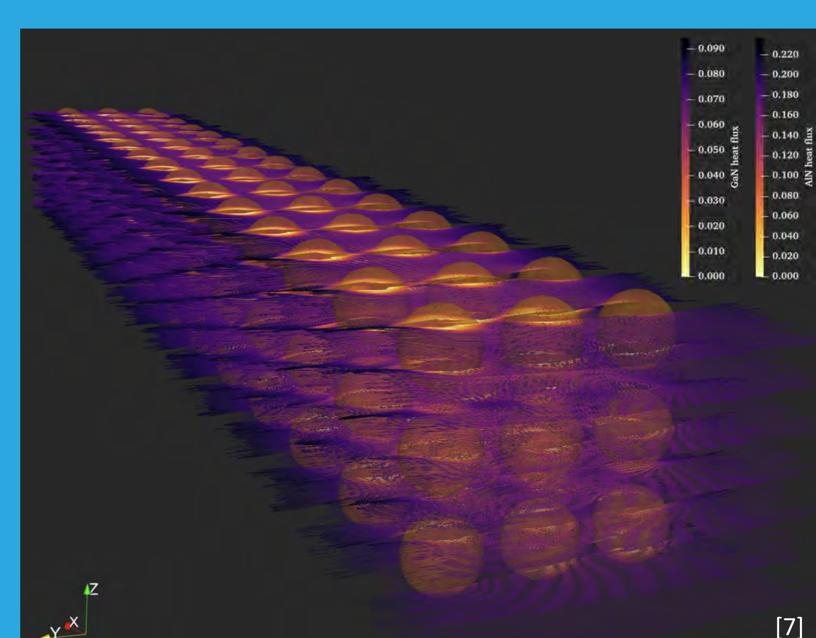


Deposition of lanthanide oxides
- PLD of Sm_2O_3
- Mn & Co alloying changes optical properties



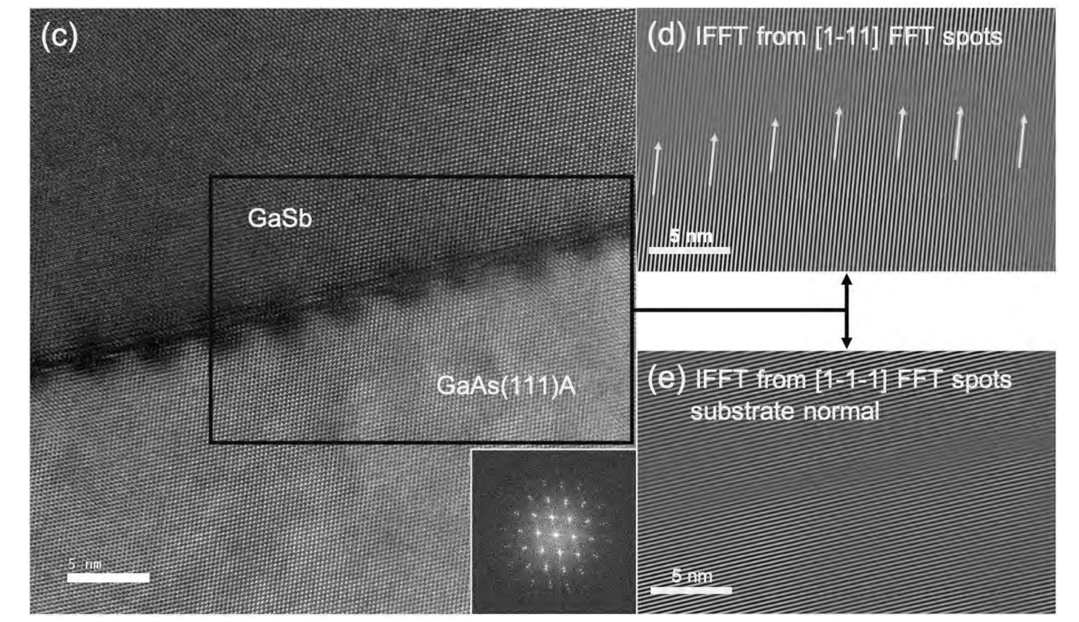


Phonon modeling in III-Ns

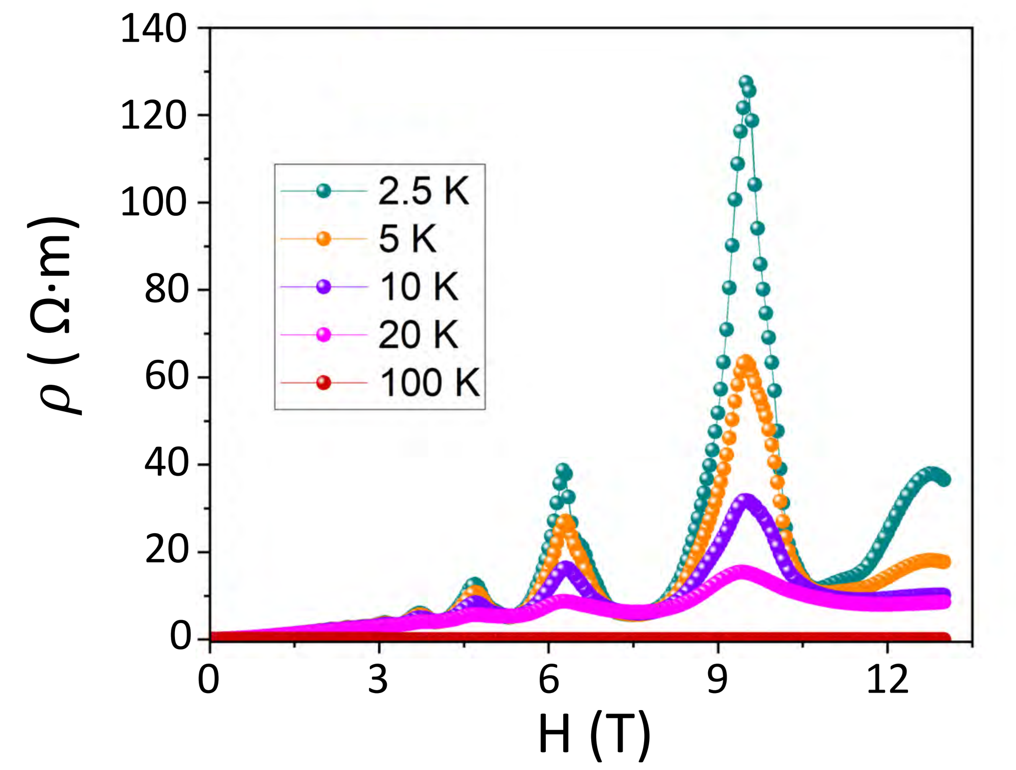


Thermal transport in the AlGaN based material system
- First-principles to finite-element
- High power optoelectronics
- Potential radiation-hard sensors

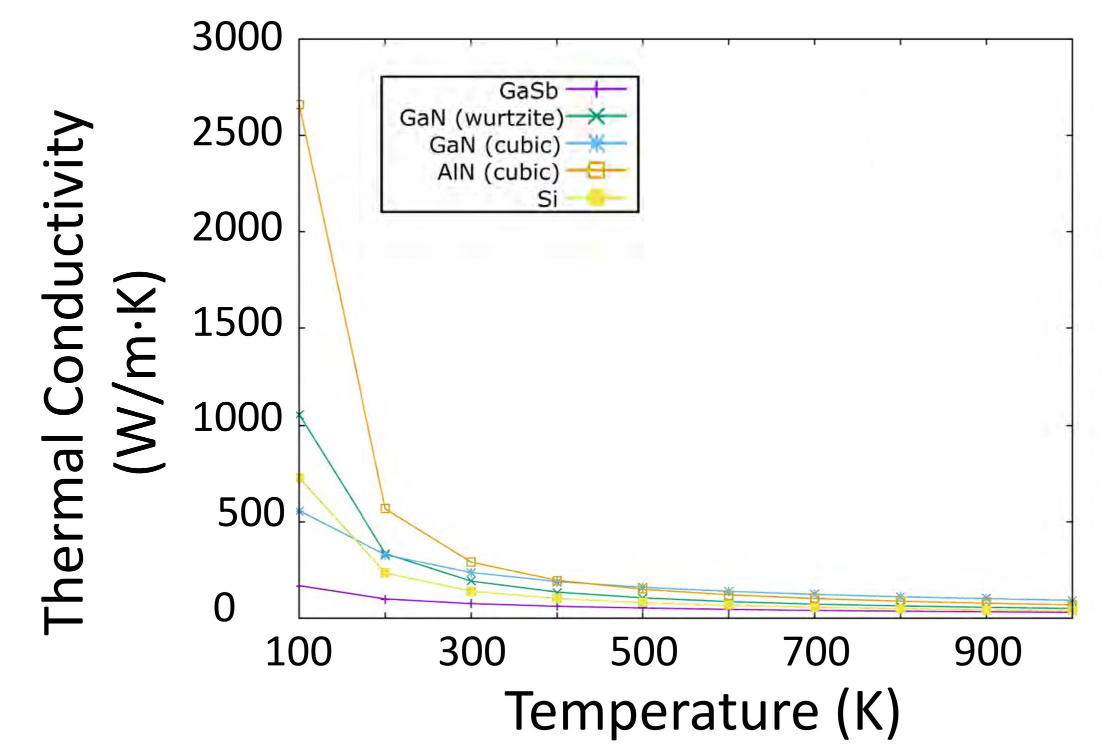
First growth of GaSb on GaAs (111)



Giant MR in GaSb >150,000%



Phonon property calculations



Papers from this project
1. Cody A. Dennett, et al. , **Nature Comm**, 13, (2022)
2. Kevin D. Vallejo, et al. **Rep. Prog. Phys**. 85 123101 (2022)
3. Madison D. Nordstrom, et al. , **Cryst Gro Des**. (submitted)
4. Gitanjali Mishra, Ashutosh Tiwari, **APS March Meeting Abstracts**, 2022
5. Madison D. Nordstrom, et. al., (in-prep)
6. Gitanjali Mishra, et. al (in-prep)
7. Jackson Harter, Cameron Chevalier, Alex Greaney (in-prep)

INL: Cody Dennett, Narayan Poudel, Kevin Vallejo, Jackson Harter, ShuixangC Zhou, Krzysztof Gofryk, Brelon May
UoU: Gitanjali Mishra Ashutosh Tiwari,
BSU: Maddy Nordstrom, Paul Simmonds,
UCR: Cameron xx, Alex Greany
NIST: Maria Muñoz, Tehseen Adel, Angela Hight Walker

Project Number: 21A1050-052FP LRS Number: INL/EXP-23-74107

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

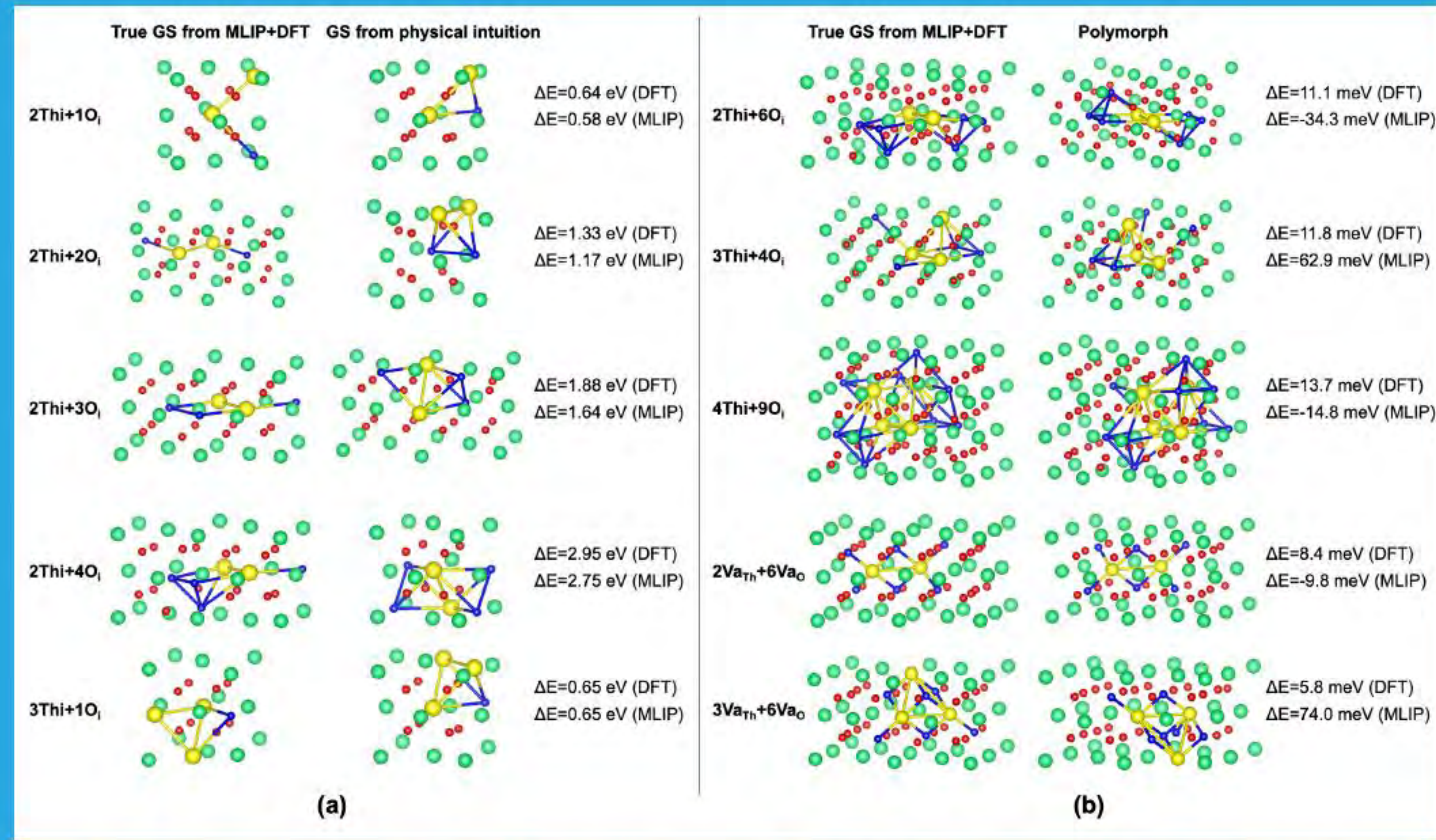
Title: Machine Learning Interatomic Potentials for Radiation Damage and Physical Properties in Model Fluorite Systems

PRESENTER: **Chao Jiang**

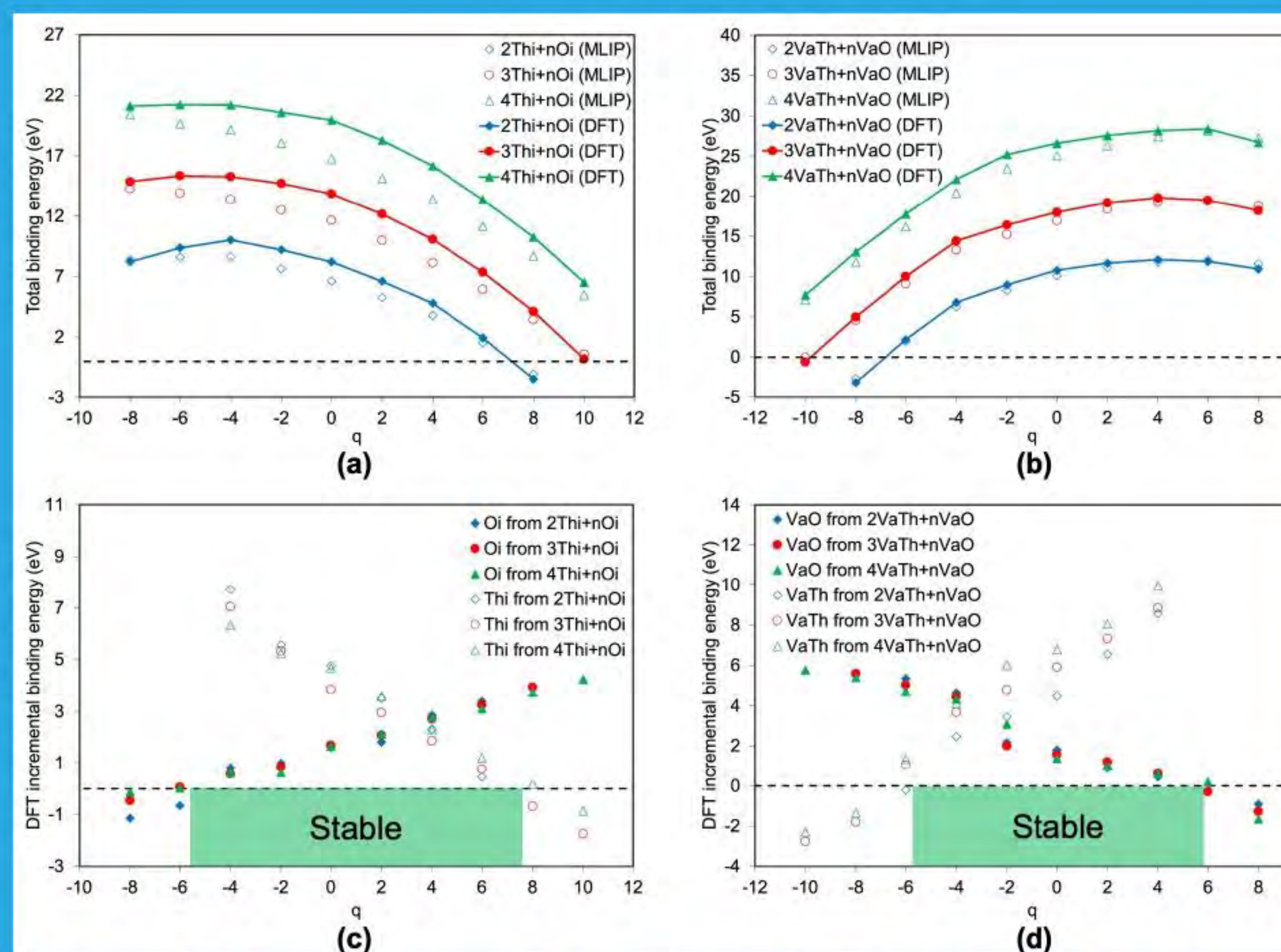
BACKGROUND: Machine learning interatomic potential (MLIP) has emerged as a powerful paradigm-shifting tool for addressing the computational challenge of modeling radiation damage in nuclear materials. In this project, we have developed MLIP to predict the structures and stabilities of small interstitial and vacancy clusters in irradiated ThO_2 with a fluorite structure, which has been proposed as an alternative nuclear fuel. While these small defect complexes are invisible under transmission electron microscopy (TEM), they can significantly downgrade the thermal conductivity of ThO_2 via phonon-defect scattering.

METHODS: A large database containing 3,672 total energies and 3,521,988 atomic forces has been constructed via high-throughput density functional theory (DFT) calculations. A neural network-based MLIP for ThO_2 has been trained using a supervised learning approach.

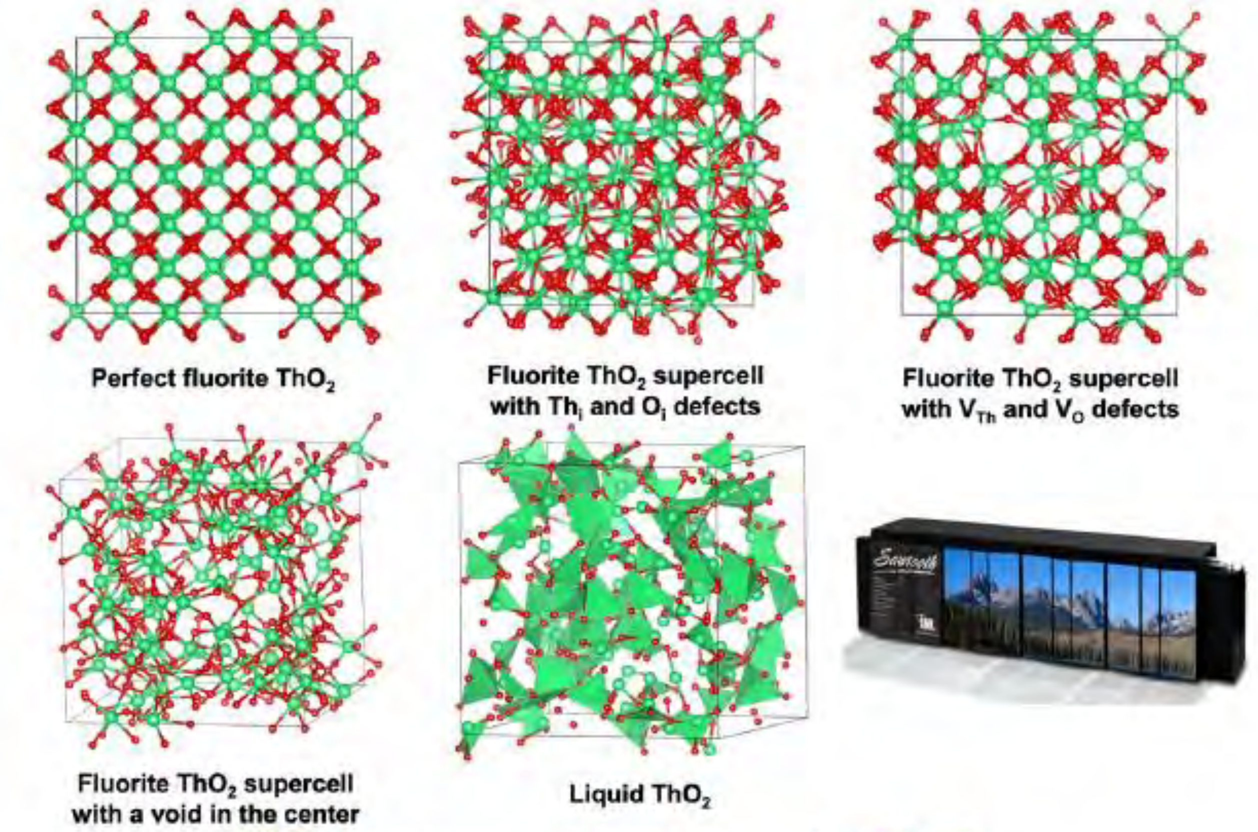
RESULTS: An exhaustive search for the ground-state (GS) defect structures has been performed using MLIP as a high-fidelity yet low-cost surrogate model for DFT. A total of 10,557,845 defect configurations have been considered. The search leads to many unexpected results such as non-compact GSs and GS polymorphism. The impact of atomic-scale defects on the thermal conductivity of ThO_2 has also been predicted.



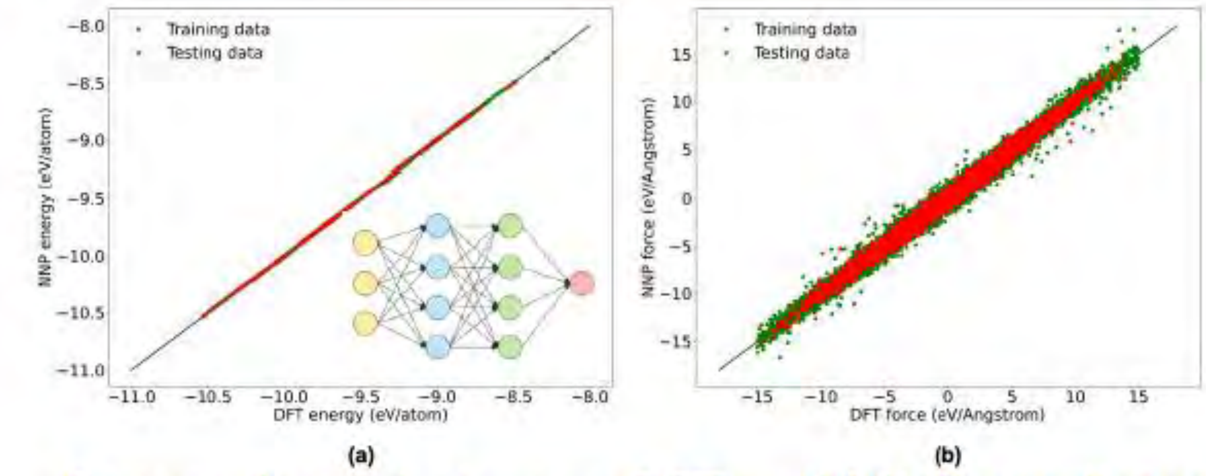
Ground-state configurations of atomic-scale defect clusters in ThO_2. (a) shows the unexpected non-impact ground-states of small interstitial clusters, while (b) demonstrates the existence of ground-state polymorphs.



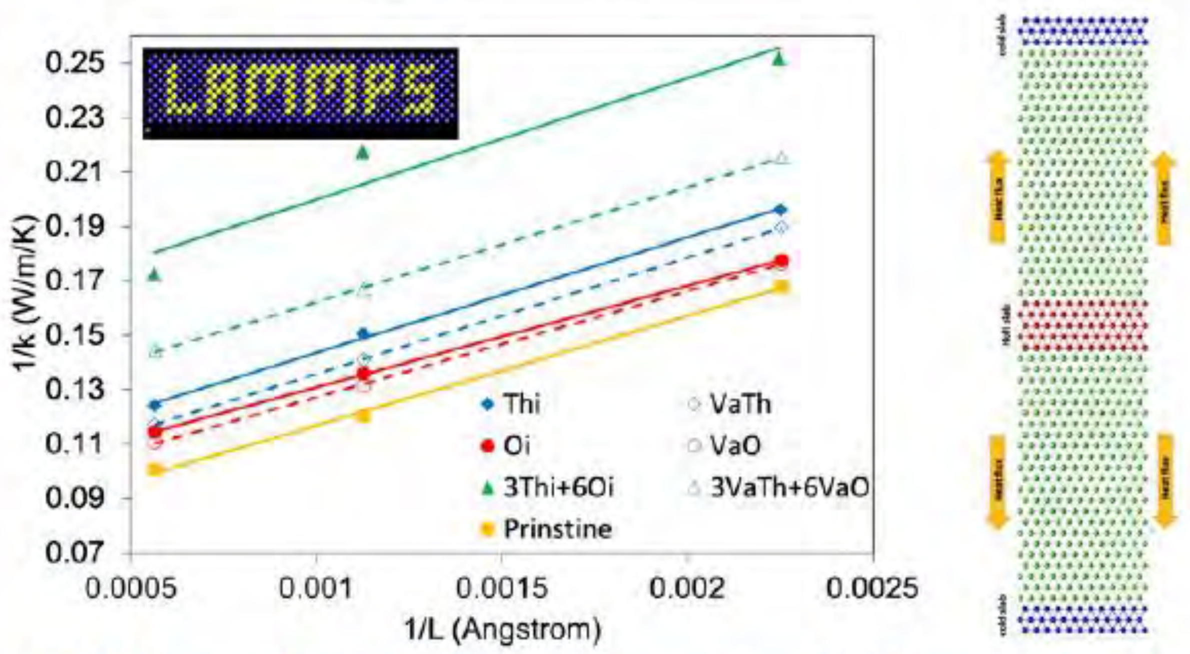
Stability of small defect clusters in ThO_2. (a) and (b) show the total binding energies of interstitial and vacancy clusters in their GS configurations. The DFT-calculated incremental binding energies are shown in (c) and (d). The shaded areas indicate the range of total charges (q) where the defect clusters are thermodynamically stable.



DFT training database for ThO_2



Comparisons between DFT and MLIP predicted (a) total energies and (b) atomic forces of ThO_2



MLIP-predicted thermal conductivities of perfect and defect-containing ThO_2 at 300 K.

Defect	MLIP (W/m/K)	Experiment
No defect	13.04	13.6*
Th_i	9.88	
Va_{Th}	10.74	
O_i	10.68	
Va_O	11.34	
$3Th_i+6O_i$	6.44	
$3Va_{Th}+6Va_O$	8.33	

*Experiment data from Acta Mater 213, 116934.

Chao Jiang and Zilong Hua

Project Number: 21A1050-078FP   LRS Number: INL/MIS-23-74117

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

An Innovative Approach for Accelerated Irradiation Studies of Materials

Cheng Sun[1], Mukesh Bachhav[1], Chao Jiang[1], Ju Li[2]

1. Idaho National Laboratory. 2. Massachusetts Institute of Technology.

Introduction

The objective of this project is to develop an innovative approach to accelerate irradiation studies of materials in nuclear reactors. For many years, ion irradiation has been used as a surrogate for neutron irradiation as the ion flux can be readily tuned to achieve high irradiation flux. However, ion irradiation creates a number of features in materials that are not observed in neutron irradiated specimens, such as irradiation polarization artifacts, defects imbalance, etc. We propose to develop a new approach to accelerate irradiation damage studies of materials in nuclear reactors using Boron neutron capture (BNC) approach.

Materials, methods, and results

Titanium-aluminum-tungsten-boron (Ti-Al-W-B) alloys have been fabricated using spark plasma sintering (SPS) process under 50 MPa at 1375°C . The alloys were irradiated in NRAD reactor and the post-irradiation examination was performed using transmission electron microscopy at IMCL at INL.

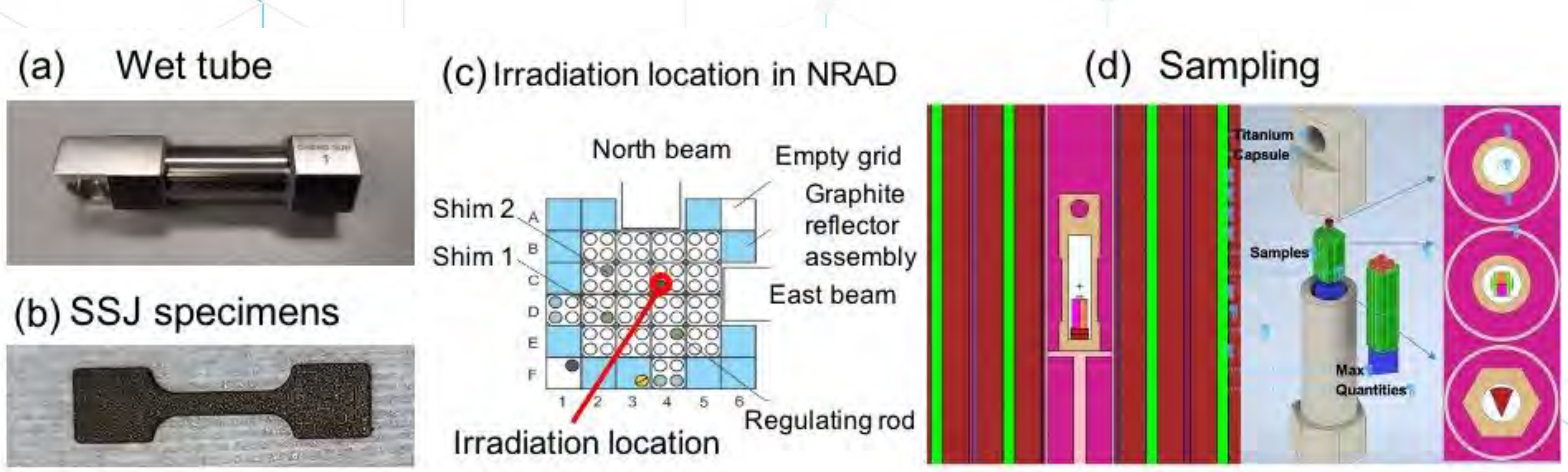


Figure 1. Neutron irradiation in NRAD reactor at INL. (a) Fabricated wet tube and small-scale J-type specimens. (b) The position (red spot) of the loaded capsule in the reactor. (c) Schematics of irradiation capsule and its irradiation location.

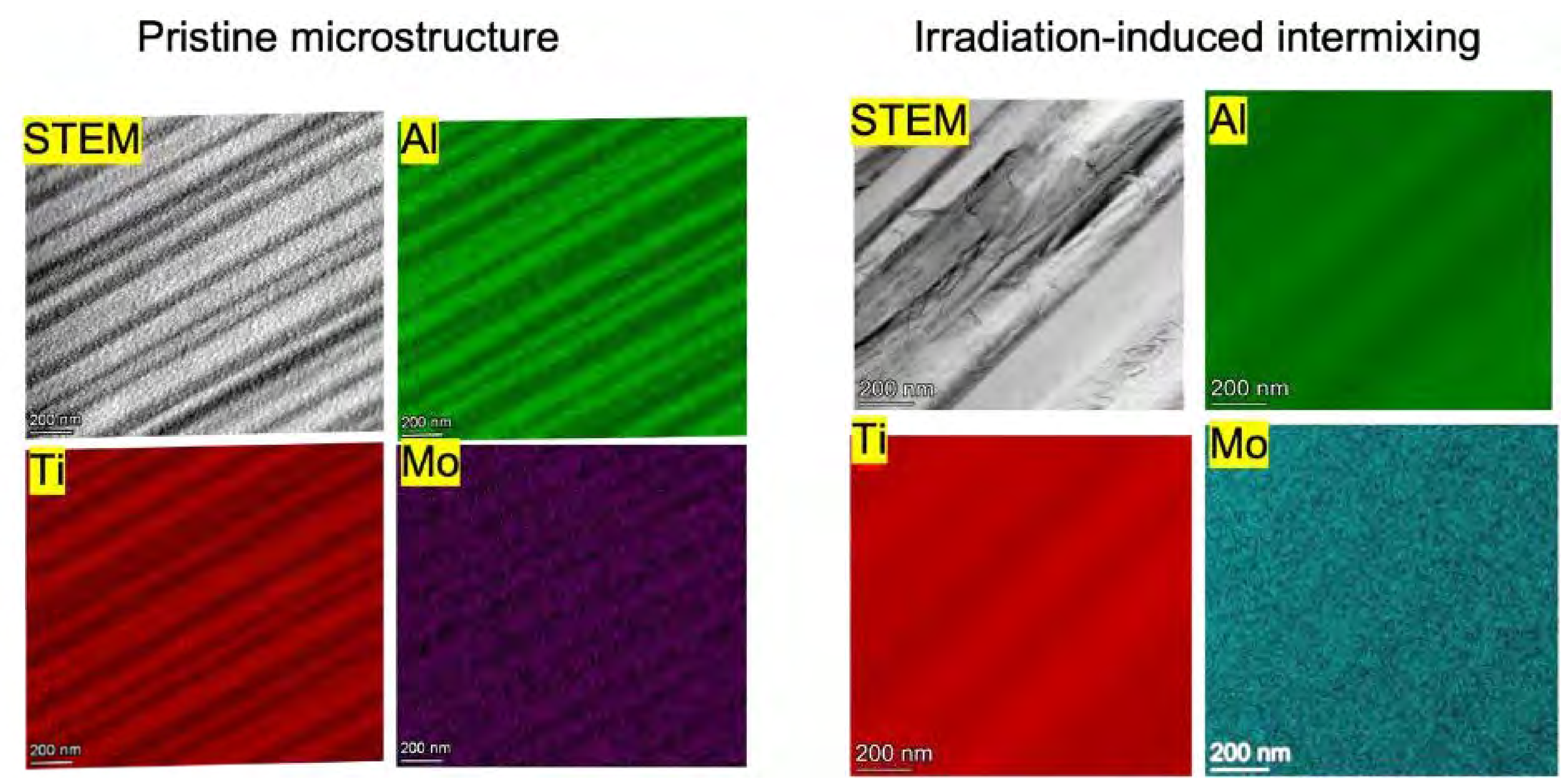


Figure 2. Chemical distribution of Ti-Al-W-B alloy. (left) Before irradiation. Ti-Al alloys showing two-phase nano-lamellar structure with Mo segregated in the α phase. (right) After neutron irradiation. Irradiation-induced intermixing occurs at such low dose irradiation due to the accelerated irradiation flux caused by boron addition. Mo is uniformly distributed in both α and β phases after irradiation.

Conclusions and impact

This project used the concept of BNC therapy to accelerate in-pile irradiation damage in research reactors. By using this approach, the desired irradiation doses can be achieved with much shorter time and lower cost. This approach dramatically decreases the cost and time required for irradiation testing in reactors and expedite the qualification of new nuclear materials and validation of computational models.

Publications

1. H. Xu, S. Kim, D. Chen, J. Monchoux, T. Voisin, C. Sun, J. Li, *Advanced Science*, 32, 2022, 2203555.
2. D. Morgan, G. Pilania, A. Couet, B. P. Uberuaga, C. Sun, J. Li, *Current Opinion in Solid State and Materials Sciences,* 26, 2022, 100975.

Project Number: 21A1050-099FP LRS Number: INL/EXP-23-74104

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

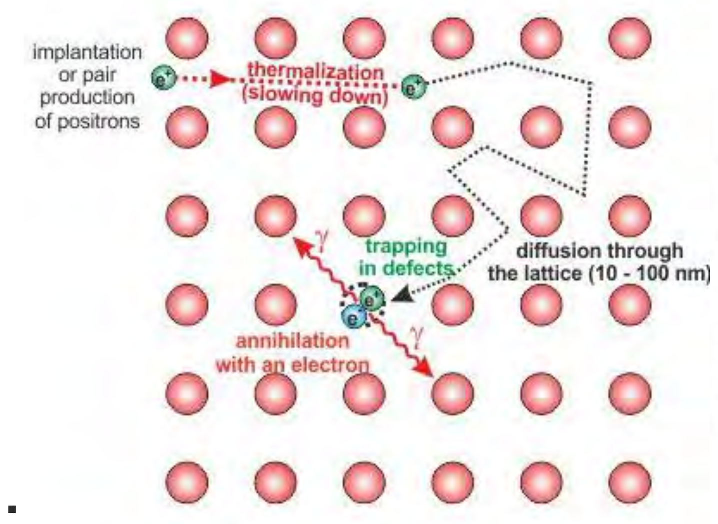
Idaho National Laboratory

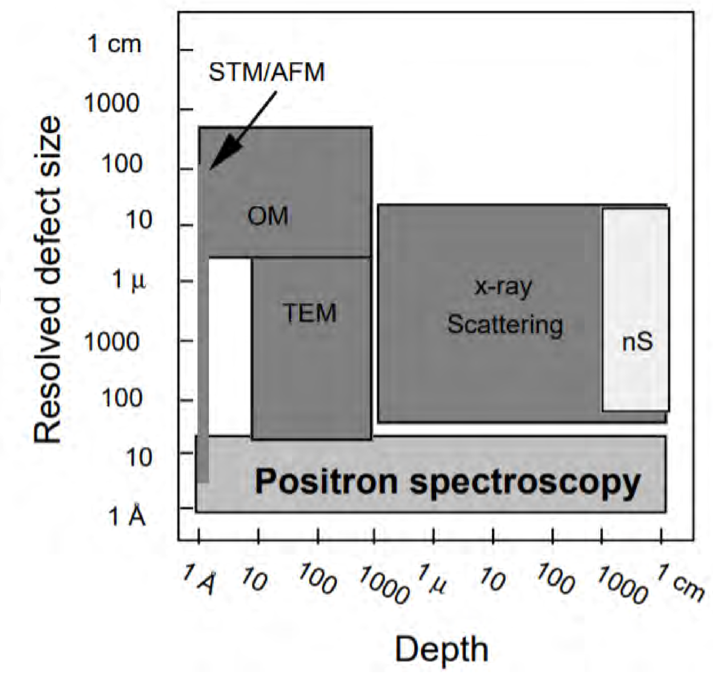
In-situ Positron Annihilation Spectroscopy

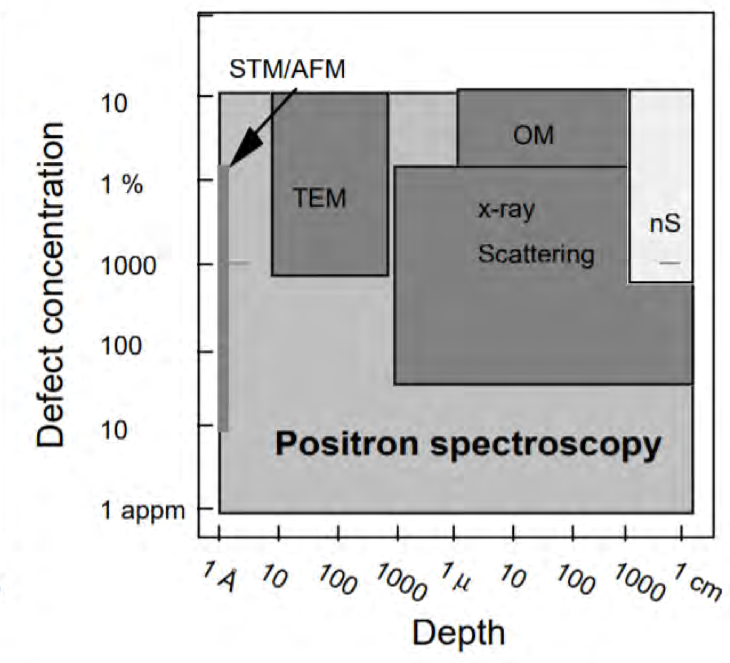
Chuting Tsai, Jagoda Urban-Klaehn, Chase Taylor, Connor Harper

Motivation

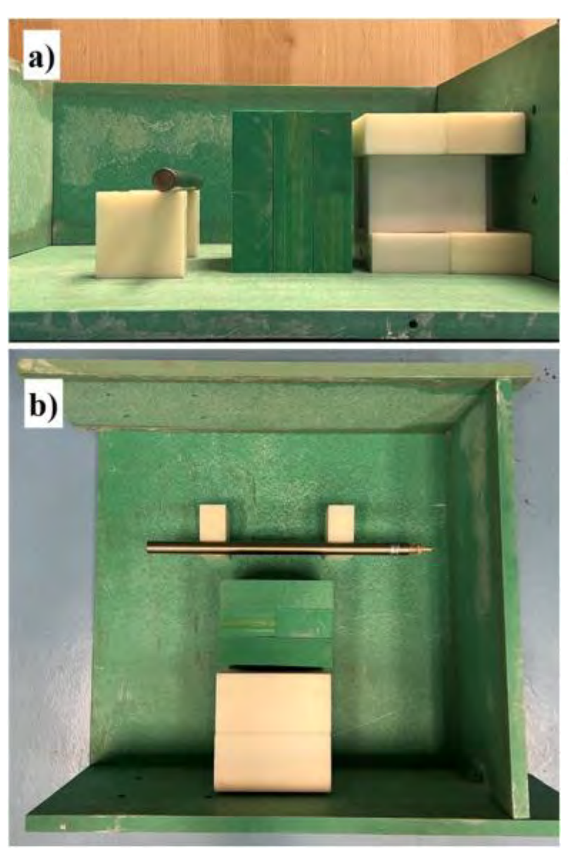
- PAS is sensitive to low vacancy concentration (~10^{14} cm^{-3}) and small defect size (sub nanometer). It can probe the formation of vacancy defects well below 1 dpa.
- Experimentally observe the generation and the evolution of point defects by probing the size, density and type of the vacancy type of defects.

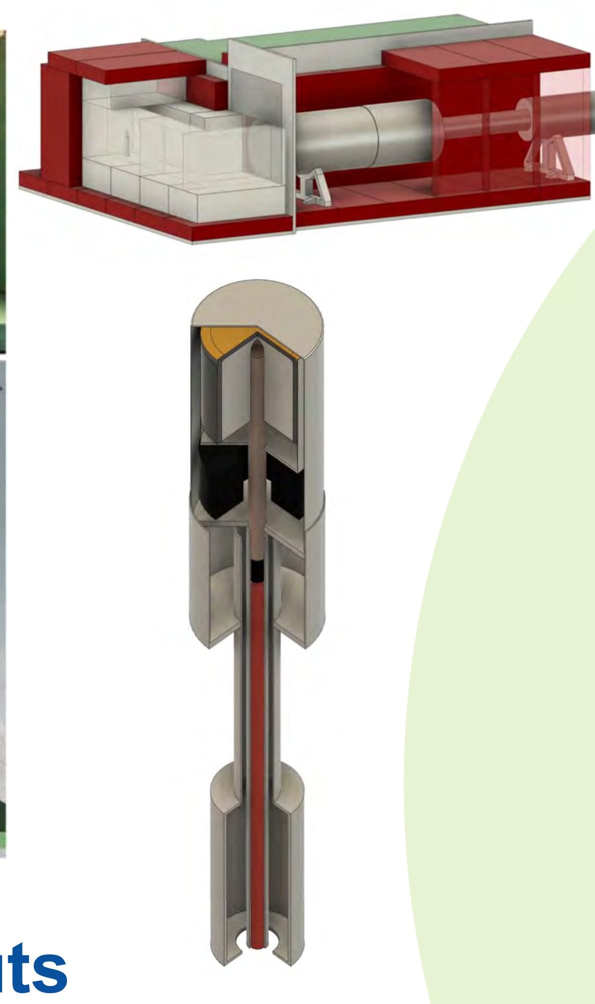






Method development - Experiment

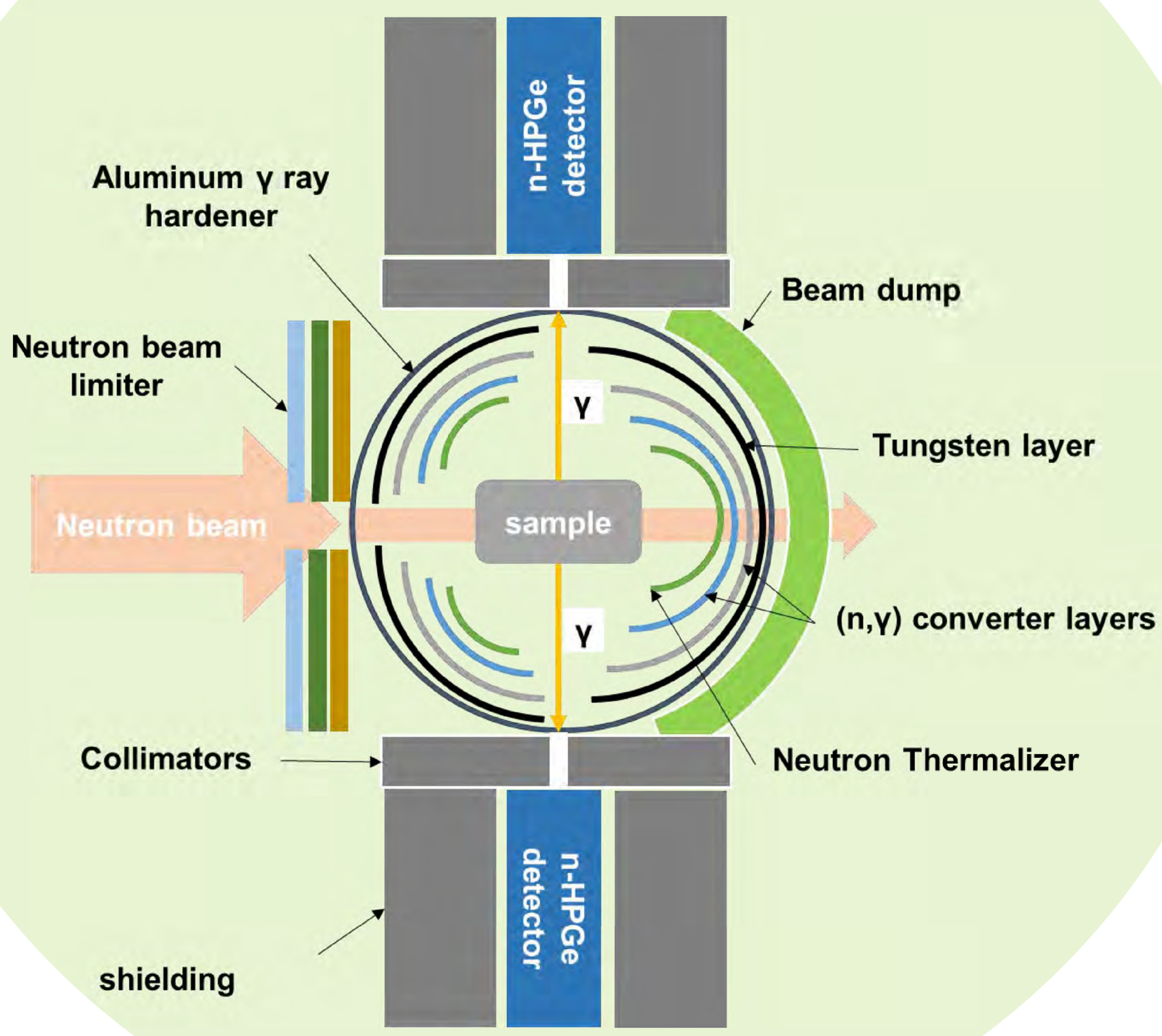




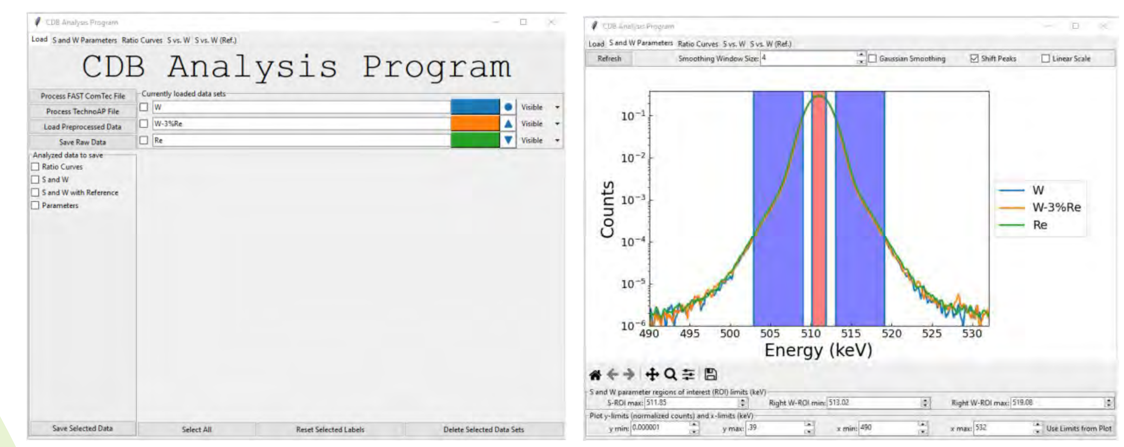
Research Outputs

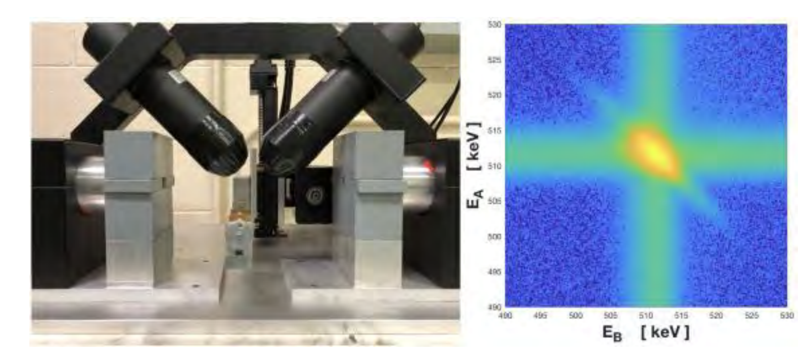
- Method for neutron source activity determination
- Optimization of n,γ reaction
- Accurate detector efficiency determination

Overarching conceptual



Method development - Software

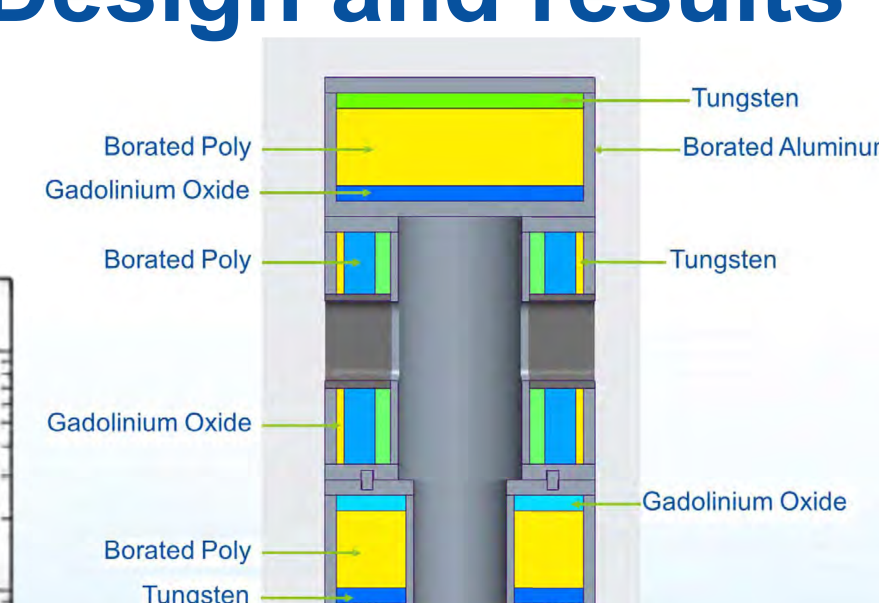


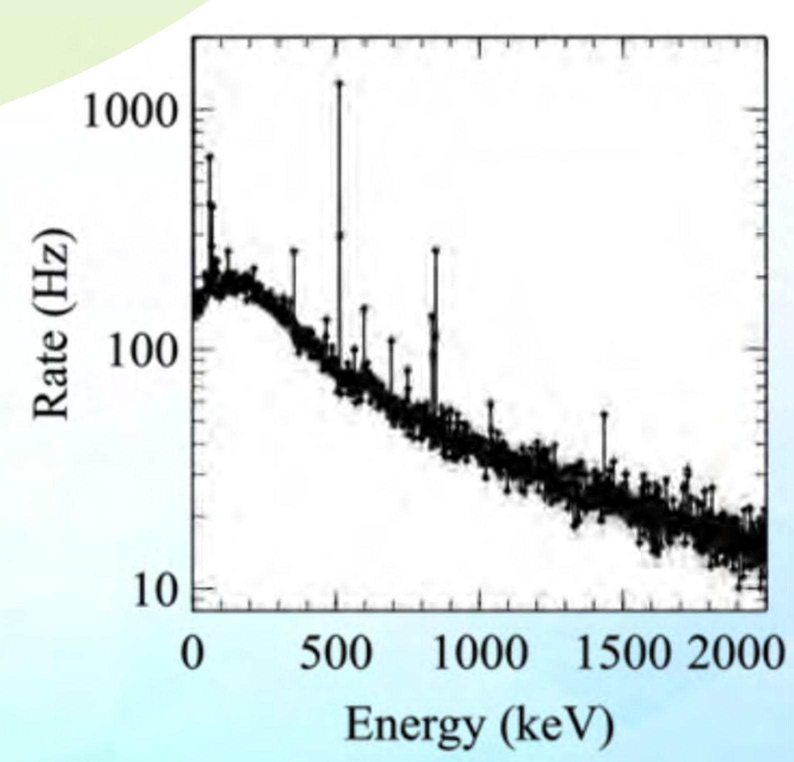


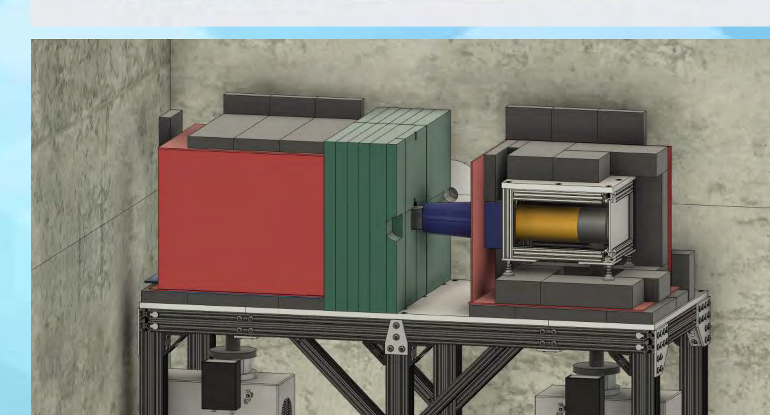
Research Outputs

- Open-source software
- Versatile, transparent, and fast Coincidence Doppler Broadening data analysis tool

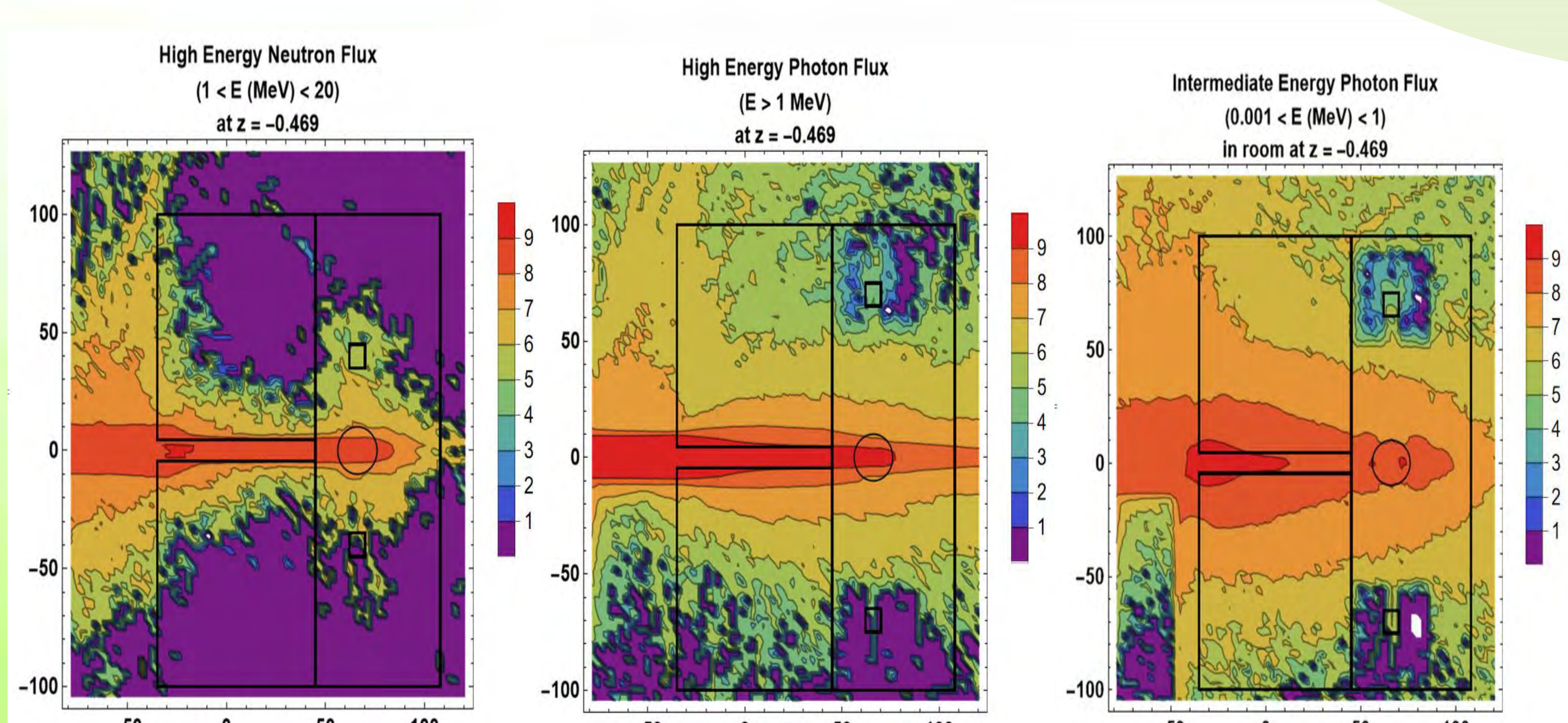
Design and results







Experiment theoretical



	Chamber in place
Total Gamma Rate (cps)	163,000 +/- 7,000
Coincidence Rate (cps)	157 +/- 23 1E6 counts in 1.77 hrs
Signal to noise (505keV < E < 517keV)	0.679

Research Outputs

- Drawings released for NRAD, experiment at university assembled
- Binned data would indicate hourly evolution of defects
- Coincidence rate 157hz at NRAD, 2.9hz at OSURR

Reference and acknowledgement

- Howell, Richard H., Thomas E. Cowan, Jay H. Hartley, and Philip A. Sterne. "Positron beam lifetime spectroscopy at Lawrence Livermore National Laboratory." In AIP Conference Proceedings, vol. 392, no. 1, pp. 451-454. American Institute of Physics, 1997.
- Positron Annihilation at Martin-Luthen-University Halle: http://positron.physik.uni-halle.de/
- Stonaha, P. J., C. Harper, C. Tan, J. Urban-Klaehn, C. N. Taylor, T. Forest, and D. Dale. "Accurate activity determination of a californium neutron source." Applied Radiation and Isotopes 194 (2023): 110712.
- Evans, George S., Joseph M. Watkins, Chase N. Taylor, Jagoda Urban-Klaehn, and Chuting T. Tsai. "CDB-AP: An application for coincidence Doppler broadening spectroscopy analysis." SoftwareX (2023): 101475.

- Work supported through the INL Laboratory Directed Research& Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

An accelerated assessment of the creep mechanisms in uranium zirconium model alloys

Principal Investigator: David Frazer, Co-PIs: Dewen Yushu, Tianyi Chen
Contributors: Tzu-Yi Chang, Gavin Vandenbroeder, Stephanie Pitts

Nanoindentation creep was demonstrated on nuclear fuel materials up to 200ºC. Temperature dependency of the obtained creep exponent was observed, agreeing with the creep theory. The load-dependency and stress relaxation were also identified for future investigation.

Creep in nuclear fuel

Creep is generally observed in nuclear fuel, cladding, and structural materials. It limits the lifetime of the nuclear components. Various factors such as high temperature, stress, irradiation, and the material microstructure evolution, simultaneously complicate the deformation mechanism behind the creep phenomena. Thus, understanding the creep on fuel and structural materials in a nuclear reactor is essential for safe reactor operation but remains challenging.

Challenges

Conventional creep measurements are expensive and time consuming. This makes it difficult to gather data quickly and efficiently for new structural and fuel material development. In addition, the microstructural heterogeneity in irradiated fuels prevents conventional testing methods to obtain microstructure-dependent creep properties.

Nanoindentation method

With a smaller amount of sample, nanoindentation creep measurements hold promise as they have been shown to measure the creep stress exponent that is comparable to the macro-scale values but at a significantly reduced time scale. It also gives localized material information regarding a specific area of interest.

Significance

This project combined modeling and nanoindentation creep measurements to better understand the deformation that is taking place under the tip. Specific areas of interest are the examination of the interface between plastic deformation and elastic deformation regions under the indent.

The understanding of the size of the plastic zone and its growth as compared with the elastic zone during the indent would give insights into the deformation process taking place in the material.

Methodology

Creep test

(1) Annealed U-50 wt% Zr samples were polished to a mirror finish for the nanoindentation creep test in vacuumed SEM chamber.

(2) Nanoindentation creep tests were conducted with a Berkovich tip under the force-controlled mode.

(3) The force dependency, temperature dependency, and loading rate dependency were examined.

(4) The data was processed with classic creep theory.

Stress relaxation test

(1) The stress relaxation tests were conducted with a Berkovich tip under the displacement-controlled mode.

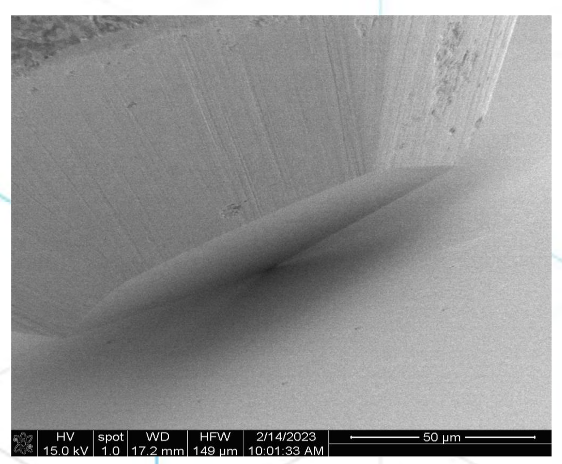
(2) Stress relaxation tests were performed on both U-50Zr and pure-aluminum.

(3) The data was processed with power law and general-Maxwell models.

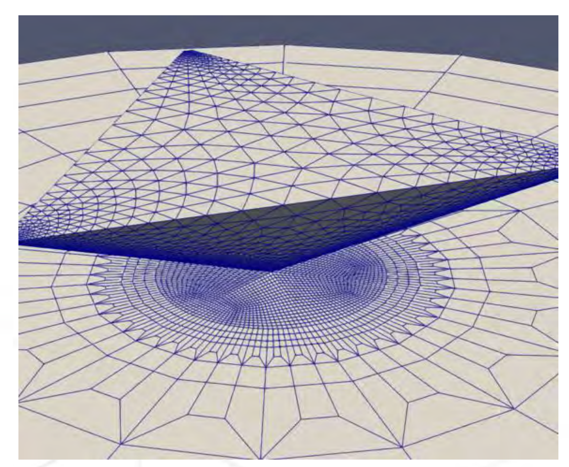
Computational modeling

(1) Modeling and simulation of the indentation process are carried out using MOOSE [1] and the mesoscale code, Marmot [2], for the aluminum and alpha uranium crystal plasticity capabilities, respectively.

(2) The modeling visualized the microstructural evolution and stress distribution under the Berkovich tip.



Berkovich nanoindenter

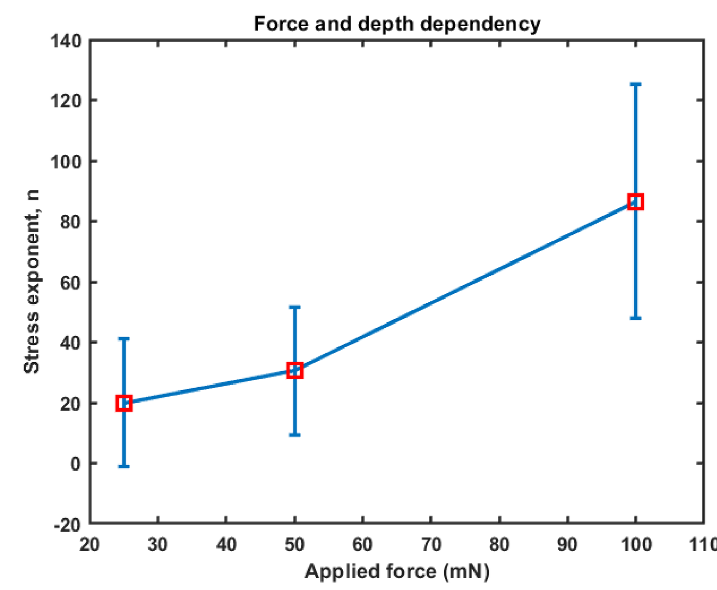


Berkovich tip in modeling

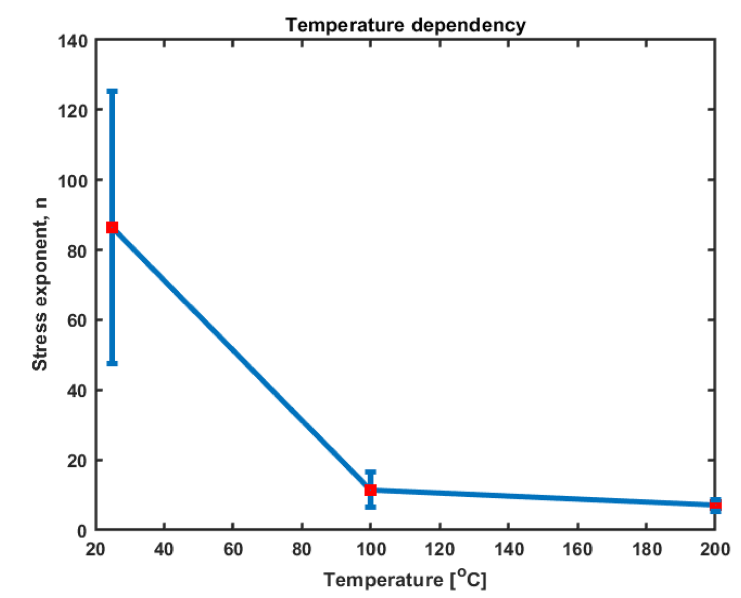
[1] Lindsay, Alexander D., et al. "2.0-MOOSE: Enabling massively parallel multiphysics simulation." SoftwareX 20 (2022): 101202.
[2] Idaho National Laboratory, Virginia Polytechnic Institute and State University "MARMOT Mesoscale Simulation Code" https://inlsoftware.inl.gov/product/marmot

Creep

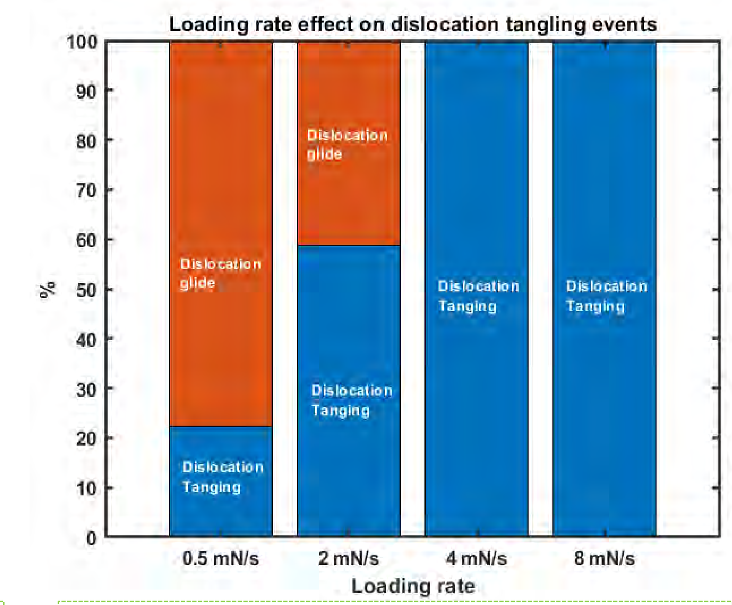
Creep is a time-deformation phenomenon that can relate to stress, temperature, and microstructure. The stress exponent based on the classic creep theory is an experimental value of stress sensitivity used to infer a possible mechanism and structural evolution of the deformation. Our results show a force effect, temperature effect, and loading-rate effect on creep behavior via nanoindentation method.



The force (25mN, 50mN, and 100mN) effect on creep at room temperature shows an increasing stress sensitivity to the deformation rate along with the depth. The dislocation glide is the dominant deformation mechanism.



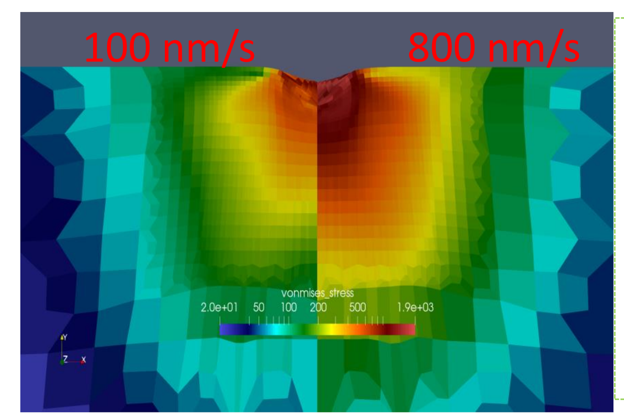
The temperature effect (25°C, 100°C, and 200°C) shows a decreasing stress sensitivity. The higher temperature initial a vacancy diffusion leading to dislocation climb mechanism.



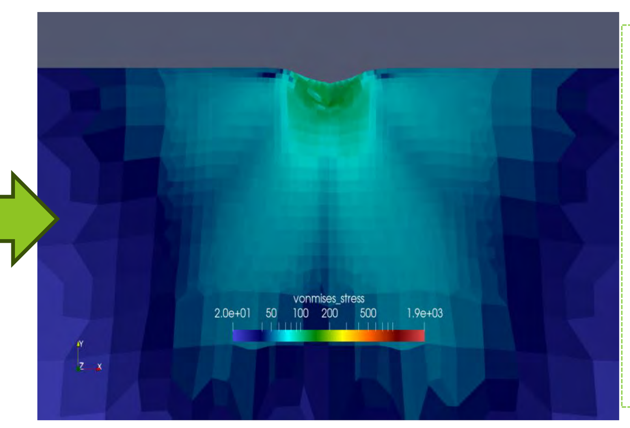
A higher applied loading speed leads a higher chance to dislocation tangling events and thus induces a longer stress relaxation which influences the stress rate sensitivity during steady state creep.

Stress Relaxation

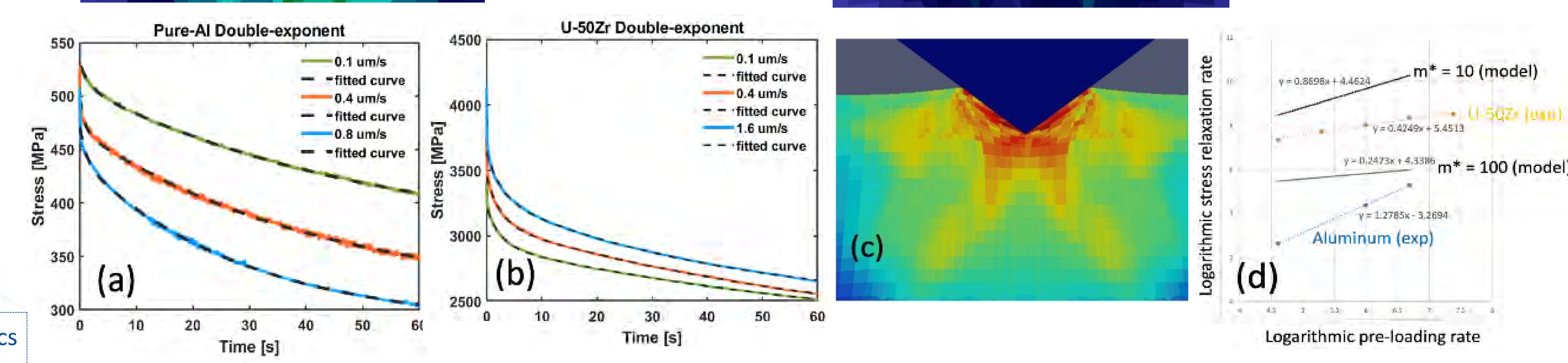
Stress relaxation is a phenomenon of atom re-arrangement during material deformation. Our results from both experiment and modeling show a loading rate dependency on stress relaxation, and a new approach for stress sensitivity estimation is developed.



Von Mises stress 0.0 seconds into the holding phase comparing loading rates of 100 and 800 nm/s with a stress exponent of 10. The stress in 800 nm/s is much higher.



Von Mises stress 2.0 seconds into the holding phase comparing loading rates of 100 and 800 nm/s with a stress exponent of 10. Both loading rates relax to nearly the same stress distribution.



Nanoindentation stress relaxation in aluminum (a) and U-50Zr (b) following different pre-loading displacement rates. This relaxation process was simulated using MOOSE with crystal plasticity model (c) and the relationship between stress relaxation and pre-loading rate is demonstrated as a new approach for stress exponent estimation (d).

Project Number: 22P1068-002FP LRS Number: INL/EXP-23-74126

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Modeling and Separate Effect Tests to investigate the microstructure of at the top of metallic fuel pins

Fidelma Di Lemma (PI)
PRESENTER Jake Fay
fidelmagiulia.dilemma@inl.gov

*The porous **(fluff)** structure at the top of the metallic fuel pins may influence reactivity and the source term.*

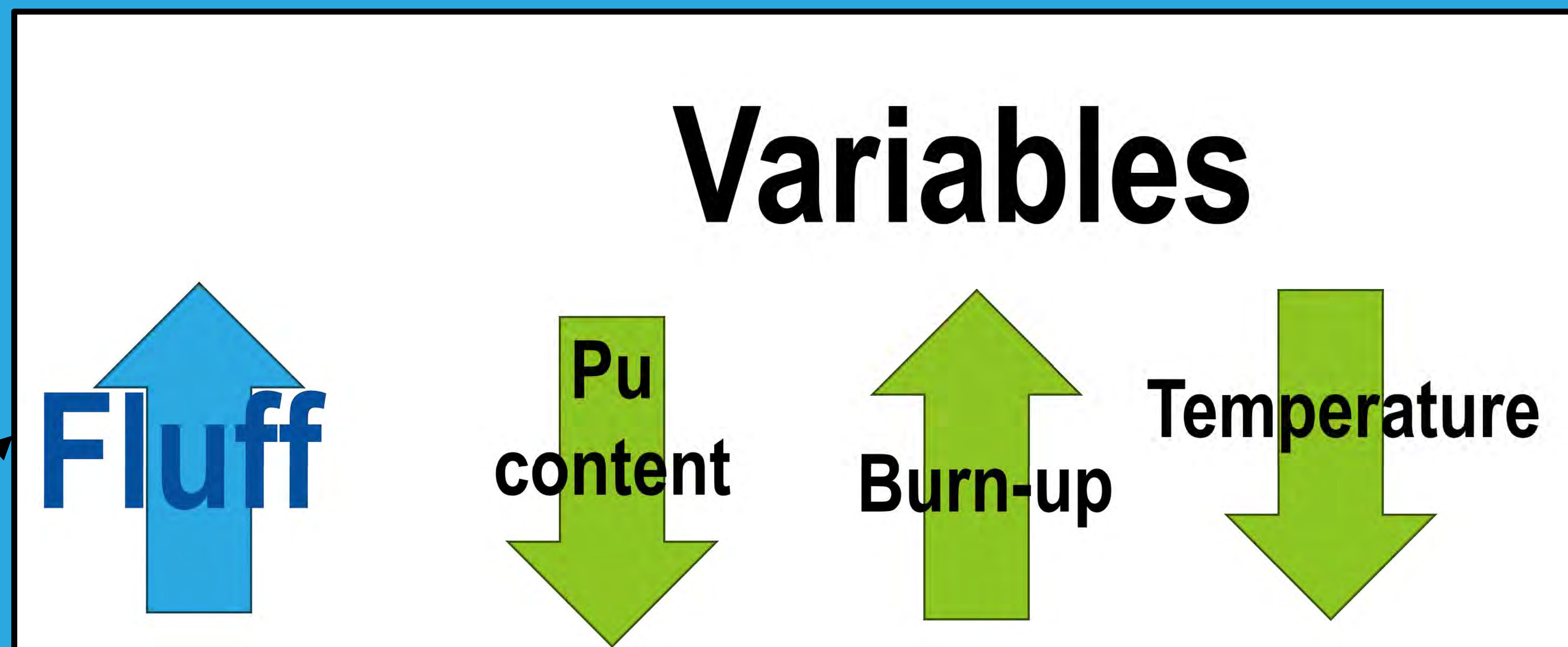
METHODS

1. Review of available database to develop correlations.
2. Image analyses to avoid subjectivity.
3. BISON simulation to provide insight on the phenomena.
4. Separate effect test for creep and thermal gradients.

RESULTS

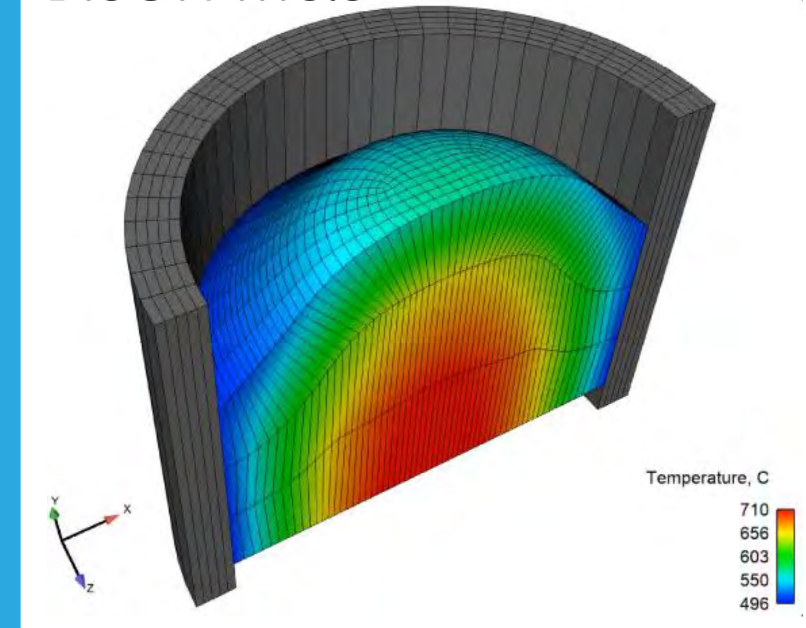
- Quantified relations between fluff length and fuel parameters/irradiation conditions.
- Developed an image analysis method using new parameters to describe the fluff.
- Modelling indicates the source of this structure to be Fuel/Cladding Mechanical iInteraction or fission gas and porosity growth.
- Creep Separate Experiments show that current models are unable to simulate this structure.
- Developed a furnace with prototypical temperature gradients and sodium cooling.

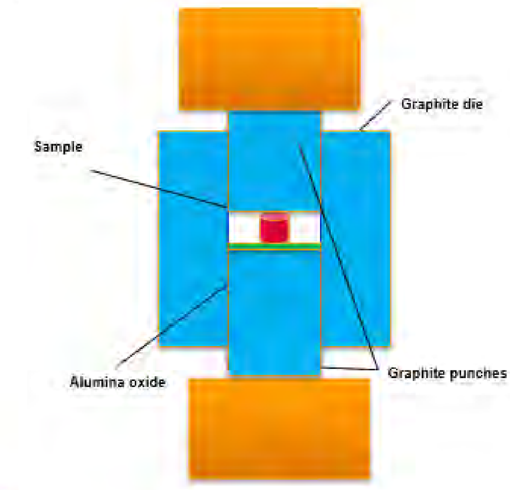
The fluff length has a direct relation to burn-up, temperature and fuel composition.



A
B
F. Di Lemma, L. , Capriotti, P. Medvedev, A. Gribok, B. Spencer, J. Lian[A], J. Fay[A], T. Knigth[B], X. Huang[B], J. Bao[B]

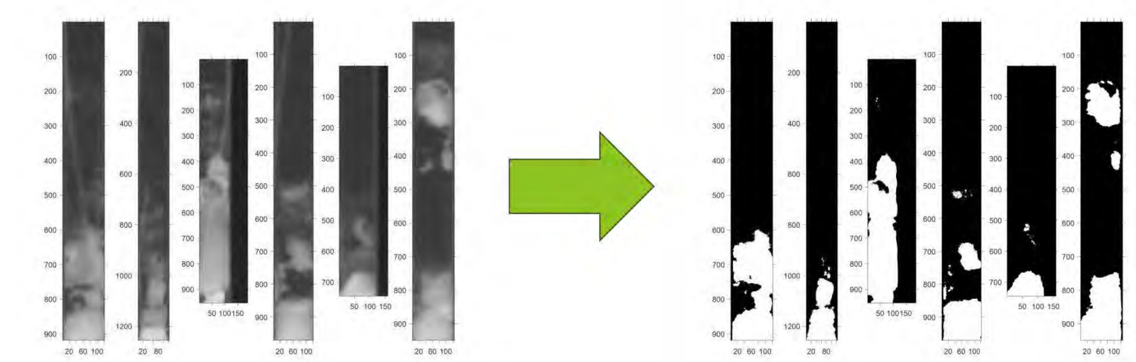
BISON M&S



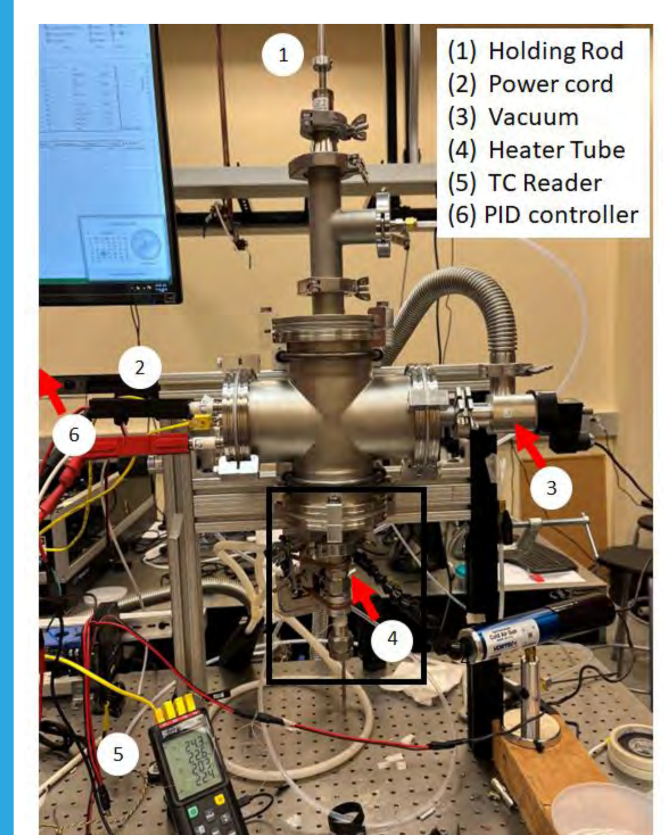


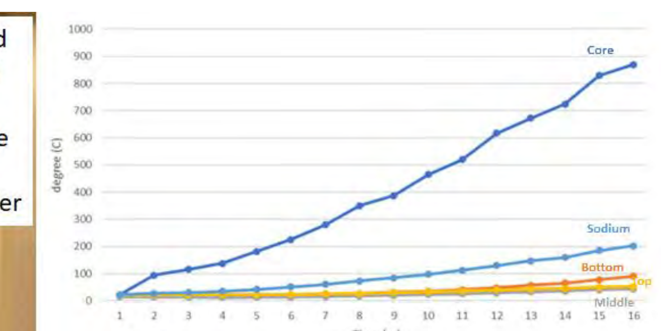
Creep tests

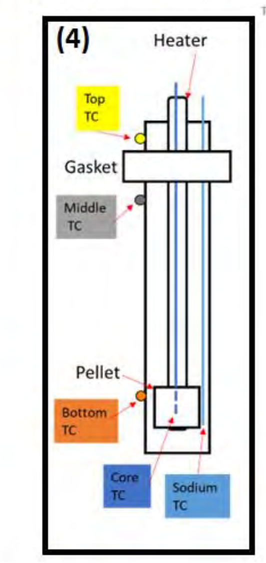
Image analyses



Property	Description
Total area of the porous matter, cm^2	Calculates the total number of pixels in all porosity regions and converts the number to cm^2. Measures the total amount of porous matter present for each pin.
Total convex area of the porous matter, cm^2	Calculates the area of the smallest convex polygon containing all porosity regions, called convex hull. Measures the dispersion of the porosity for each pin.
Solidity, unitless	Total area/total convex area, calculates the ratio of the porous matter area within the convex hull to the area of convex hull. Solidity is bounded from above by one.
Average extent, unitless	Total area/region's bounding box area, extent is bounded from above by one. Measures the density of the porous matter region within its bounding box.
Average eccentricity, unitless	Eccentricity measures the average roundedness of the porosity regions. For a single region, the eccentricity is equal to 0 if the region is a perfect circle, and it is 1 if the region is a line segment. The eccentricity and average eccentricity are between 0 and 1.
Average equivalent diameter, cm	Diameter of a circle with the same area as a porosity region averaged over all regions within bounding box. Measures granularity of the porous matter.
Average perimeter, cm	Measures perimeter of each porosity region for a pin and takes the average.







Furnace tests

OUTCOMES

5+ journal papers and 1 graduate fellow

Project Number: ***21A1050-006FP*** LRS Number: **INL/EXP-23-73840**

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Unattended Operation through Digital Twin Innovations

PI: Jeren Browning

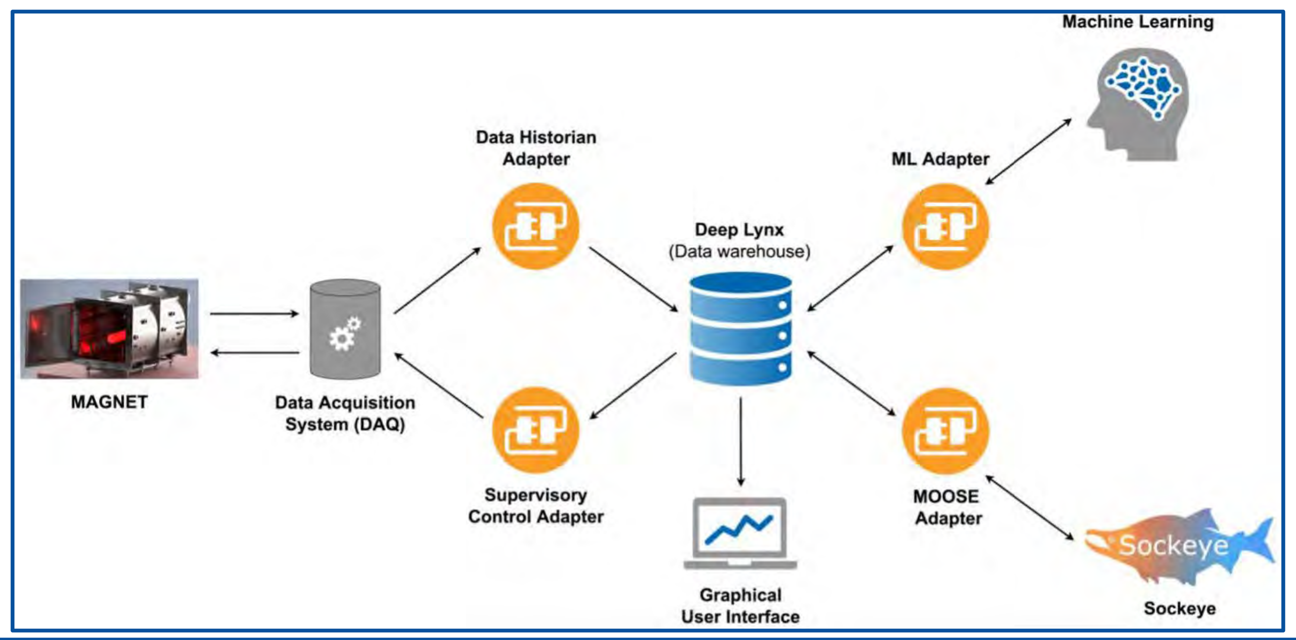
First digital twin to control a non-nuclear microreactor.

Jeren Browning, Katherine Wilsdon, Joshua Hansel, Bri Rolston, Adam Pluth, Ross Kunz, Andrew Slaughter

4 Parts of a Digital Twin:

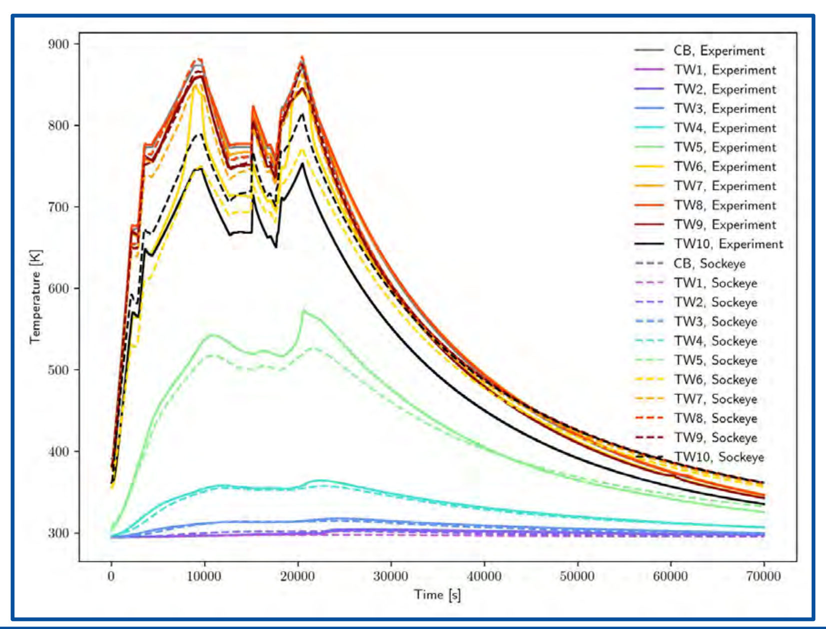
1 Bi-directional Communication

- Sensor data in real-time
- Controls sent from digital twin



2 Models & Predictions

- Physics modeling (MOOSE)
- Machine learning & AI



Listed as a **Nuclear Milestone** and one of **11 Big Wins for Nuclear Energy** in 2022 by the Office of Nuclear Energy

SCAN ME ⟵ *See* the digital twin **in action**

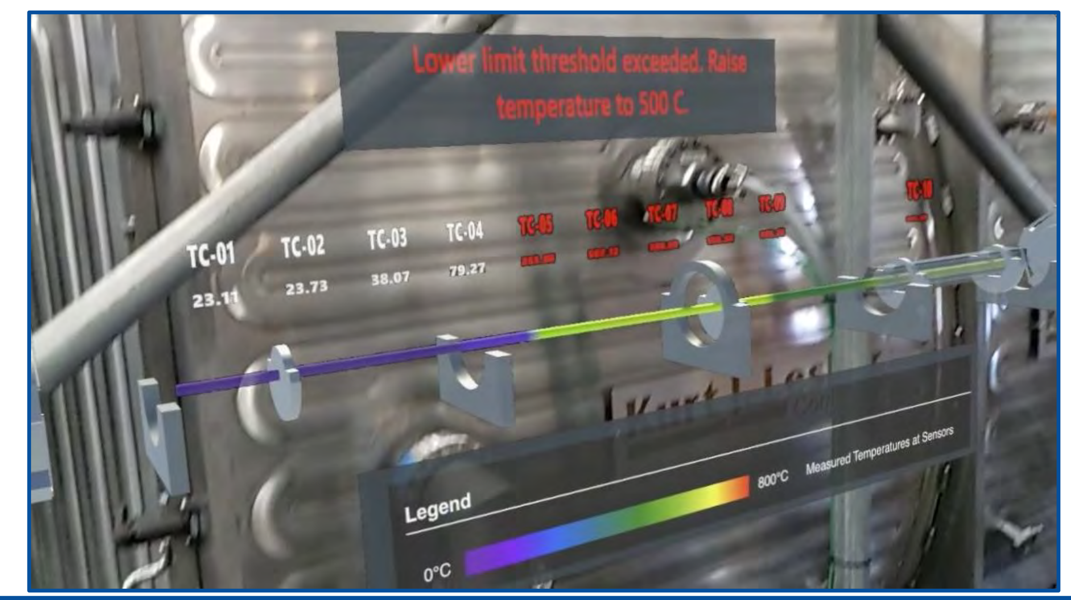
Read about the *demonstration* ⟶ SCAN ME

Digital Twin Framework

- ▻ 6 open-source software tools
- ▻ Supports ongoing efforts

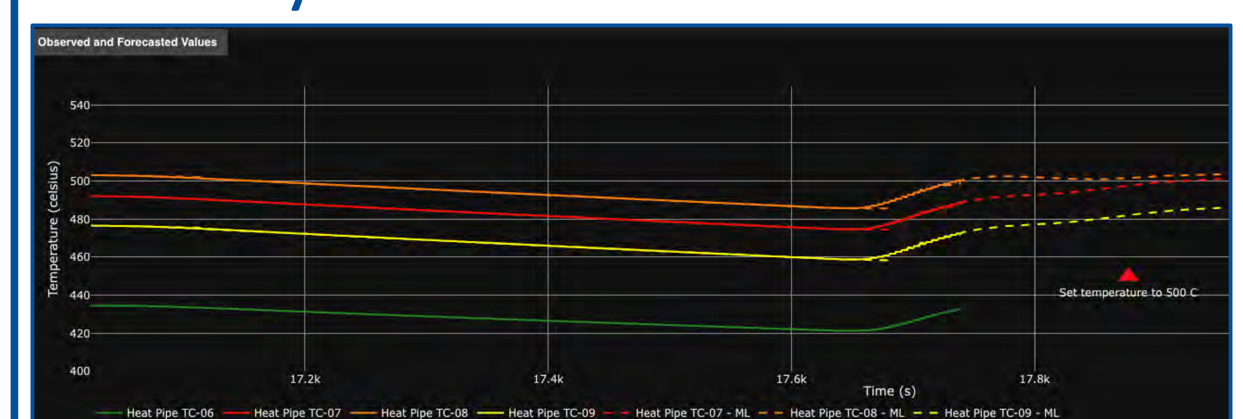
3 Visualization

- Human-centered
- Real-time data and alerting
- Scalable and interactive



4 Automated Control

- Predictions of heat pipe state used to avoid undesirable states or anomalies before they occur



Project Number: 21A1053-007FP LRS Number: INL/EXP-23-74083

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

INL Idaho National Laboratory

PRESENTER:

Kyle A. Gamble

Modeling and Measurement of Axial Gas Transport in Nuclear Fuels

PI: Kyle A. Gamble

Co-PIs: Fabiola Cappia, Seongtae Kwon, Chase Christen, Kaustubh Bawane, Chiara Genoni, Tommaso Bergomi

Background

- Axial gas transport plays a crucial role in **determining pressure equilibrium** in nuclear fuel rods
  - Spent fuel storage [1]
  - Loss-of-coolant accident (LOCA) [2]
  - Helium-bonded fast reactor fuel rods
- Permeability currently determined **a posteriori** [3,4]
- Current models assume **instantaneous** pressure equilibrium and laminar flow

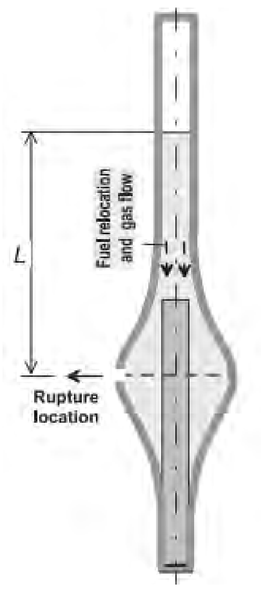


Figure 1: Schematic of gas flow during LOCA

Methodology

- **Verify scalability** of axial gas transport to **enable full microstructural characterization** of specimens for use in model development
- Develop a model for **permeability as a function of microstructural features**

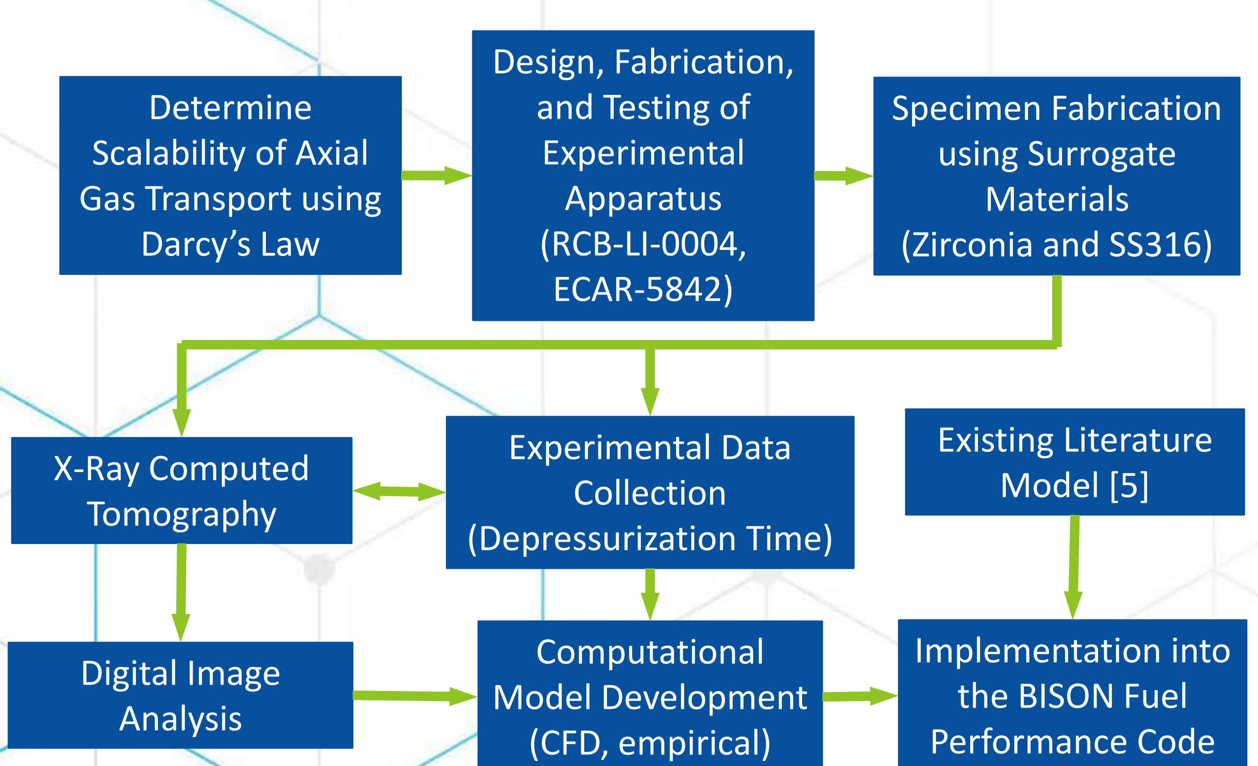


Table 1: List of experimental specimens. Crushed and quenched pellets indicate fracture induced by mechanical and thermal loading, respectively.

Specimen ID	Pellet Status	Number of Pellets	Gap Status
Test tube 1 (TT1)	Crushed	4	Open
Test tube 2 (TT2)	Crushed	8	Open
Control tube 1 (CT1)	Fresh	4	Open
Control tube 2 (CT2)	Quenched	4	Open
Control tube 3 (CT3)	Fresh	6	Closed
Control tube 4 (CT4)	Quenched	4	Closed
Control tube 5 (CT5)	Fresh	8	Closed
Control tube 6 (CT6)	Fresh	4	Closed
Control tube 7 (CT7)	Fresh	4	Closed

Main Research Findings

- Scalability of axial gas transport **confirmed**
- More accurate fracture patterns obtained by **quenching**
- Pressure equilibration is **not instantaneous**
- Gas flow is **turbulent** for short decay times
- Permeability equation developed as a function of **smeared porosity** obtained from image analysis

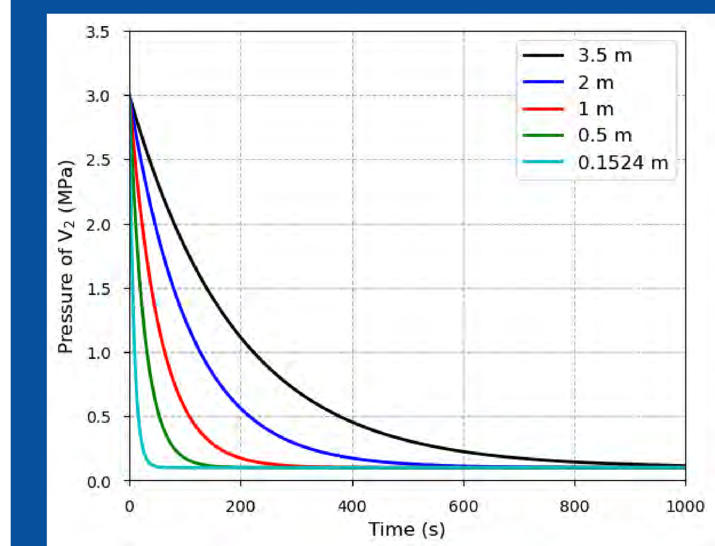


Figure 2: Depressurization as a function of time for varying specimen length

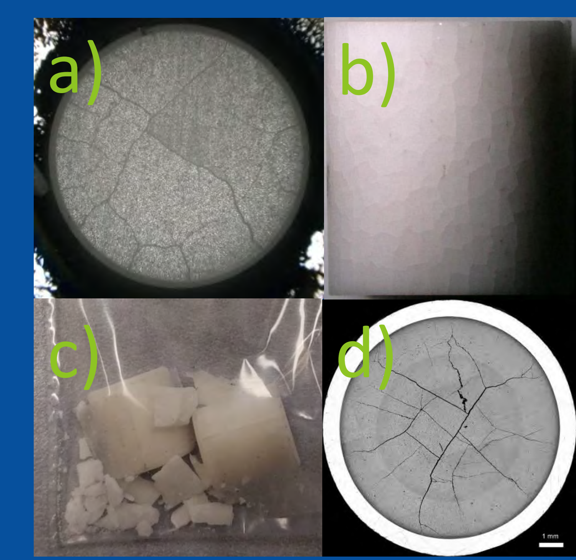


Figure 3: a) Thermal quench (top view) b) thermal quench (side view), c) mechanical crushing, and d) experimental micrograph of irradiated fuel

Laminar Friction Factor (Darcy's Term) **Turbulent Friction Factor (Forchheimer's Term)**

$$\frac{\mu \bar{u}}{K_1} + \frac{\rho \bar{u}^2}{K_2}$$

$$K_1 = C_1 \frac{\epsilon_s^3}{(1-\epsilon_s)^2} \qquad K_2 = C_2 \frac{\epsilon_s^3}{(1-\epsilon_s)}$$

ϵ_s = smeared porosity, $\bar{u}$ = velocity

μ = dynamic viscosity, ρ = density

C_1, C_2 = pressure-dependent constants

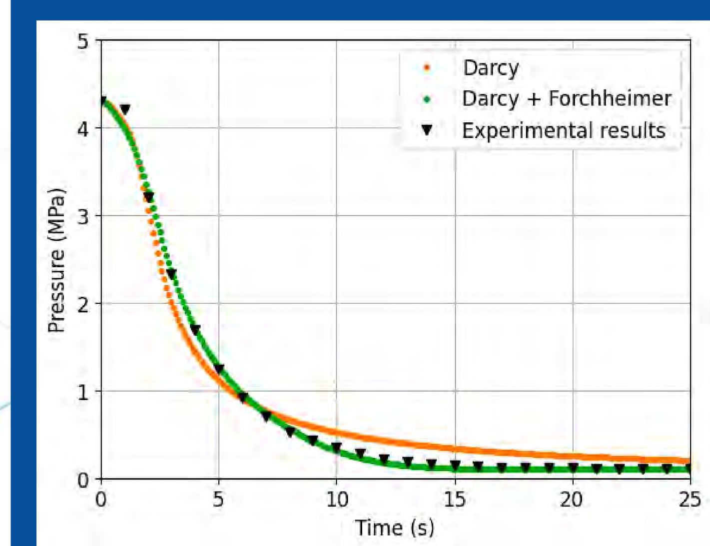


Figure 4: Best-fit curves included and excluding Forchheimer coefficient for experiment TT1 at an initial pressure of 4.3 MPa

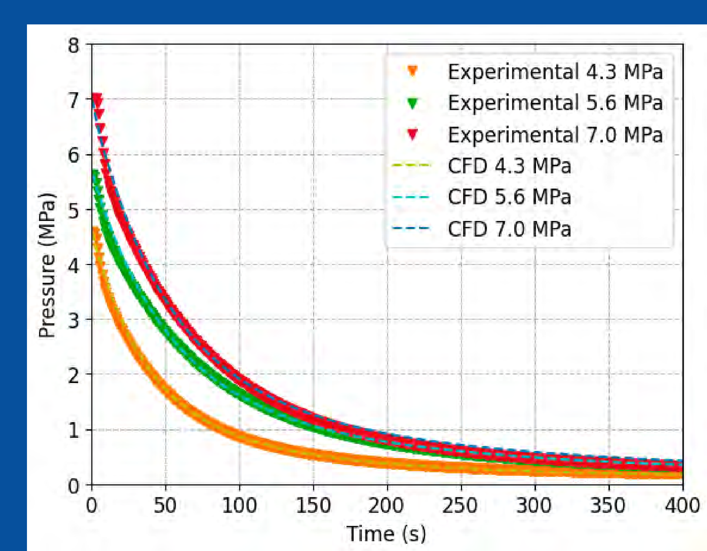


Figure 5: Best-fit curves excluding the Forchheimer coefficient for experiment CT4 at different pressure levels

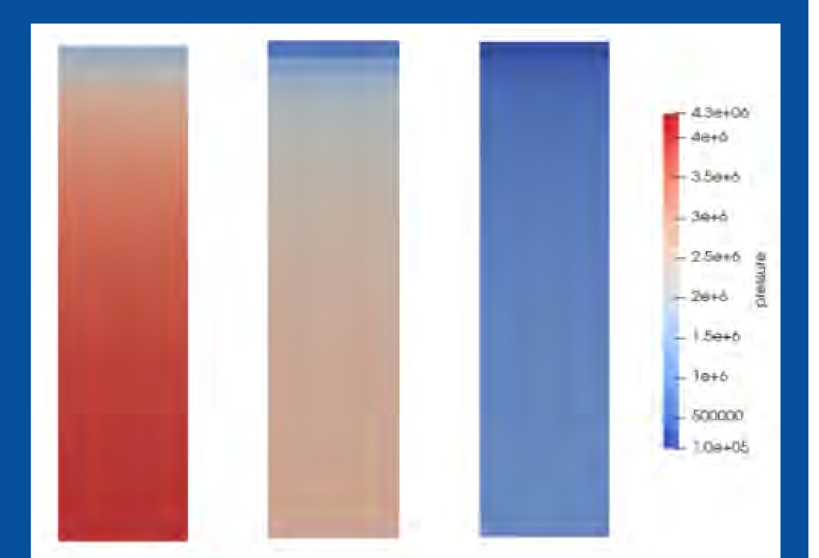


Figure 6: Snapshots of computational fluid dynamicssimulation of CT4 with initial pressure of 4.3 MPa

Publications

[1] C. Genoni, et al., "Modeling and Measurement of Axial Gas Transport in Nuclear Fuels," ANS Annual Meeting, June 2023.

[2] S. Kwon, et al., "Fabrication of Surrogate Oxide Spent Fuel with Various Cracking Patterns and the Design of an Axial Gas Transport Apparatus," to be submitted to the Journal of Nuclear Materials.

[3] C. Genoni, et al., "Investigation of the Impact of Non-Uniform Permeability on Axial Gas Transport within Light Water Reactor Fuel Rods during a Loss-Of-Coolant Accident," to be submitted to Nuclear Engineering and Design.

[4] T. Bergomi, "Fuel Pellets Three-Dimensional Properties Reconstruction Exploiting Image Analysis: A Bridge Between Experiments and Modeling", Masters Thesis, Politecnico Di Milano, expected 2024.

Specimen Fabrication and Experimental Apparatus

- Decay of **inlet pressure measured** as a function of time
  - 4.3, 5.6, and 7 MPa analyzed
- Quenching and mechanical crushing used to **induce** fracture
- Mylar wrapping used to **preserve** pellet position

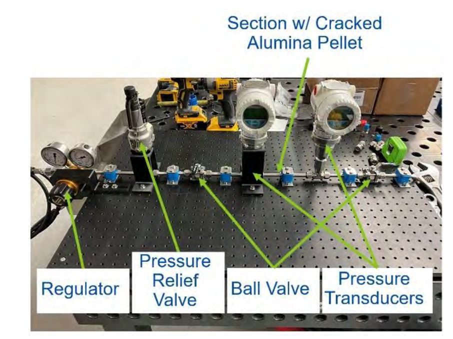


Figure 6: Experimental apparatus

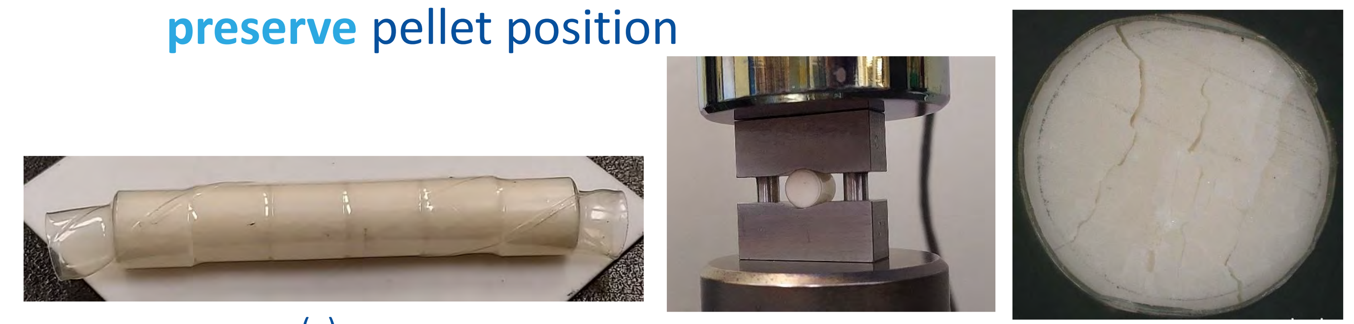


Figure 7: Photo of (a) pellets with mylar wrapping, (b) mechanical compression of individual pellet, and (c) resulting separation-crack formation

Digital Image Analysis

- **Hundreds** of two-dimensional (2D) images obtained per specimen by x-ray computed tomography (CT)
- Image analysis used to estimate features
  - Crack tortuosity
  - Specific surface
  - Porosity distribution
- **3D reconstruction** of the pellets can be performed

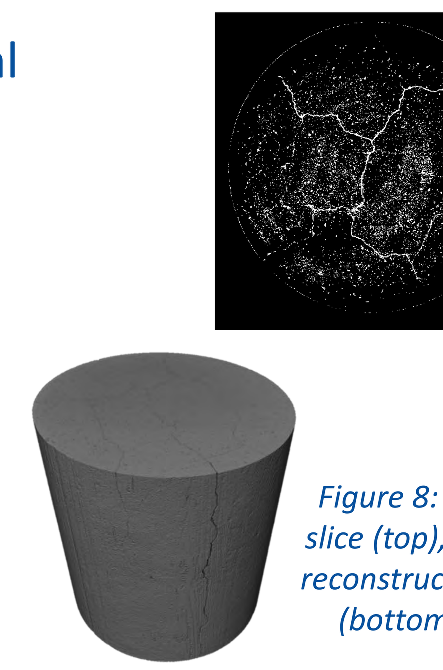


Figure 8: CT slice (top), 3D reconstruction (bottom)

References

[1] V. Rondinella et al., TopFuel 2015. JRC94524.

[2] W. Wiesenack, et al. International Conference on the Physics of Reactors, 2008.

[3] R. Montgomery and R. N. Morris, doi: doi.org/10.1016/j.jnucmat.2019.05.041.

[4] S. J. Dagbjartsson, et al., TREE-NUREG-1158, 1977.

[5] Khvostov, G., et al., doi: doi.org/10.1016/j.nucengdes.2011.03.003.

Acknowledgments

- William Chuirazzi for performing the x-ray CT of the specimens
- Fei Xu for supporting the digital image analysis
- Davide Pizzocri (Politecnico Di Milano) for modeling discussions
- This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

Project Number: 21A1050-028FP

LRS Number: INL/MIS-23-74111

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

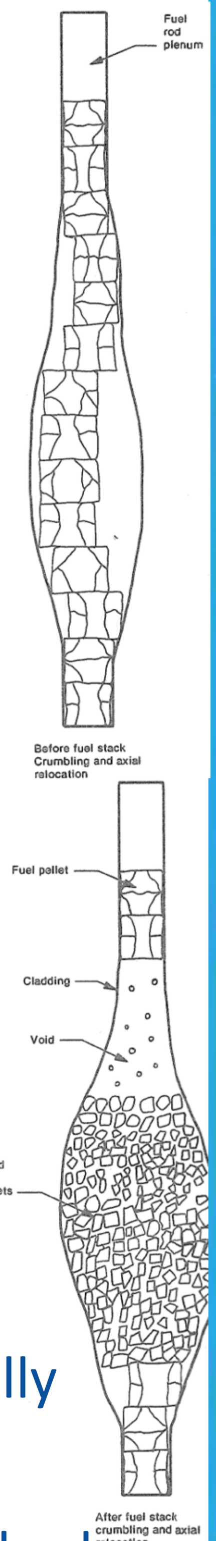
Idaho National Laboratory

High-fidelity multiscale model development for accelerated fuel qualification for high discharge burnup

Finite element-informed, discrete element modeling of fuel fragmentation, relocation, and dispersal (FFRD) phenomena during a simulated loss of coolant accident (LOCA)

PRESENTER:

Ahmed Hamed



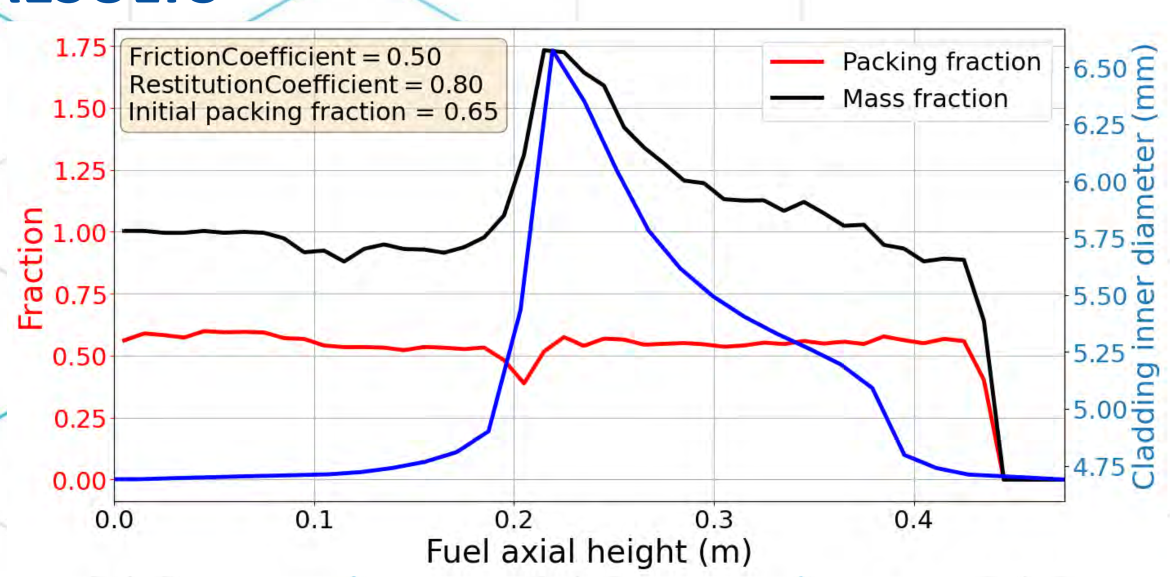
BACKGROUND:

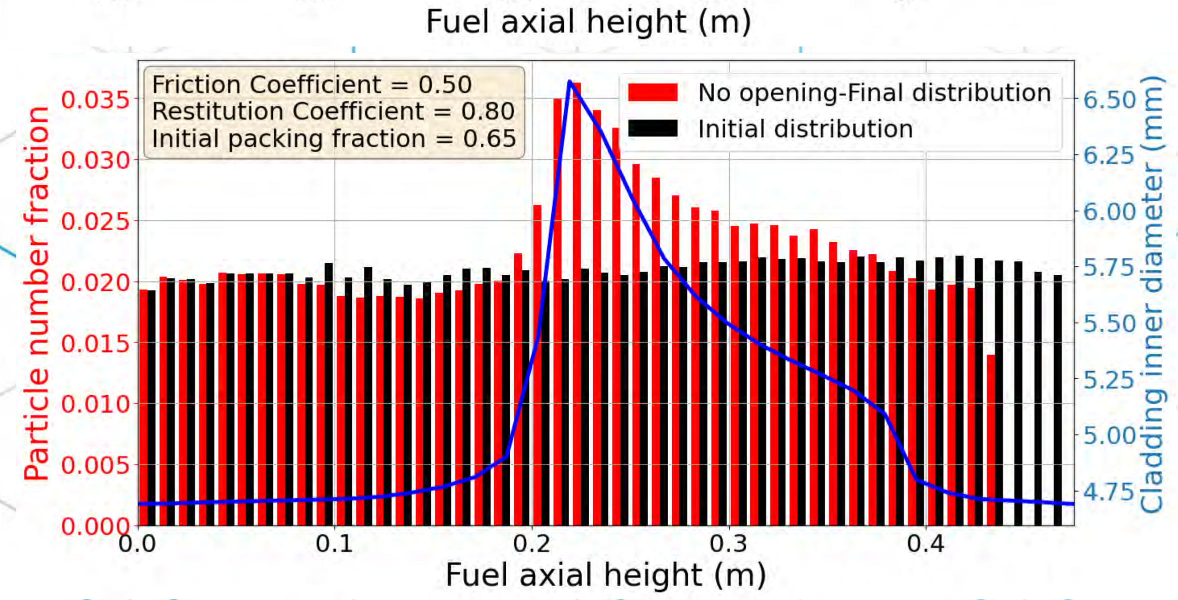
Reactor vendors seek economic benefits associated with increasing nuclear fuel service lifetime in the existing light-water reactors fleet. FFRD phenomena represent a major safety concern which still needs to be addressed. Formation of high burnup structure (HBS) in conjunction with LOCA can lead to relocating fuel to escape the fuel pin and get dispersed into the primary coolant system.

METHODS

1. BISON is used to simulate experimentally observed scenarios leading to FFRD.
2. BISON-informed Discrete Element Method is used to simulate FFRD dynamics and analyze controlling parameters.

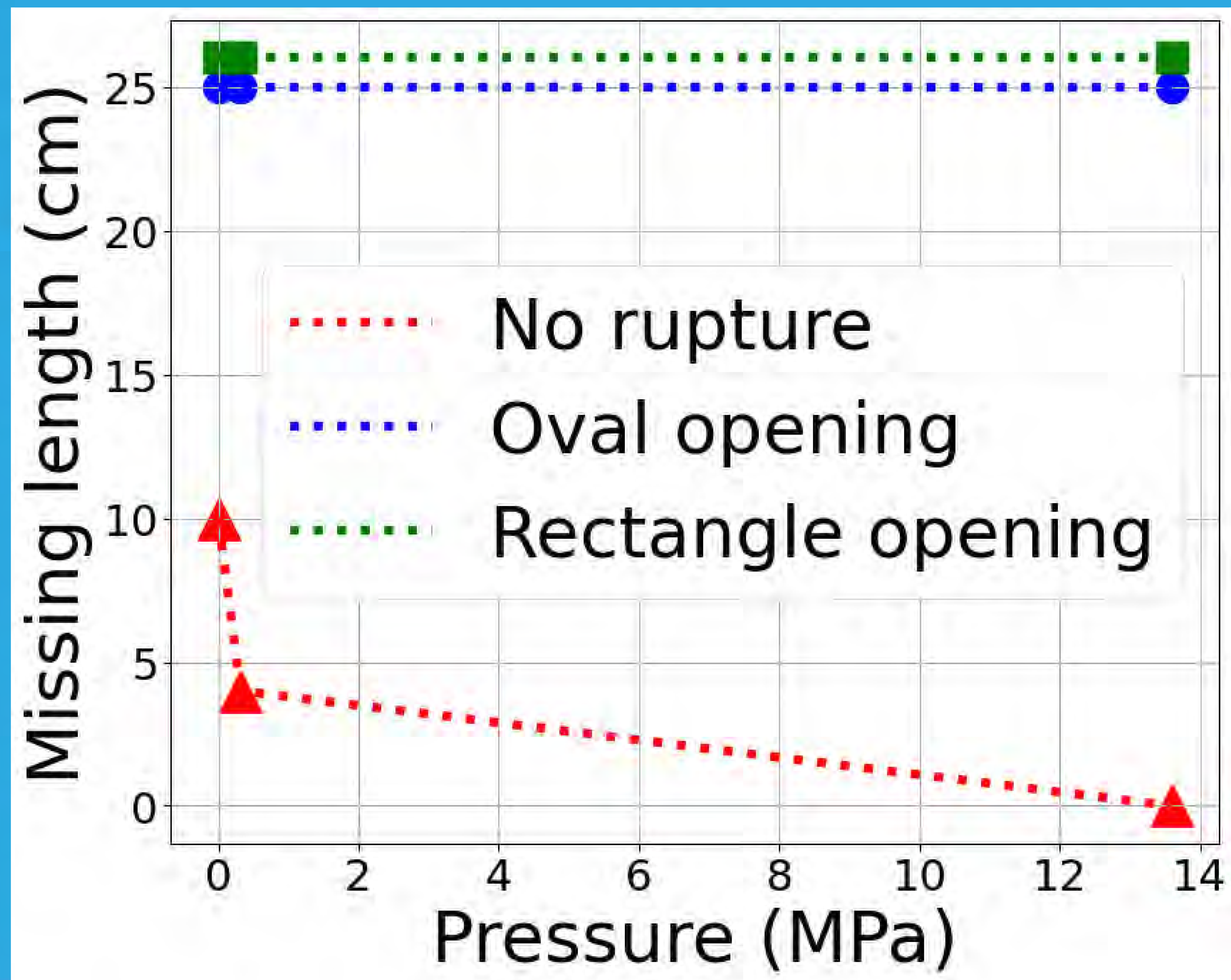
RESULTS

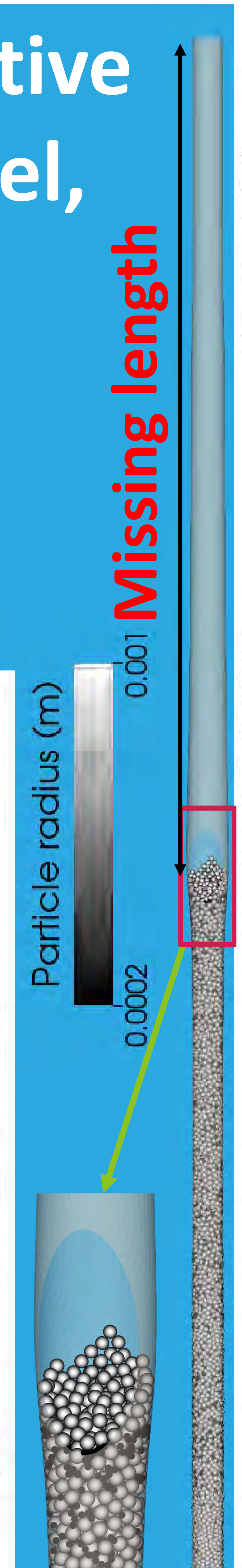




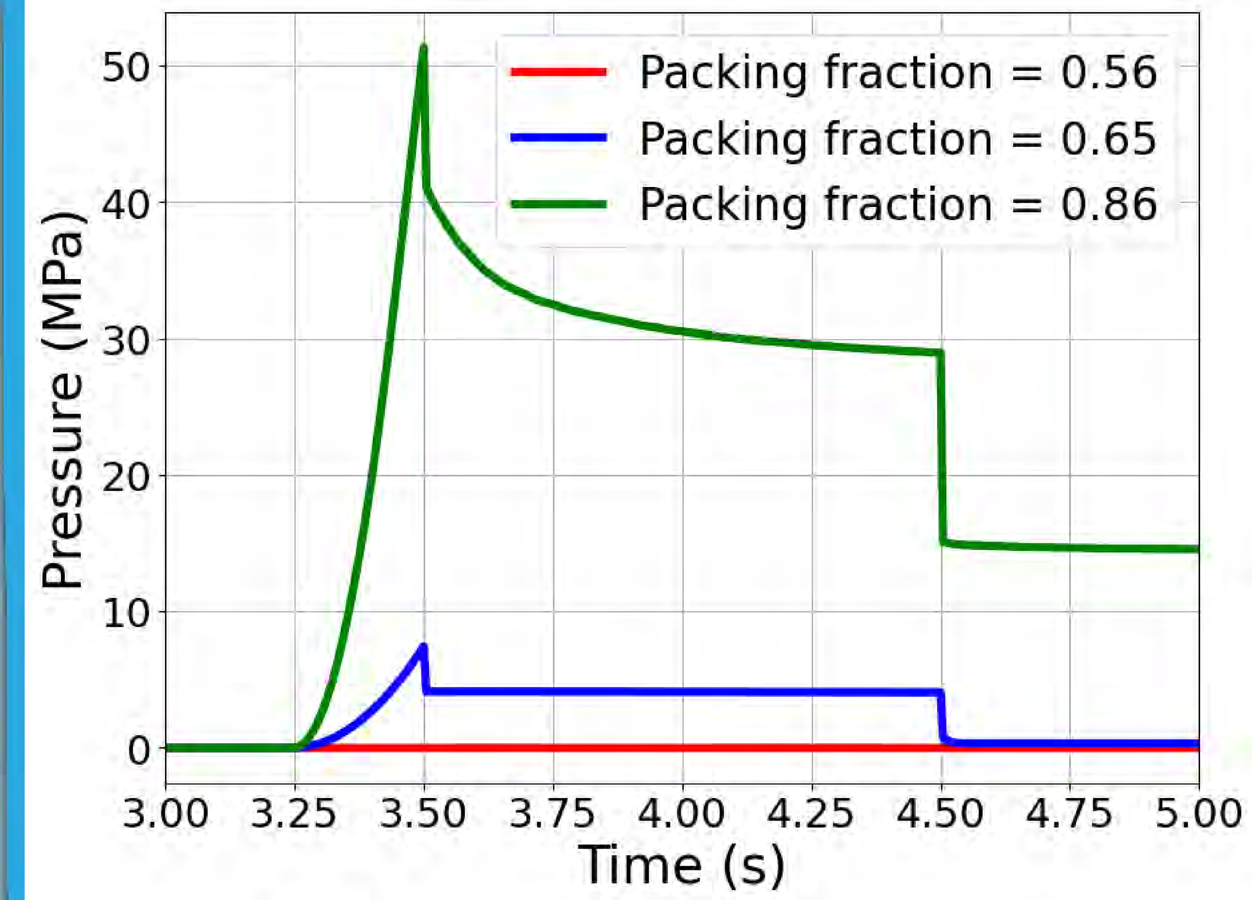
FFRD dynamics are very sensitive to particle features, stress level, and burst opening geometry.

High pressure suppresses the axial fuel relocation until the onset of clad rupture.

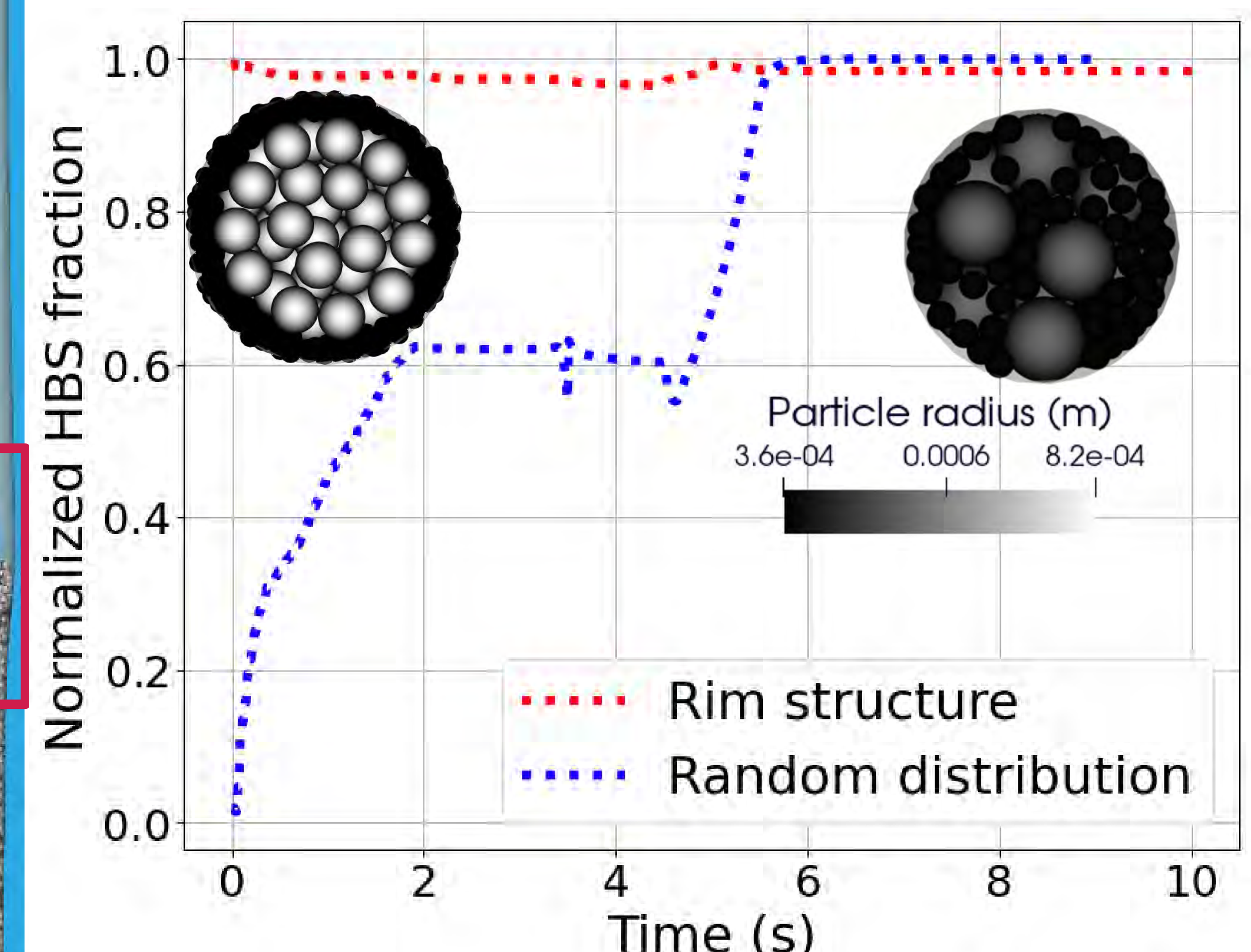




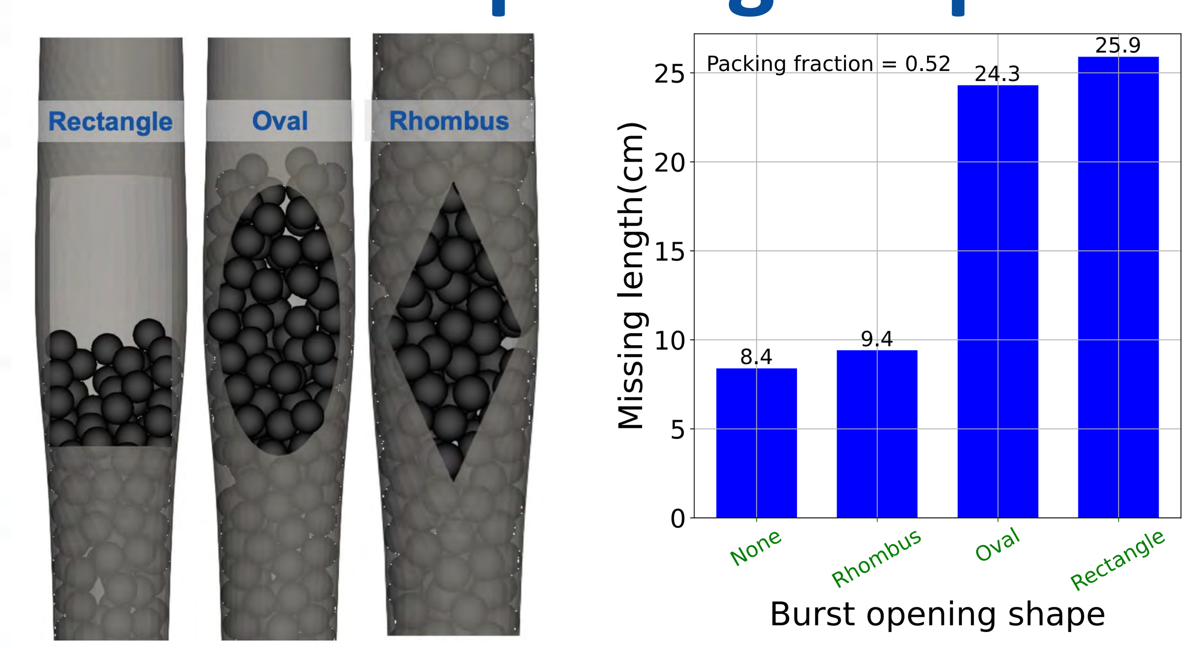
Packing fraction effect



Radial structure effect



Burst opening shape



Ahmed Hamed, Kyle Gamble (PI), and Yidong Xia

Project Number: 22P1074-009FP

LRS Number: INL/MIS-23-74169

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

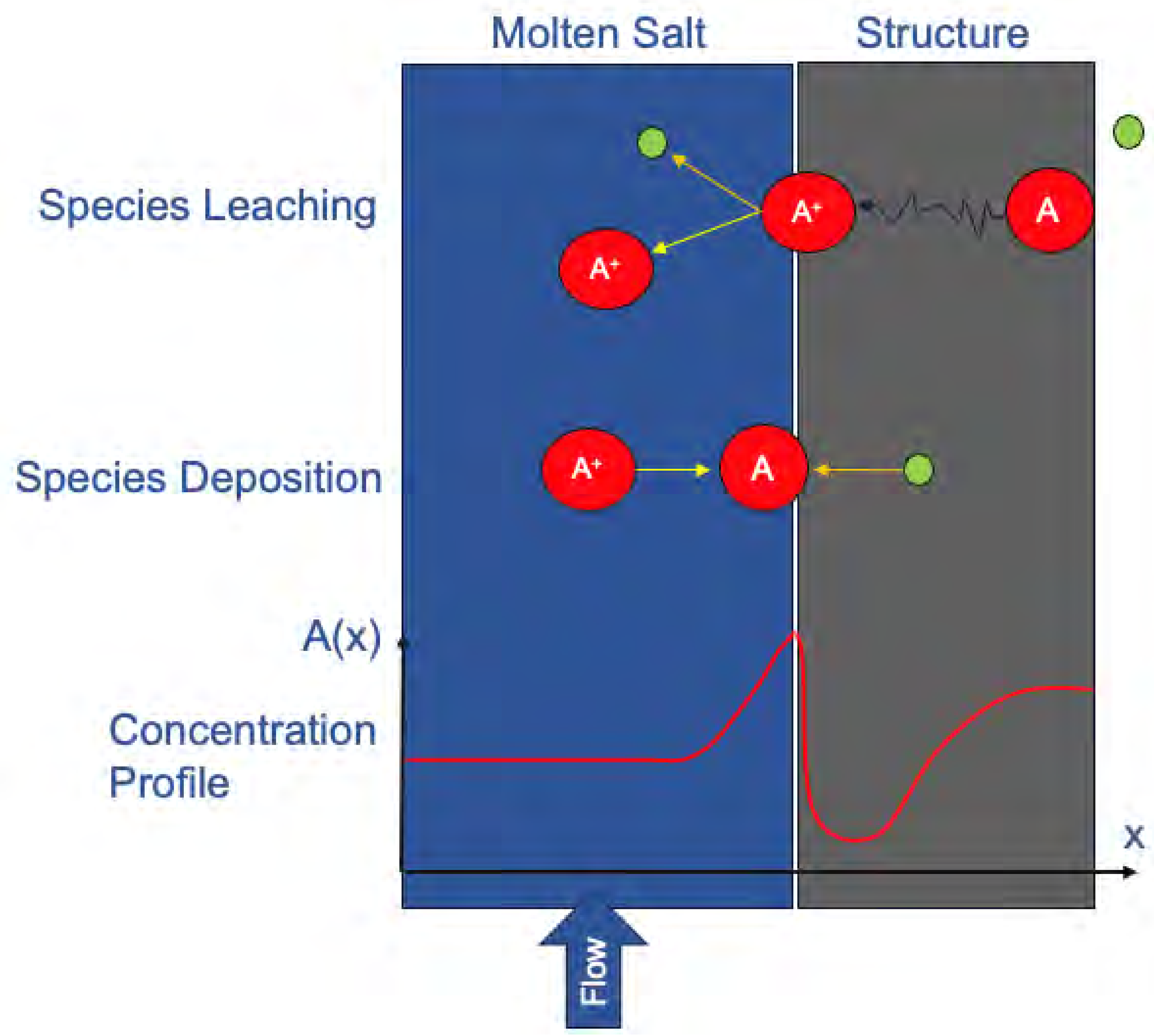
Idaho National Laboratory

* FFRD schematic is adopted from Siefken, Int. Conf. on Structural Mechanics in Reactor Technology, 1983

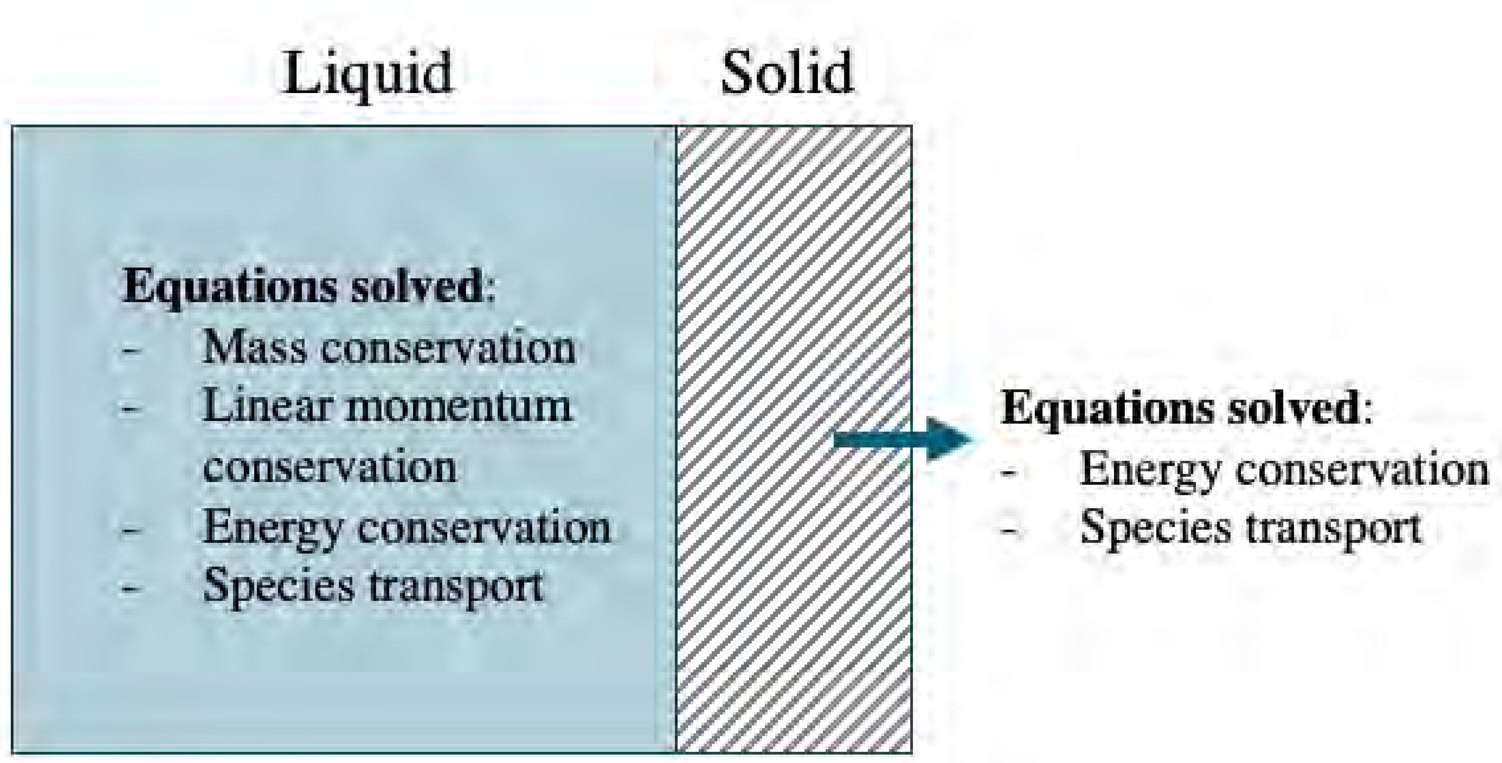
Modeling Flow-Informed Corrosion in Molten Salts

Poisson-Nernst-Planck Model

PI - Mauricio Tano (C130); Co-PIs: Samuel Walker (C120) & Abdalla Abou-Jaoude (C120)



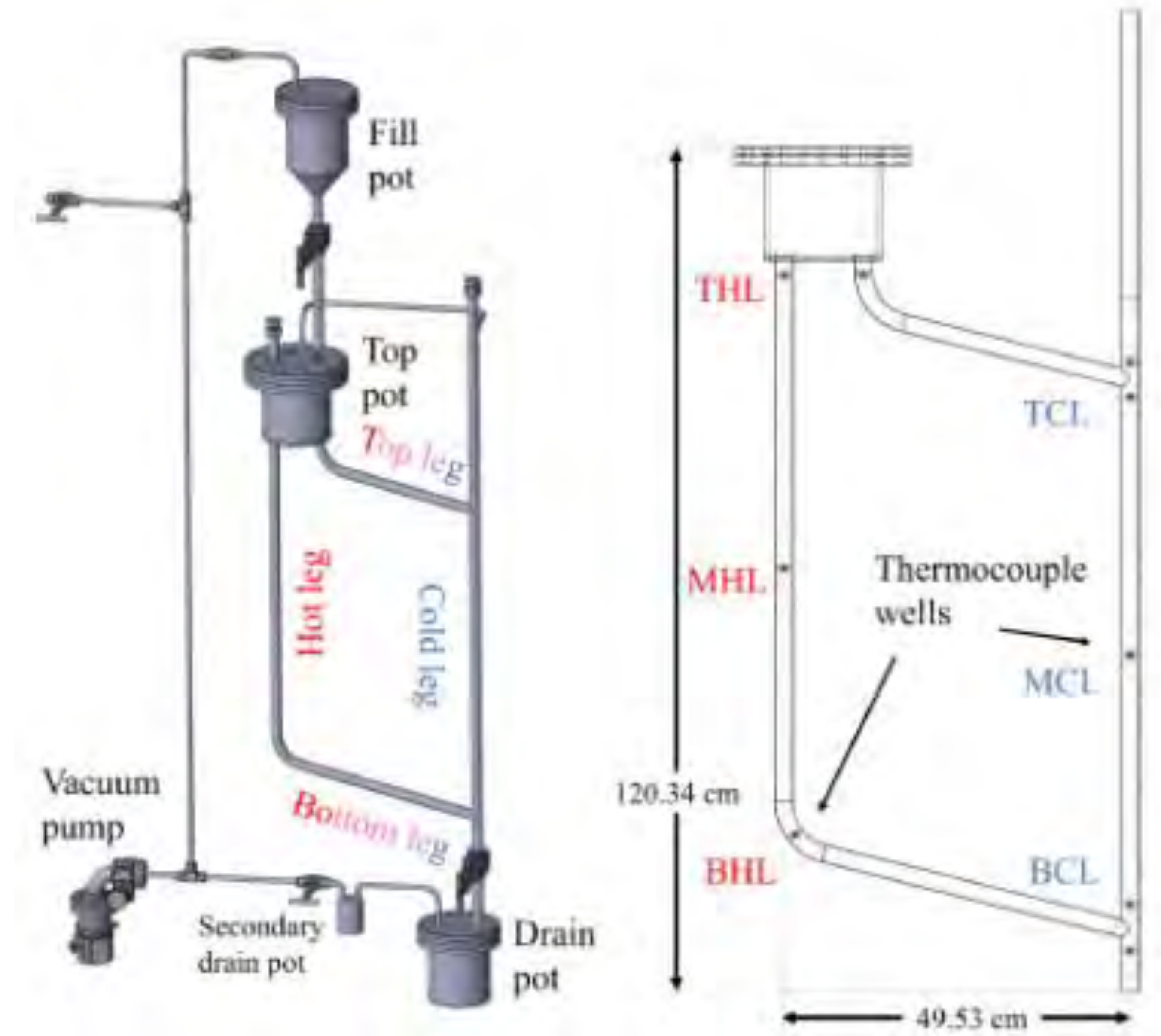
Mechanistic model for Redox Corrosion in Molten Salts



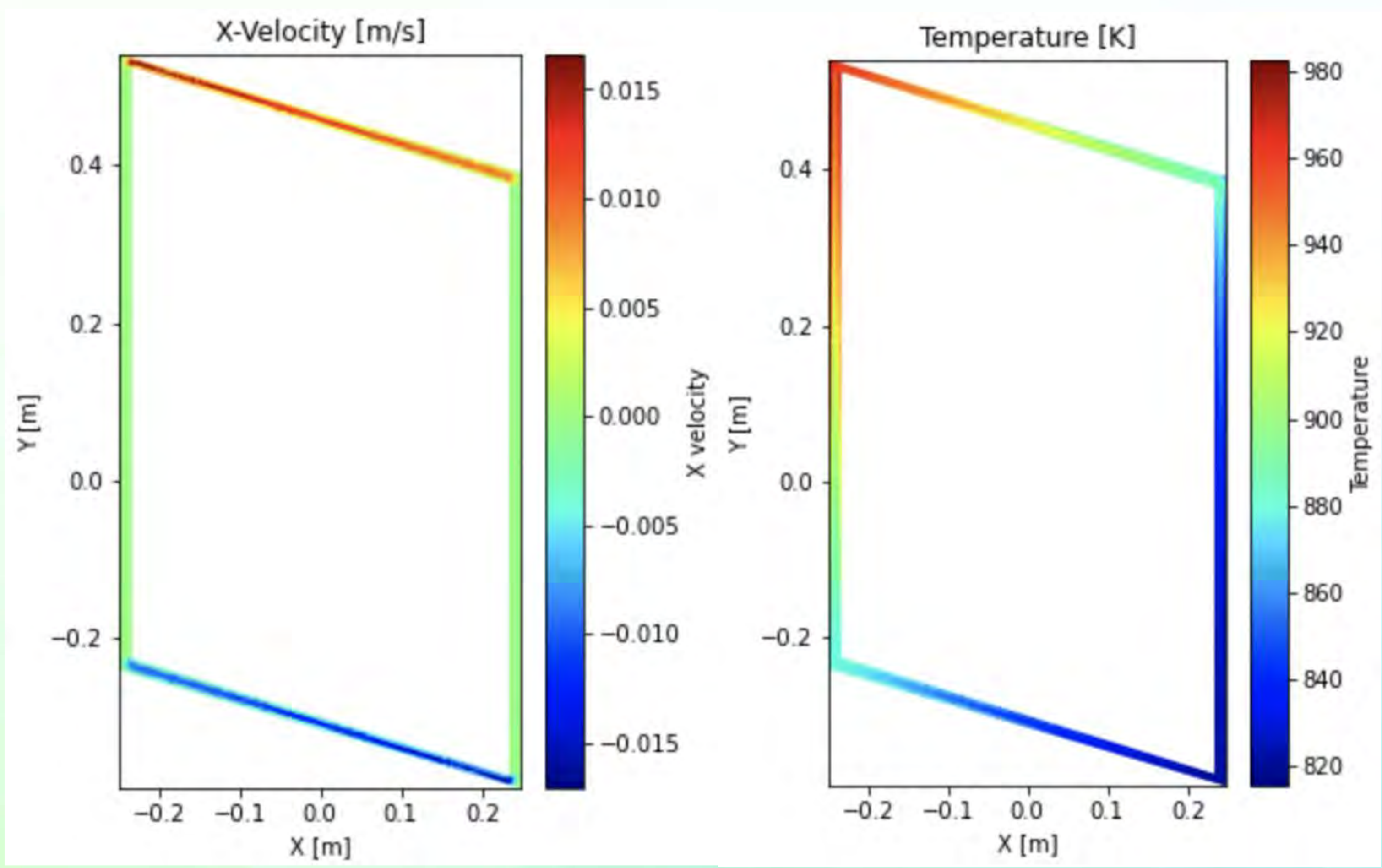
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\boldsymbol{u} c_i) - \nabla \cdot (D_i \nabla c_i) = 0 \text{ --- Liquid}$$

$$\nabla c_{i,FLiNaK}|_{r_{in}} = -\frac{D_{leach,i}}{D_i} \nabla c_i|_{r_{in}} \text{--- Interface}$$

$$\frac{\partial c_i}{\partial t} + a_{dep,i} \nabla c_i - \nabla \cdot (D_{leach,i} \nabla c_i) = 0 \text{ --- Solid}$$

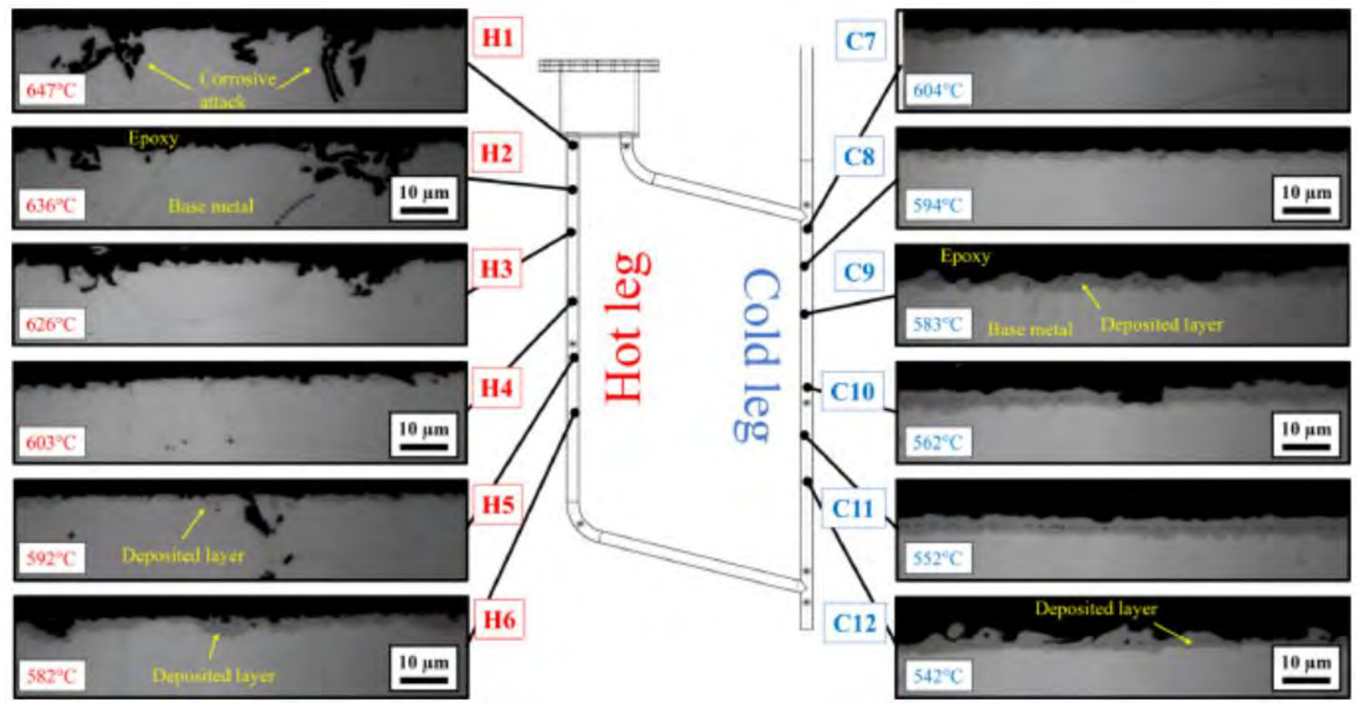


Experiment: Raiman, S. S., Kurley, J. M., Sulejmanovic, D., Willoughby, A., Nelson, S., Mao, K., ... & Pint, B. A. (2022). Corrosion of 316H stainless steel in flowing FLiNaK salt. *Journal of Nuclear Materials*, *561*, 153551.

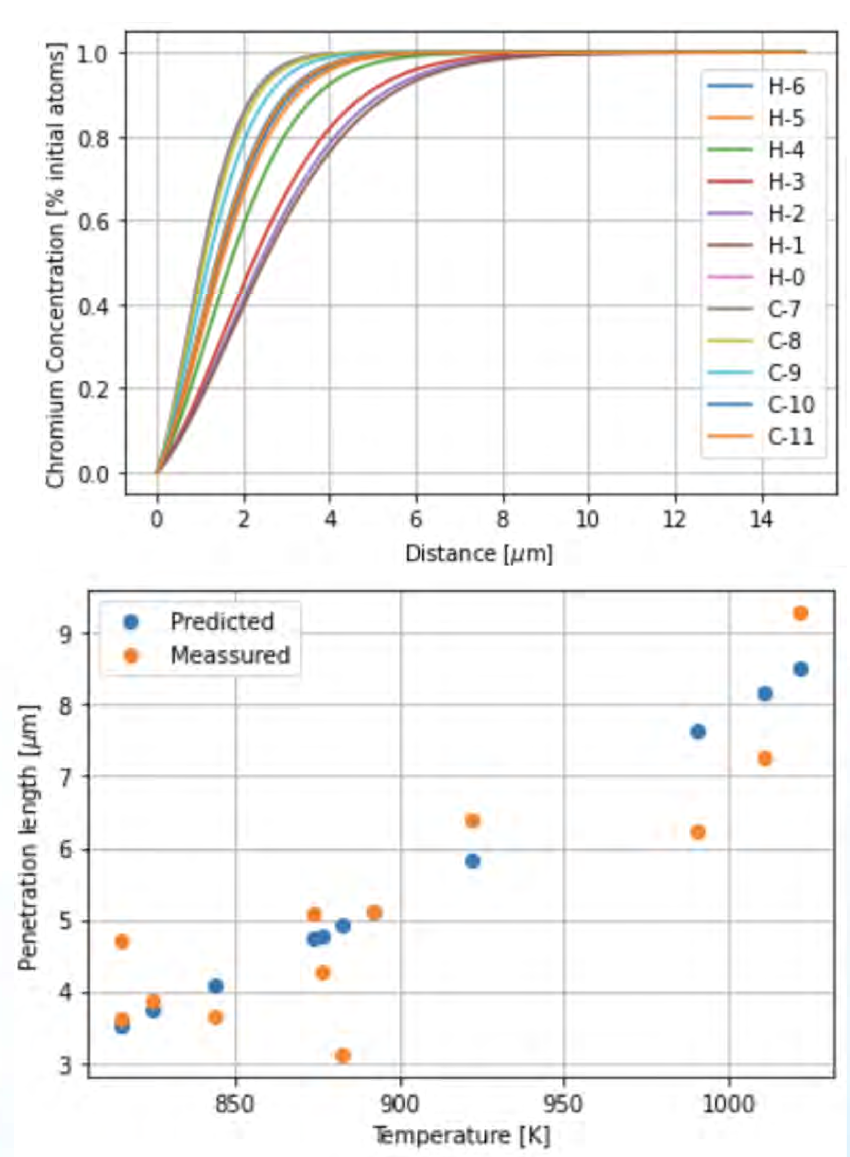


Thermal Hydraulic Field Solutions of FLiNaK Salt Loop Experiment

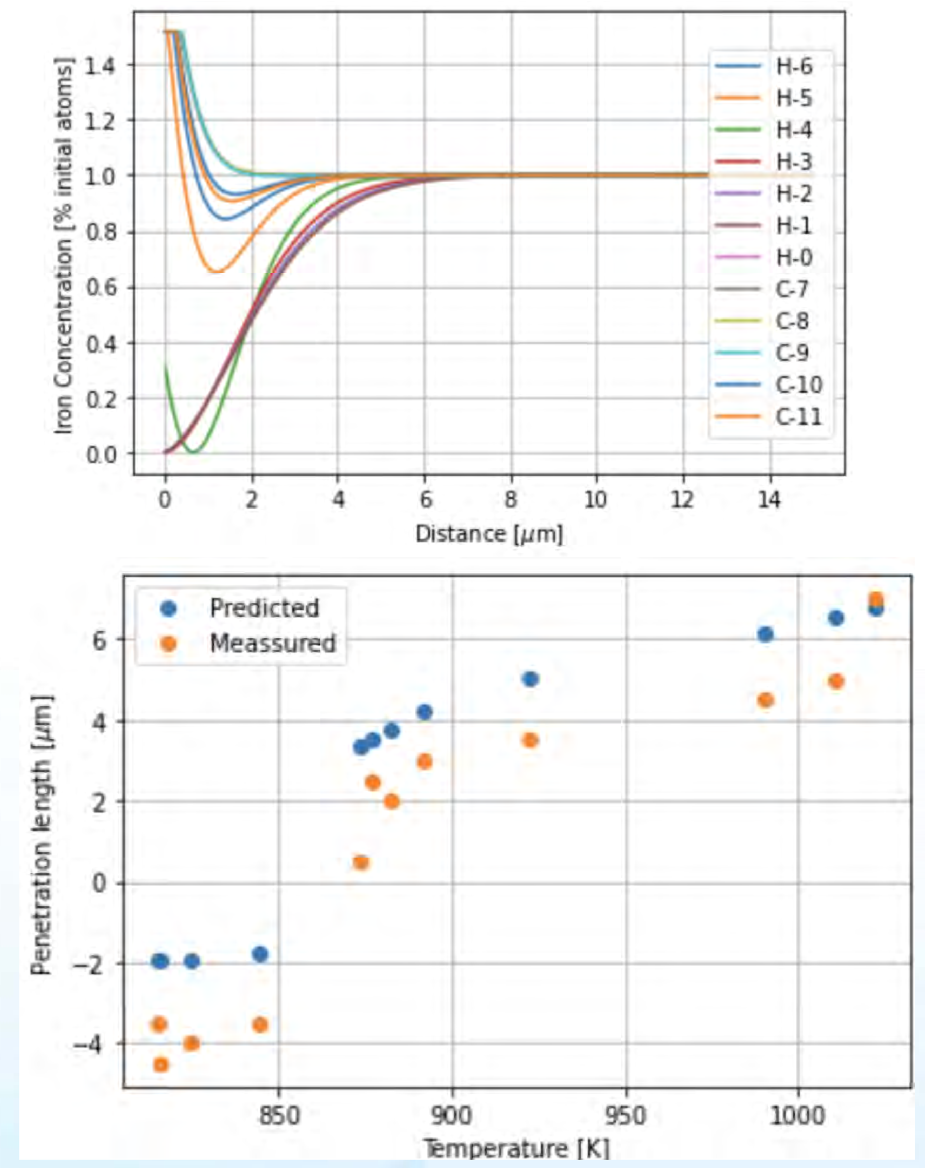
Hot Leg Corrosion in FLiNaK Loop



Cold Leg Deposition in FLiNaK Loop



PNP Cr Concentration Gradient and Corrosion Penetration Length



PNP Fe Concentration Gradient and Corrosion Penetration Length

Main finding:
- A Poisson-Nernst-Plank model has been developed that can accurately predict structural corrosion in molten salts

Next step:
- Further validation of the model and transition to programmatic and vendor usage of the model

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Scaling, Validation and Uncertainty Characterization

Mohammad Abdo (PI), Congjian Wang (CoPI), Aaron Epiney (CoPI), Ramon Yoshiura, Botros Hanna, Alexander Duenas, Charles Folsom, and From Purdue University: Shiming Yin, Hany S. Abdel-Khalik (CoPI)

BACKGROUND

- Code/model validation, Scaling, and Uncertainty Characterization are indispensable for Nuclear Digital Transformation.
- Quantitatively judge the relevance (representativity) of a prototype model to a full target model.
- Qualify experiment(s) *before execution* and design better experiments, lower cost, hence less destructive experiments.
- Parameter adjustment/calibration based of training models to reduce uncertainties for Reactivity Insertion Accidents (RIAs).

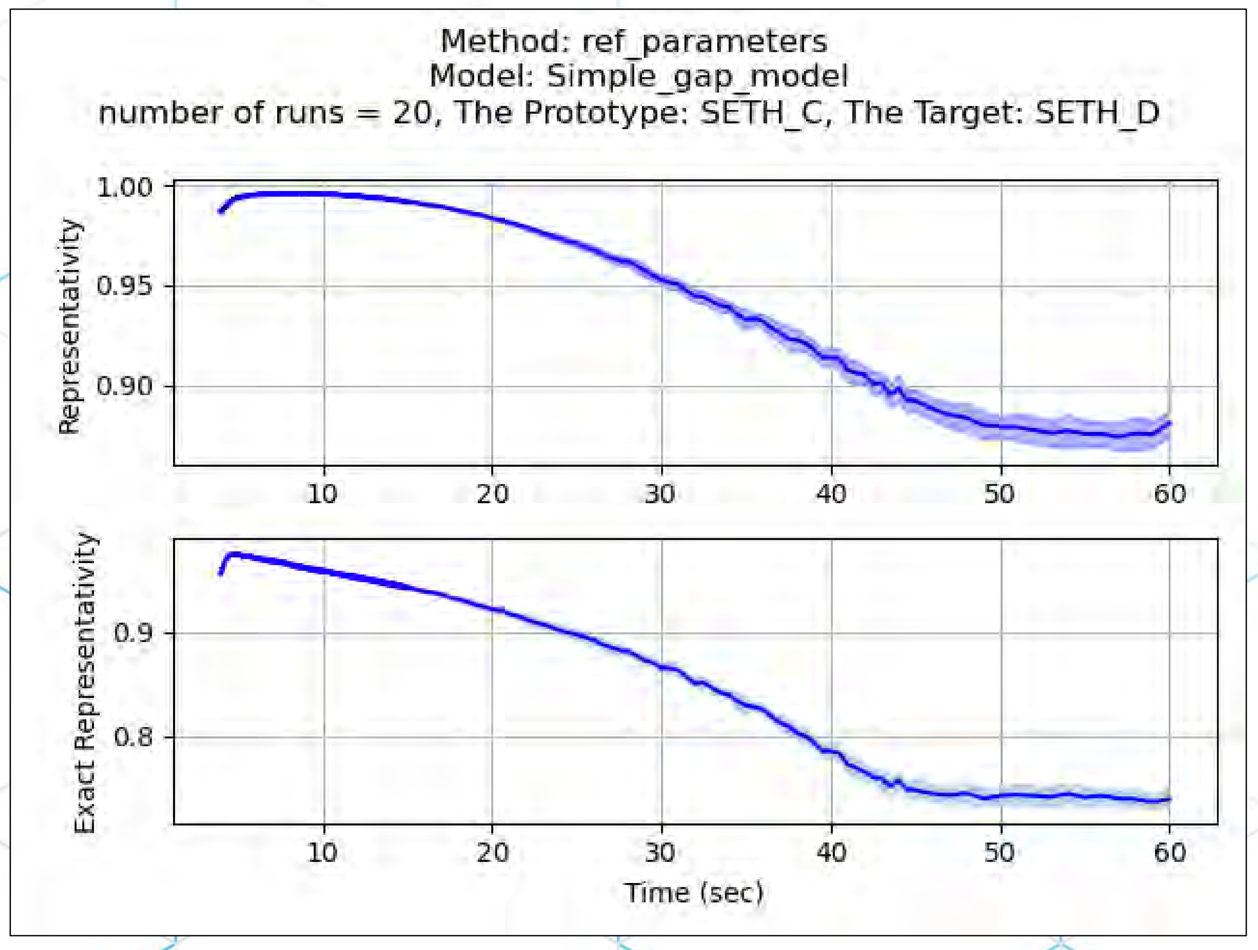
CONCLUSIONS

- Three theories: representativity, PCM, and DSS were compared for model validation.
- Representativity performed the best in case global sensitivities are present.
- Representativity and PCM can qualify experiments, based on reduction in Uncertainty.
- DSS shows the global distortion in the dimensionless transformed space and guide the judgement whether the models are ill-scaled or well-scaled.

METHODS

Representativity

$$r = \frac{S_{FOM} C_{U_p^m} S_F^T}{\sqrt{S_{FOM} C_{U_p^m} S_{FOM}^T}\sqrt{S_F C_{U_p^m} S_F^T + C_{U_F^m}}}$$

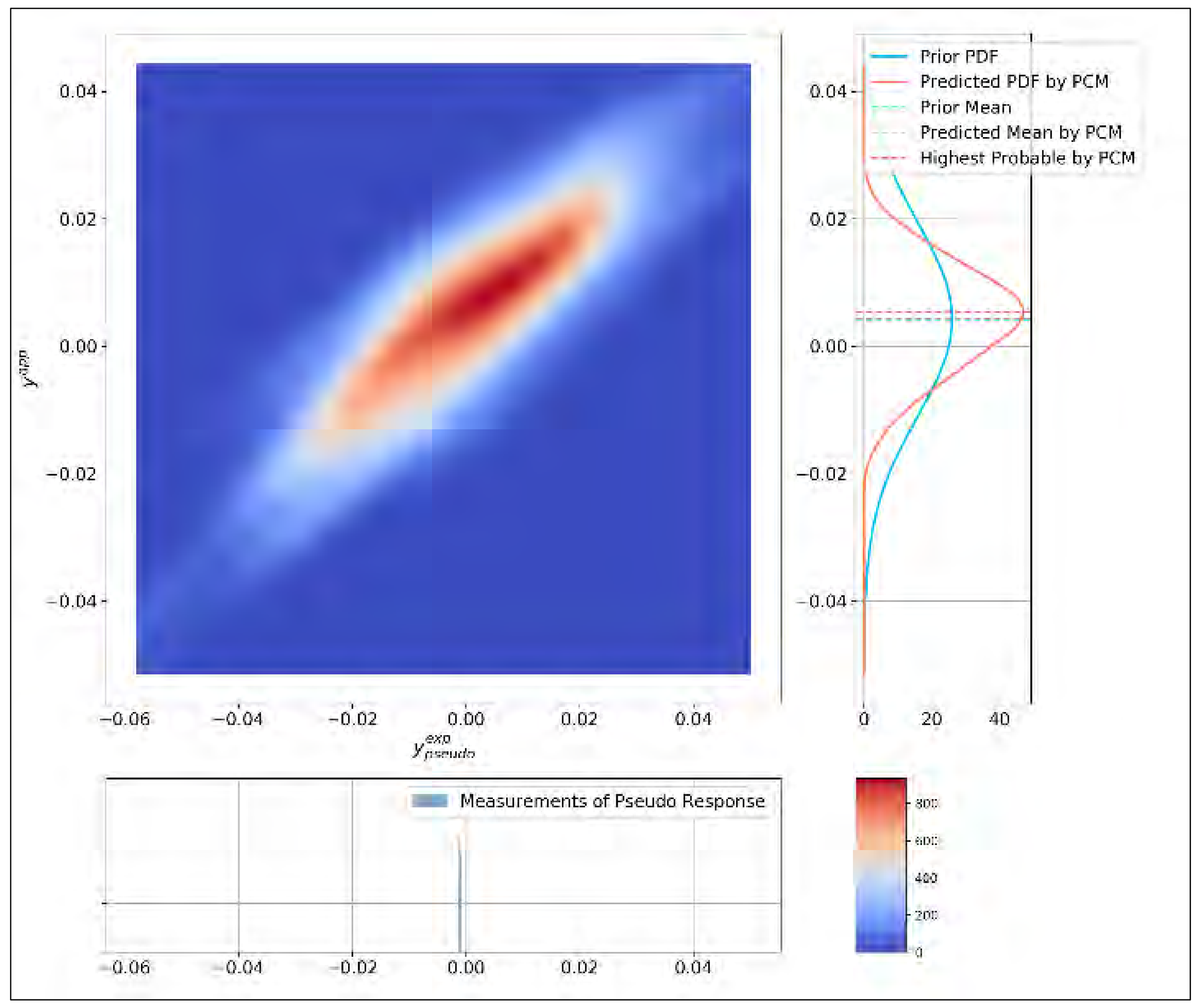


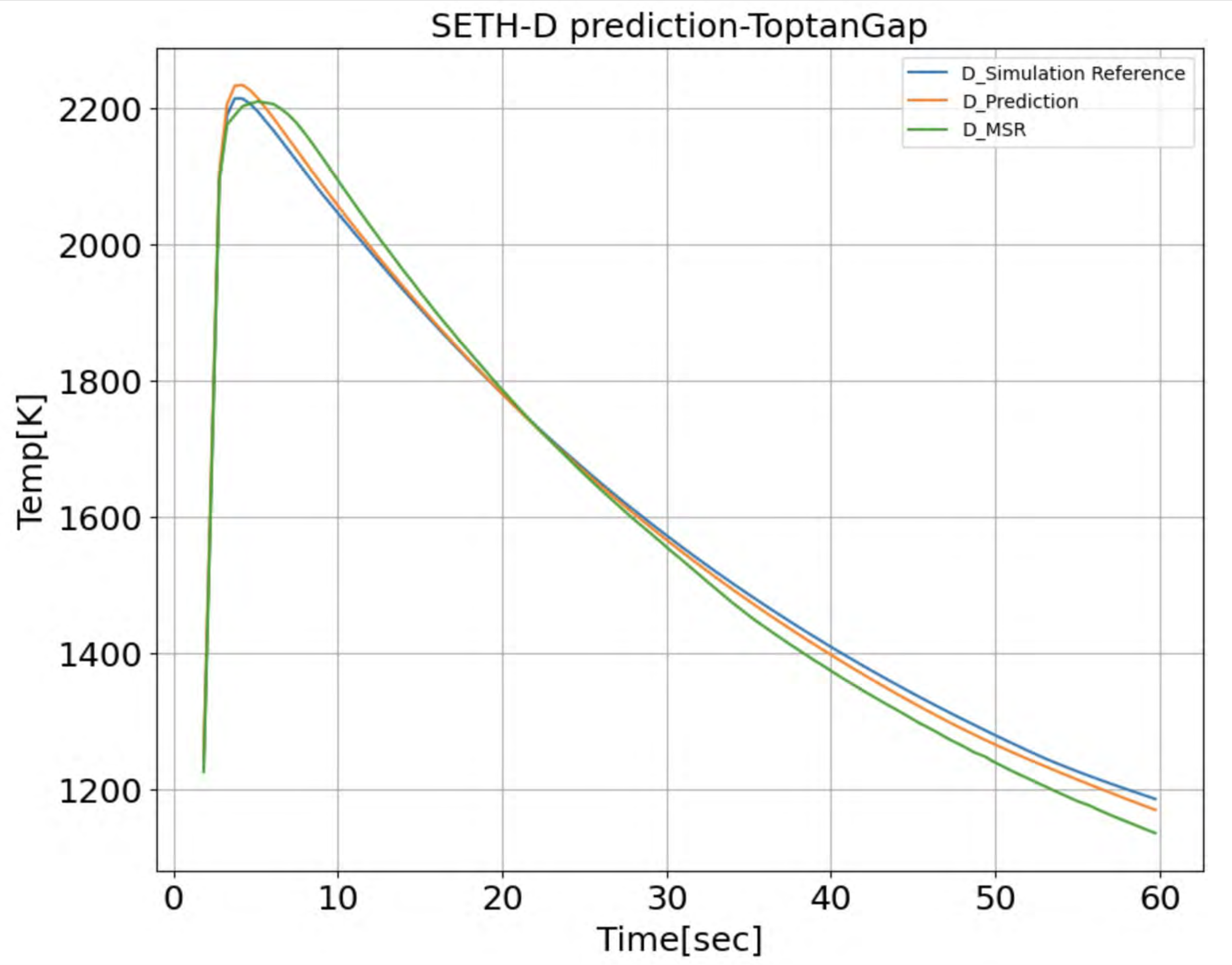
Physics-guided Converged Mapping

$$p(y_{app}^{post}) = \int_{y_{exp}^{min}}^{y_{exp}^{max}} p(y_{exp}, y_{app}) p(y_{msr}) dy_{exp}$$

$$Var(y_{app}^{post}) = E\left[\left(y_{app}^{post} - \mu_{y_{app}^{post}}\right)^2\right]$$

$$Var(y_{app}^{post}) = \int_{y_{app}^{min}}^{y_{app}^{max}} (y_{app} - \mu_{y_{app}^{post}})^2 p(y_{app}^{post}) dy_{app}$$



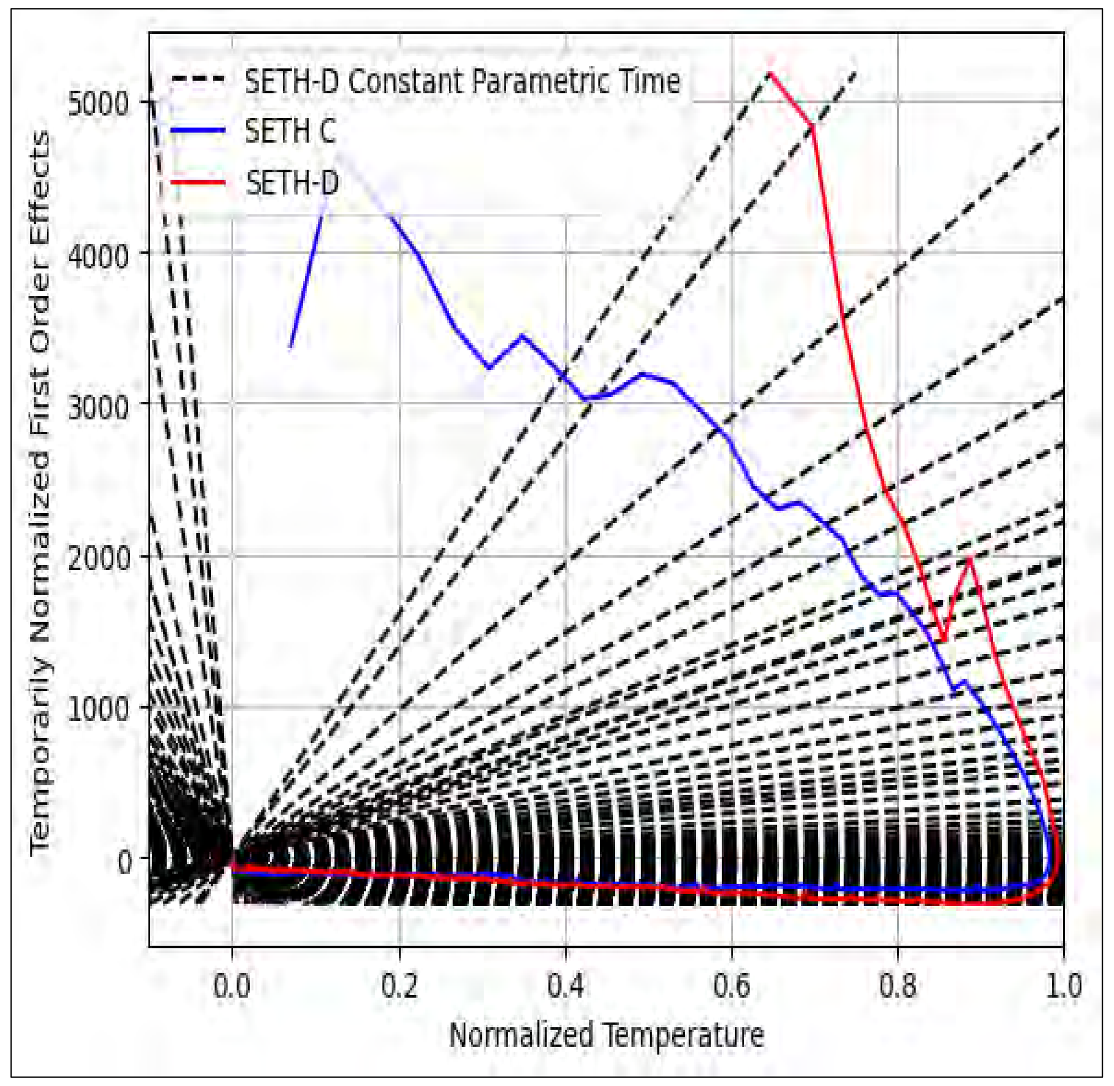


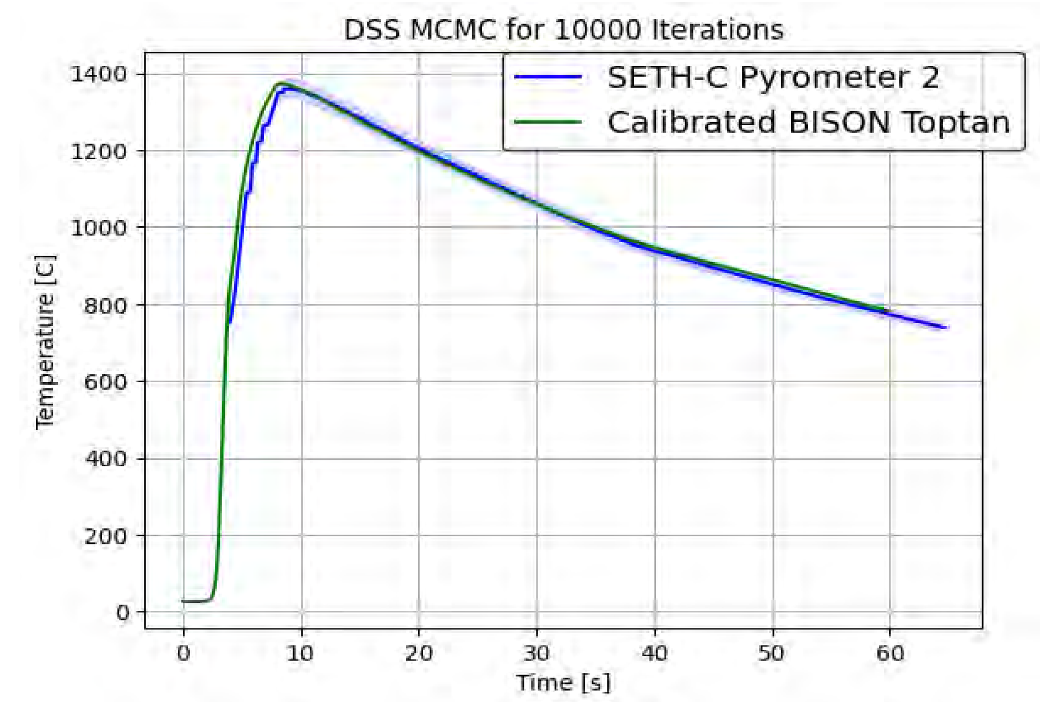
Dynamic System Scaling

$$\beta(t) = \frac{1}{\Psi_0}\iiint_V \Psi(\vec{x}, t) dV$$

$$\omega(t) = \left.\frac{d\beta}{dt}\right|_t = \sum_{i=1}^{n} \omega_i, D = -\frac{\beta}{\omega^2}\frac{d\omega}{dt}, \tau_s = \int (1 + D) dt,$$

$$\tilde{\Omega} = \omega\tau_s, \tilde{\beta} = \beta, \tilde{t} = \frac{t}{\tau_s}, \tilde{D} = D$$





SCAN ME SCAN ME SCAN ME SCAN ME

Project Number: LDRD 21A1050-014FP LRS Number: **INL/MIS-23-74350**

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

BACK TO THE FUTURE: HYDRIDE MODERATORS

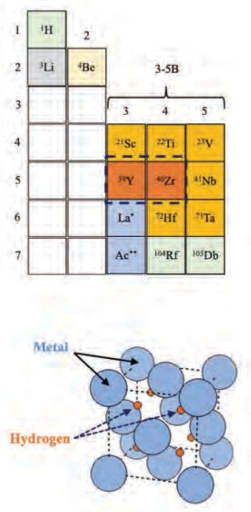
Presenter: M. Nedim Cinbiz (PI), Co-PI: Jianguo Yu

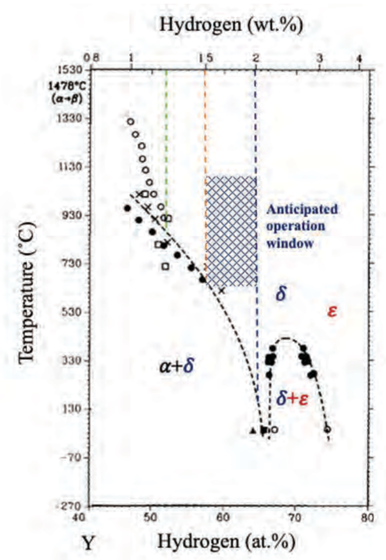
Content Collaborators: A. Sundar, Li Qi (UM), Y. Huang, J. Eapen (NSCU), T. Lach, E. Cakmak, A, Le Coq, K. Linton (ORNL)

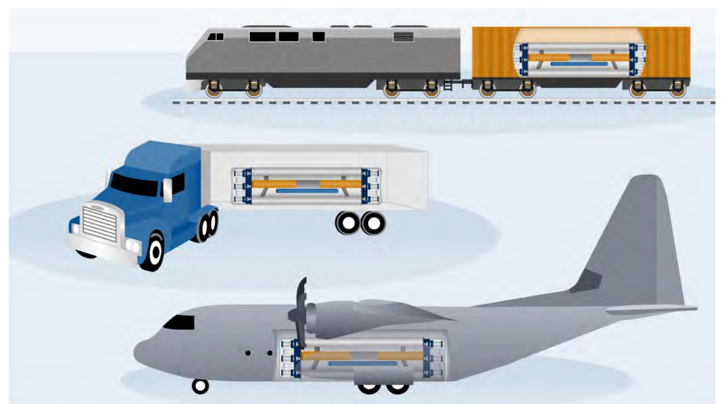
LDRD Co-PIs: C. Taylor, D. Labrier (ISU), M. Short (MIT)

University of Michigan · NC State University · Massachusetts Institute of Technology · Idaho State University · Oak Ridge National Laboratory · NSUF Nuclear Science User Facilities

BACKGROUND: Use of Solid Metal Hydride Moderators Allow Compact Transportable Nuclear Reactors

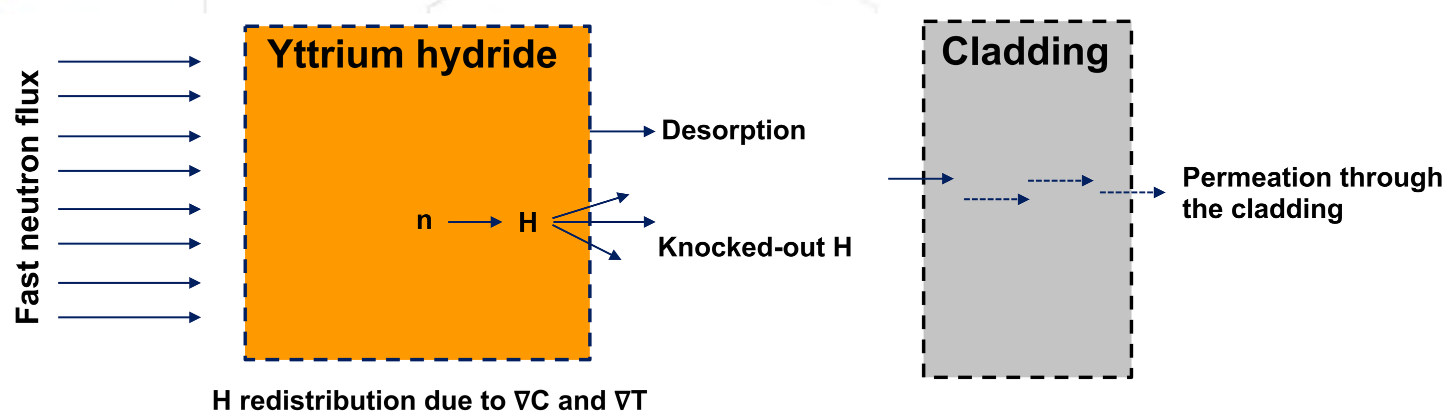




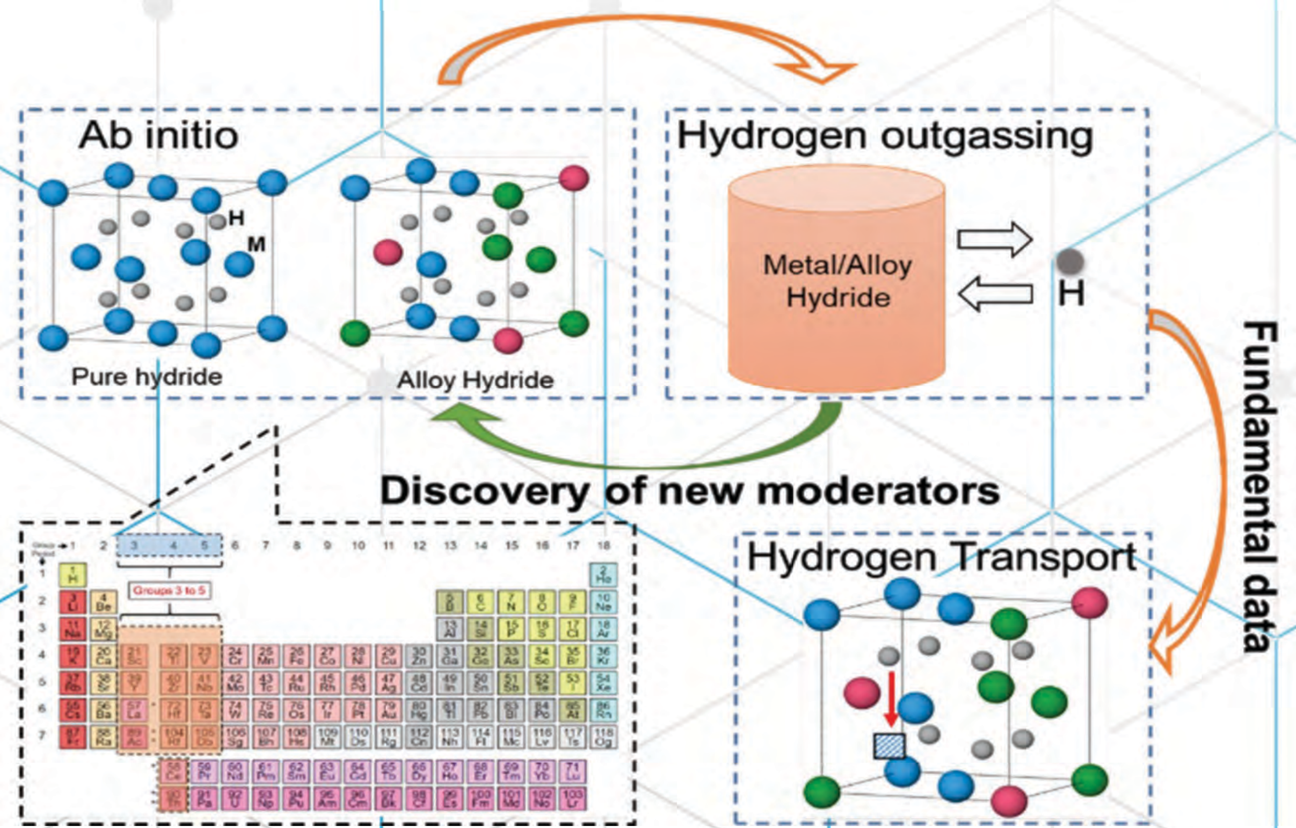


Source: GAO. | GAO-20-380SP

CHALLENGE: Hydrogen Retention at Elevated Temperatures (>500°C) For 10 Years of Operation



SOLUTION: Hydride Moderator Design Via Computations ⇆ Experiments

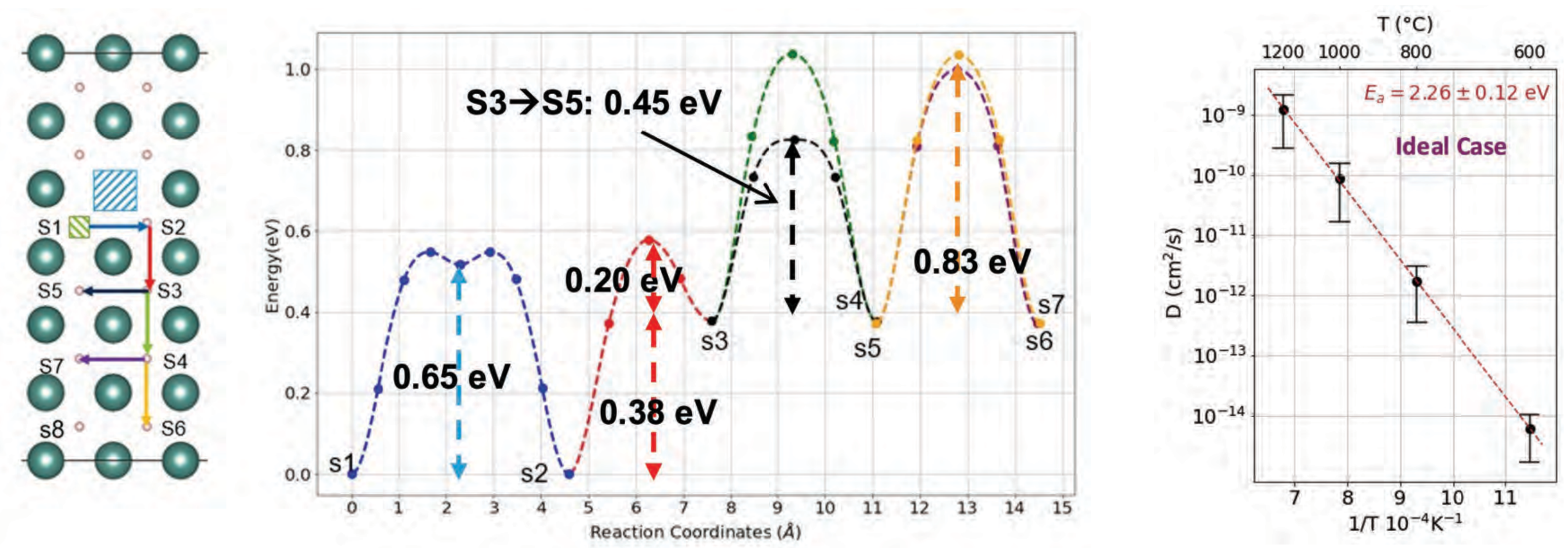


METHODS: Electronic structure ⇨ Hydrogen Diffusional Characteristics ⇨ Alloying ⇨ Irradiation

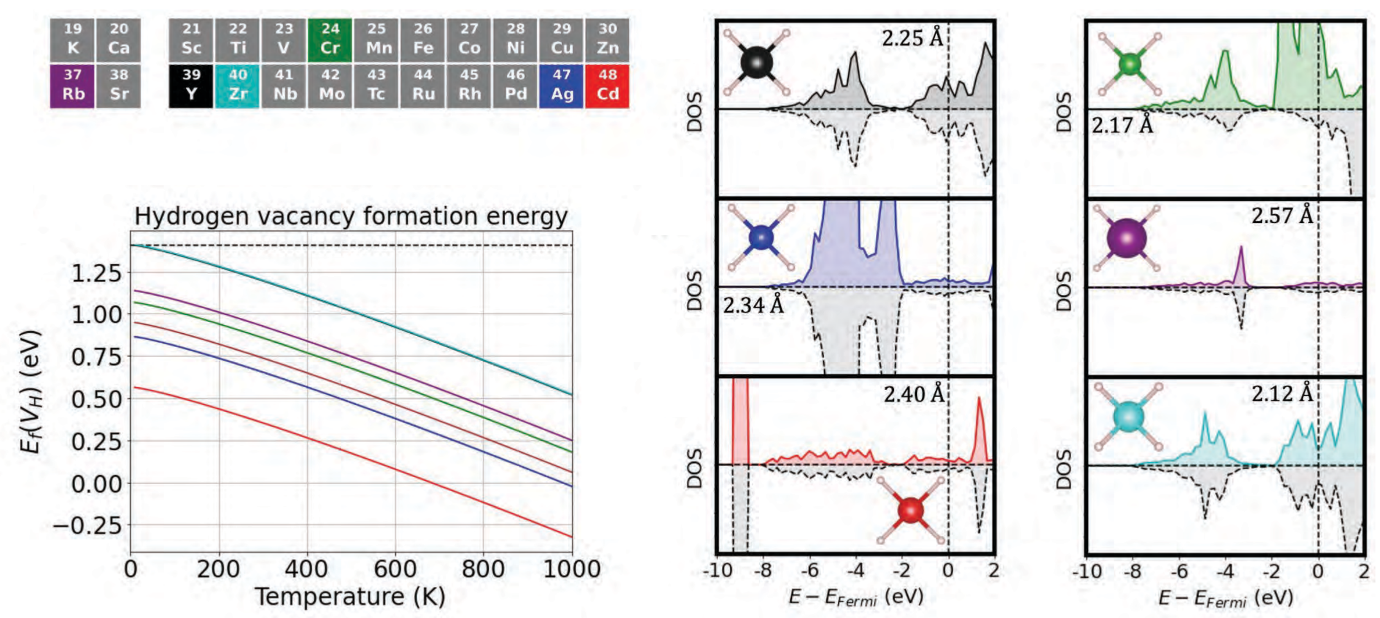
Density Functional Theory+ Ab Initio Molecular Dynamics+ Gaussian Potentials + Kinetic Monte Carlo + Incoherent Quasi Elastic Neutron Scattering + Transmission Electron Microscopy

1. HYDROGEN RETENTION IS GOVERNED BY CHARGE TRANSFER FROM HOST OR ALLOYING ELEMENT TO HYDROGEN, CHARGE LOCALIZATION, & METALLICITY

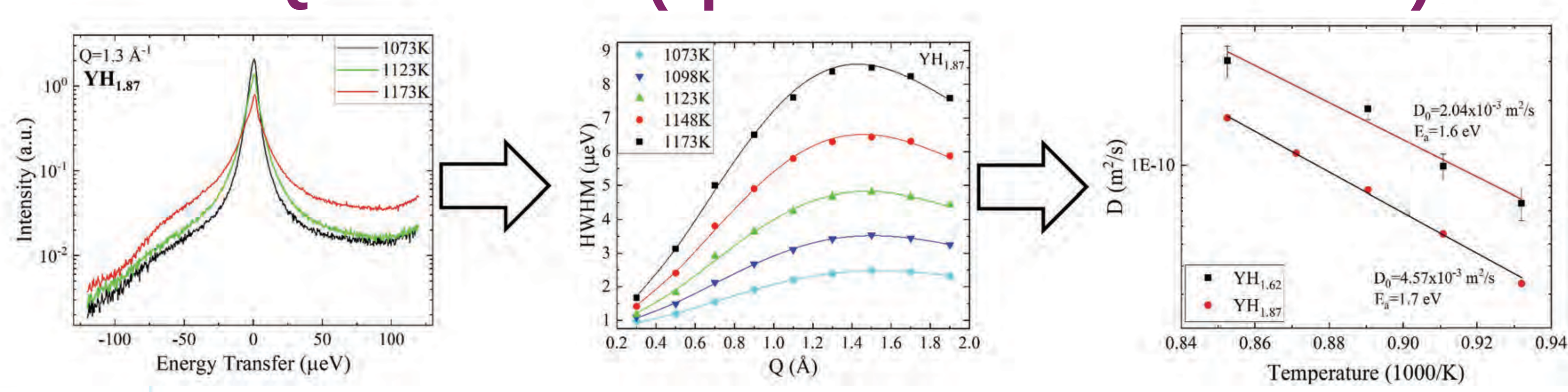
Pure Yttrium Hydride

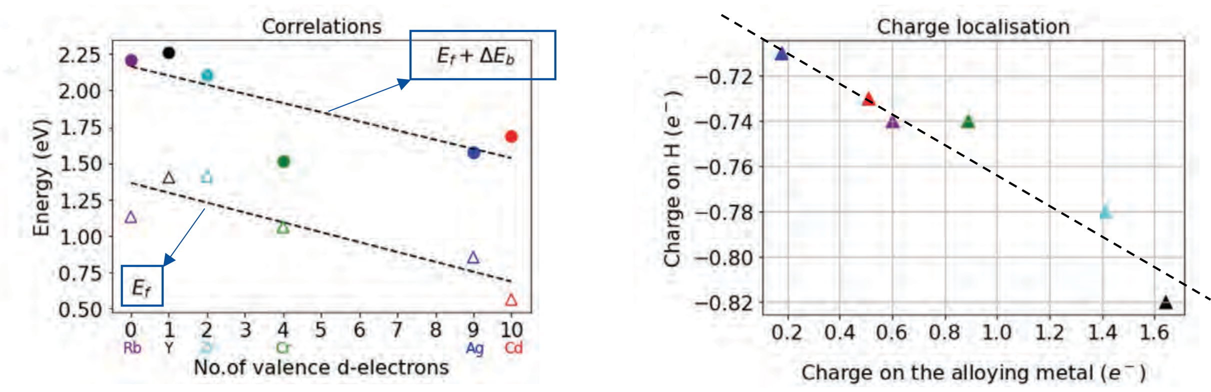


Binary Alloy Hydride



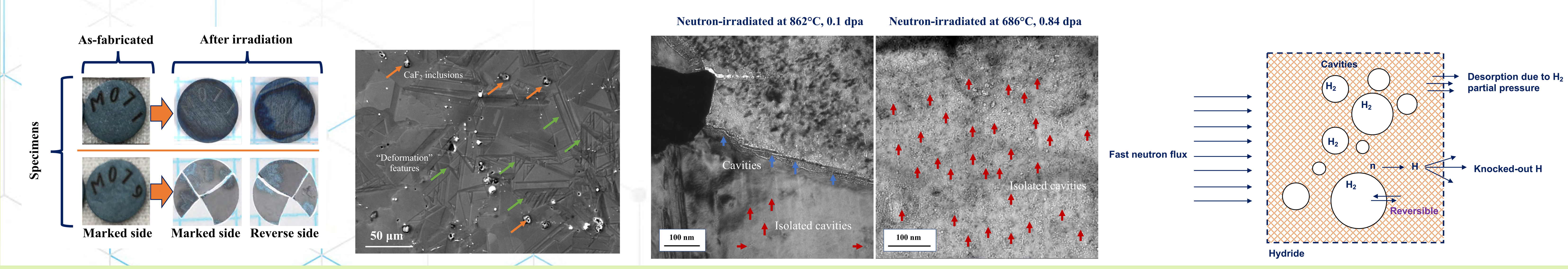
IQENS Results (Spallation Neutron Source)





2. NANO-SCALE CAVITIES ACT AS STORAGE POCKETS WHICH REGULATES THE HYDROGEN RETENTION IN NEUTRON-IRRADIATED YTTRIUM HYDRIDES

Impact of Neutron Irradiation (ORNL Donated Irradiated Specimens)



Project Number: 21A1050-020FP

LRS Number: INL/MIS-23-74174

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Accelerating Rare Events Estimation for the Safety Evaluation of Advanced Reactor Technologies

TEAM: Som Dhulipala, Ben Spencer, Vincent Laboure, Zach Prince, Peter German, Yifeng Che, Mike Shields, Promit Chakroborty, Denny Thaler

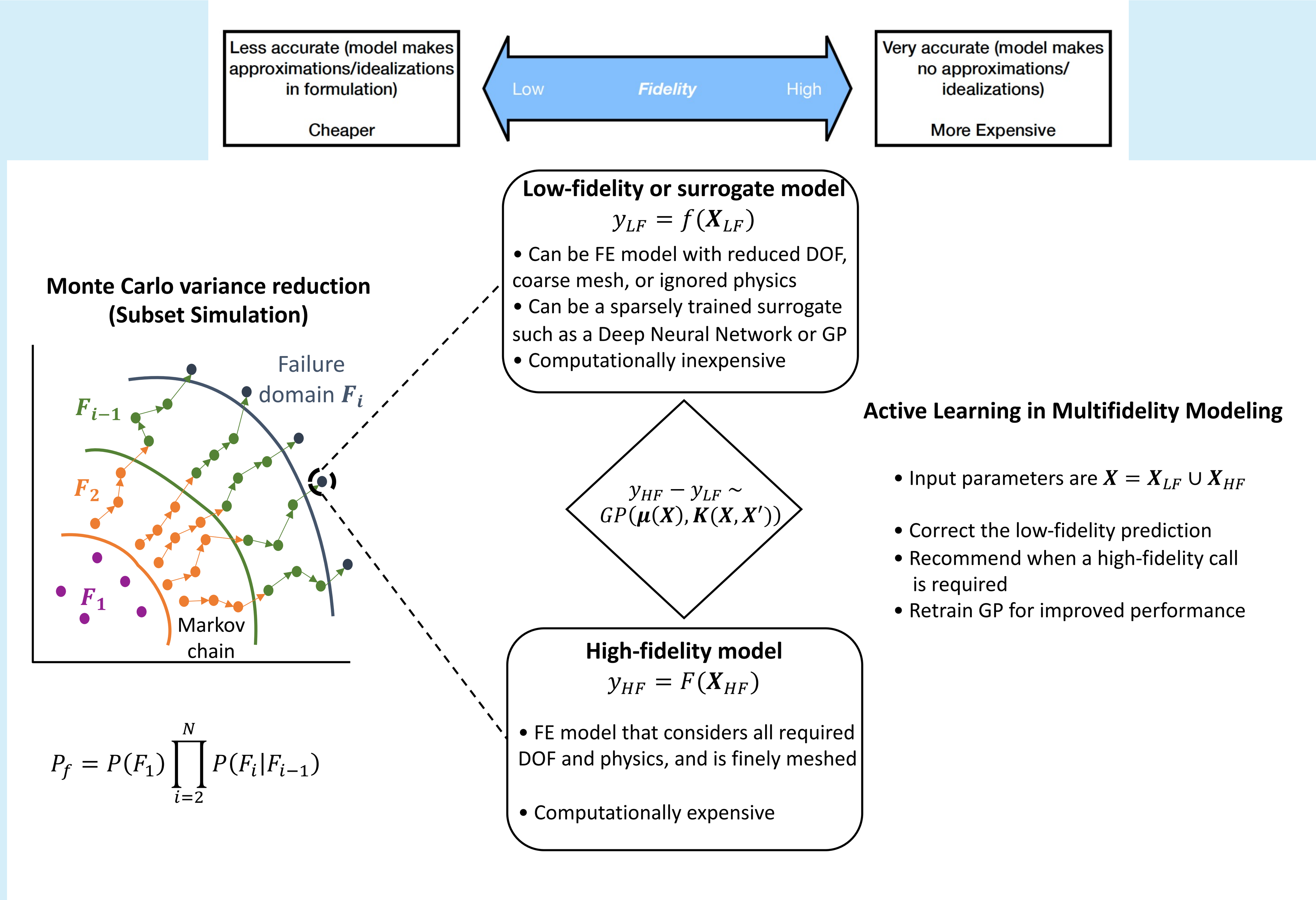
BACKGROUND: Safety evaluation of advanced reactors is computationally very expensive (failure probabilities b/w 1E-4 to 1E-8). This project employed ML-enabled UQ methods to significantly reduce this computational burden. Results will positively impact the safe design and optimization of advanced reactors.

DEVELOPED COMPUTATIONAL METHODS

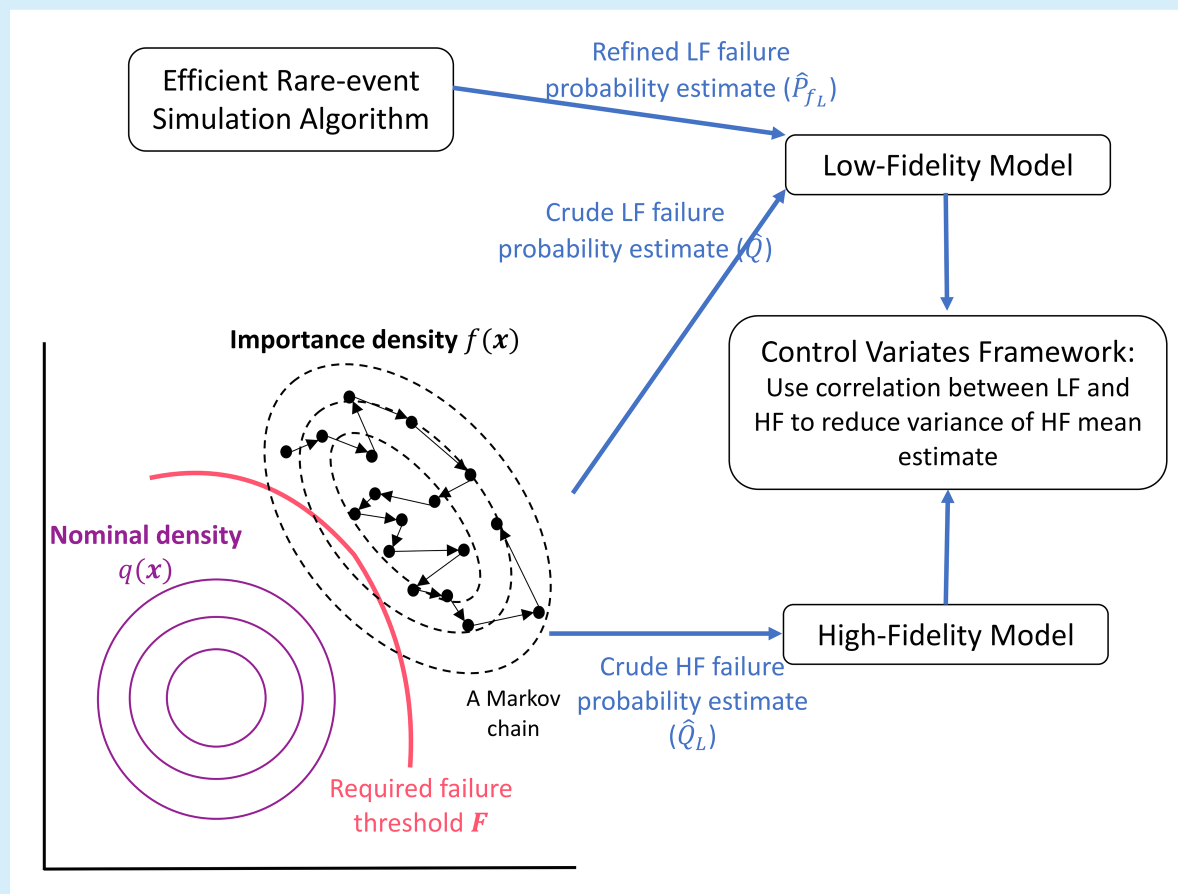
1. Multifidelity modeling in active learning
2. Control variates importance sampling
3. Uncertainty quantification with Hamiltonian Neural Networks

APPLICATIONS AND RESULTS

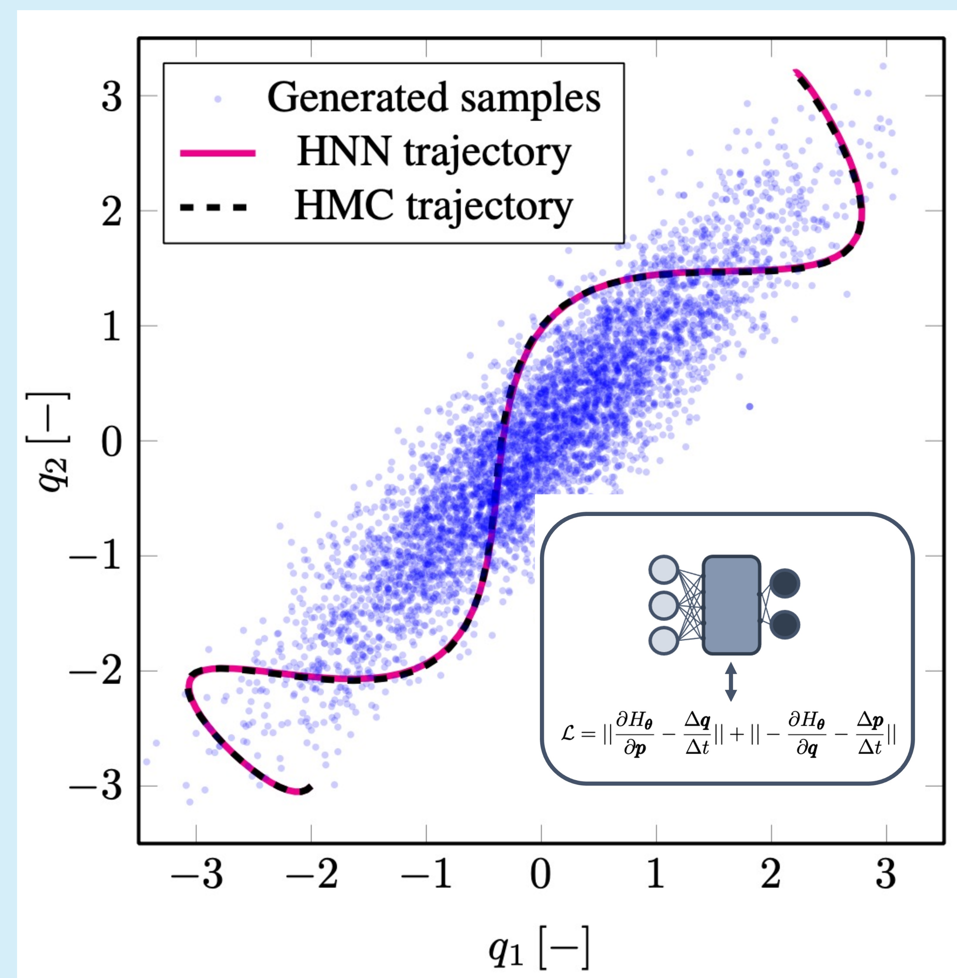
- **TRISO fuel**, **reactor pressure vessel embrittlement**, and **heat-pipe reactor**
- Developed methods accurately estimated very rare events (failure probability: 1E-4 to 1E-8)
- Computational effort reduced by 3 orders of magnitude compared to state-of-practice.



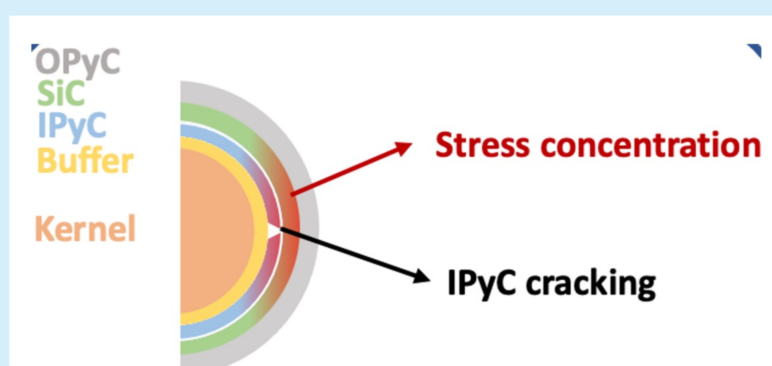
Multifidelity modeling in active learning



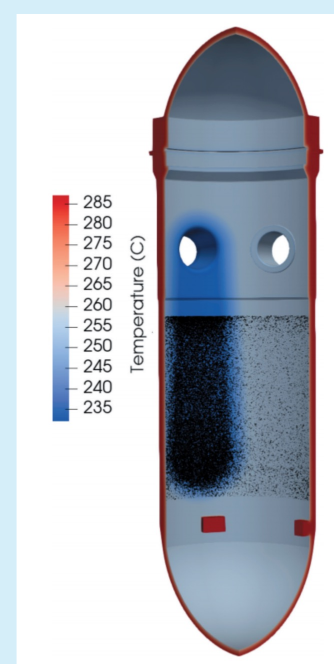
Control variates importance sampling



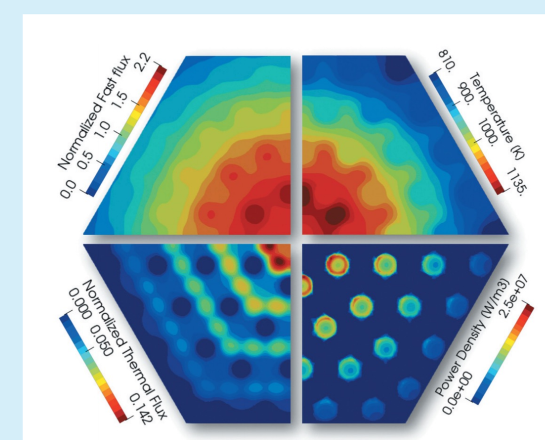
UQ with Hamiltonian Neural Networks



TRISO advanced nuclear fuel model (Jiang et al. 2021)



Flaws simulation in a reactor pressure vessel (Spencer et al. 2021)



Reactor core simulation of a heat-pipe microreactor (Matthews et al. 2021)

OUTCOMES

PUBLISHED/ACCEPTED JOURNAL PAPERS

- "Active Learning with Multifidelity Modeling for Efficient Rare Event Simulation" *Journal of Computational Physics*
- "Accelerated Statistical Failure Analysis of Multifidelity TRISO Fuel Models" *Journal of Nuclear Materials*
- "Reliability Estimation of an Advanced Nuclear Fuel using Coupled Active Learning, Subset Simulation, and Multifidelity Modeling" *Reliability Engineering & System Safety*
- "General Multi-Fidelity Surrogate Models: Framework and Active Learning Strategies for Efficient Rare Event Simulation" *Journal of Engineering Mechanics*
- "Efficient Bayesian Inference with Latent Hamiltonian Neural Networks in No-U-Turn Sampling" *Journal of Computational Physics*

JOURNAL PAPERS UNDER SUBMISSION

- "Parallel Uncertainty Quantification in MOOSE: Forward, Bayesian Inverse, Active Learning, and Multifidelity Modeling Capabilities" *Journal of Computational Science*
- "Reliability Analysis of Complex Systems using Subset Simulations with Hamiltonian Neural Networks" *Structural Safety*
- "A Coupled Control Variates and Importance Sampling Method for Efficient Bifidelity Reliability Analysis" *SIAM/ASA Journal on Uncertainty Quantification*

SOFTWARE DISCLOSURE RECORD

BIhNNs: Bayesian Inference with Neural Networks (CW-22-35)

TALENT PIPELINE

Yifeng Che (Russell Heath Distinguished Postdoc), Promit Chakroborty (Outstanding Contribution Prize), Eusef Abdelmalek (GEM Fellow), Akram Batikh

AWARDED GRANT PROPOSALS

- DOE Nuclear Safety Research & Development (NSR&D) Program
- DOE Nuclear Energy University Partnerships (NEUP)

FOLLOW-ON FUNDING FROM PROGRAMMATIC ACTIVITIES

- DOE Nuclear Energy Advanced Modeling and Simulations (NEAMS)
- DOE Advanced Materials and Manufacturing Technologies (AMMT)

JOHNS HOPKINS UNIVERSITY

RWTH AACHEN UNIVERSITY

Project Number: 21A1050-114FP

LRS Number: INL/MIS-23-74133

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Simulating Hydrogen Migration for Microreactor Applications using MOOSE-Based Tools

Stefano Terlizzi[1] (PI), Mark DeHart[1] (co-investigator), Vincent Labouré [1], Quentin Faure[2]

1. Reactor Physics Methods and Analysis Group, Idaho National Laboratory, 1955 N Fremont Ave, Idaho Falls, ID 83415
2. Department of Nuclear Engineering, North Carolina State University, 2500 Stinson Drive, Raleigh, NC 27695

Introduction

The introduction of nuclear microreactors is projected to open new markets for the nuclear power industry because of potential to be cost-competitive in non-traditional market segments. An obstacle to the deployment of many nuclear microreactor concepts is their reliance on high-assay low-enriched uranium (HALEU). In fact, despite enabling the design of compact systems and long operational lifetime, usage of HALEU entails both technical and regulatory challenges. Reduction of the fuel enrichment or quantity while maintaining the design compactness and high operating temperature can be achieved by using metal hydrides. However, it has been shown that the hydrogen contained in the hydrides tends to redistribute and leak from the moderating elements leading to reactivity losses, and, potentially, failure of the moderating elements, with consequent reactor shutdown.

This work aimed at (1) modeling **the hydrogen migration** in hydrides, with emphasis on yttrium hydride, in the Multiphysics Object-Oriented Simulation Environment (MOOSE). (2) **Gaining a better understanding** on the effect of hydrogen migration on neutronics and thermal field in prototypical nuclear microreactors, and (3) **Perform a rigorous uncertainty quantification** to assess experimental needs.

Theory

Three sub-phenomena determine the hydrogen migration in metal hydrides:

(a) Hydrogen **redistribution** of the hydrogen in the hydride's bulk is driven by the temperature and hydrogen concentration spatial gradients.

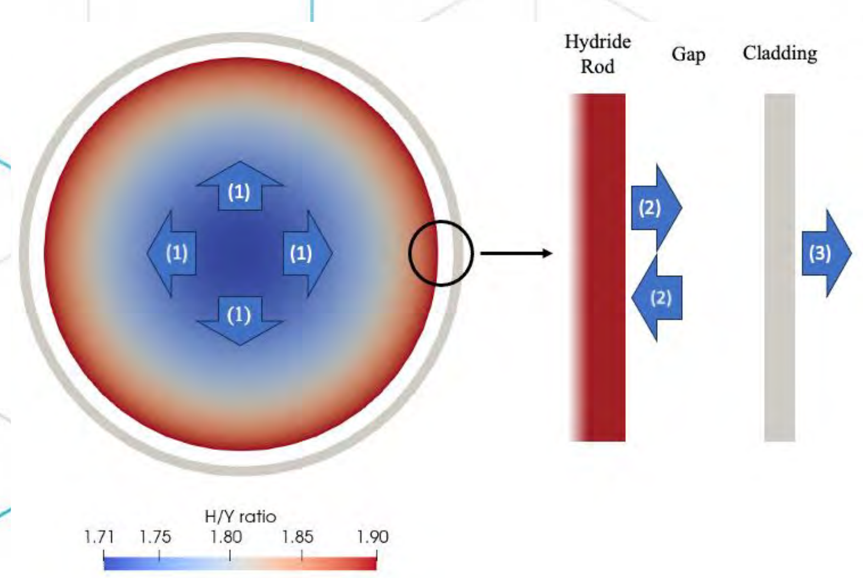
(1) $$\frac{dc_H}{dt} = \nabla \cdot \left(-D\left(\nabla c_H + \frac{Q c_H}{R\,T}\nabla T\right)\right).$$

(b) Hydrogen **dissociation** at the hydrogen surface due to material-dependent adsorption-desorption dynamics.

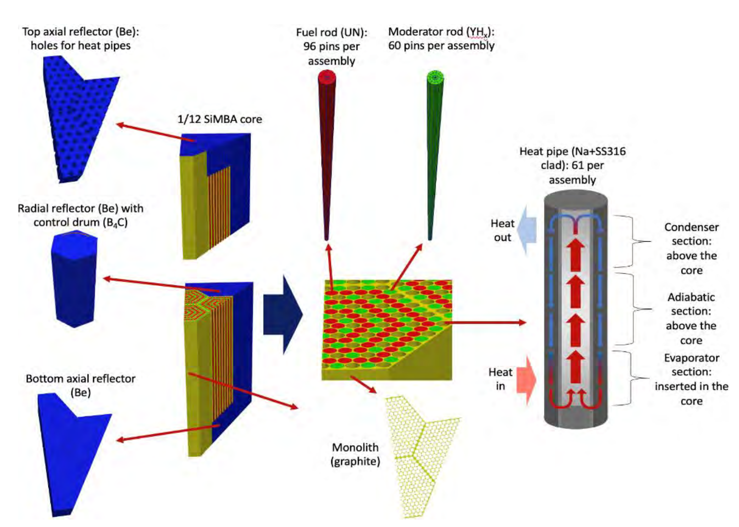
(2) $$\overrightarrow{J_H^s} \cdot \vec{n} = J_{des} - J_{ads}.$$

(c) **Leakage** through the clad surrounding the hydride can be computed through the permeability ϕ and the partial pressure of hydrogen p_H given by the pressure-concentration-temperature (PCT) curves:

(3) $$\overrightarrow{J_H^c} \cdot \vec{n} = -\phi\frac{\sqrt{p_H}}{\Delta x}.$$



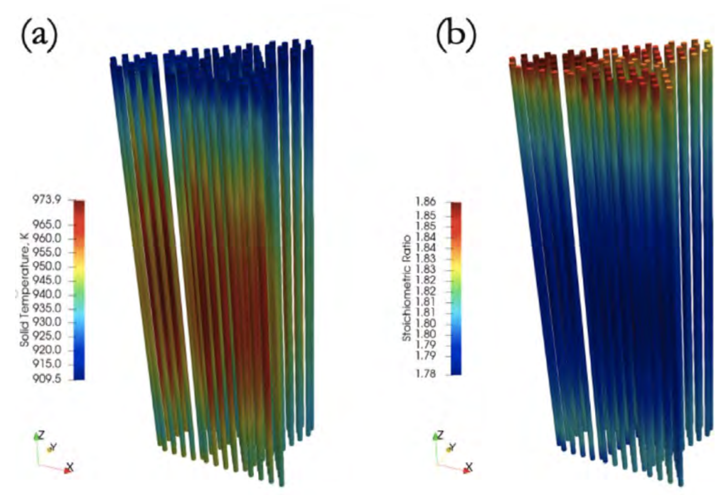
Test Problem



A test problem named the Simplified Microreactor Benchmark Assessment (SiMBA) problem was prepared as a prototypical heat-pipe cooled yttrium hydride-moderated microreactor. The coupled neutronic, heat conduction, thermal-hydraulics, hydrogen redistribution equations were solved for the full reactor.

The details of the design were made generic enough to avoid any proprietary concerns, but specific enough to capture the primary design characteristics of the envisioned HP-cooled monolithic microreactors. A model based upon will be included on the Virtual Test Bed (VTB) by the end of the fiscal year.

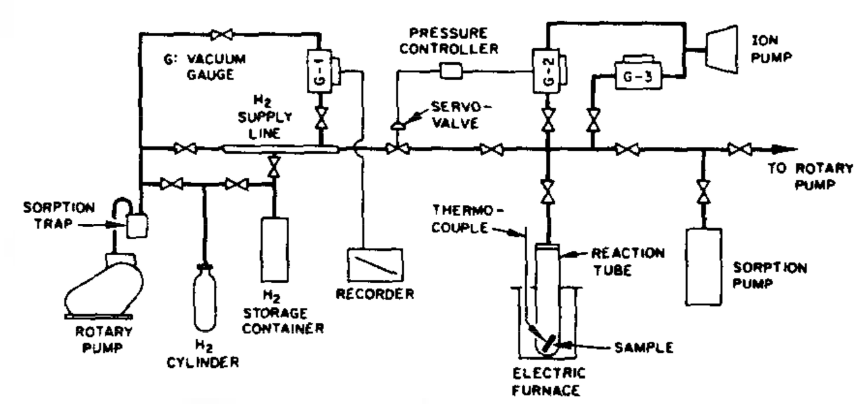
Redistribution



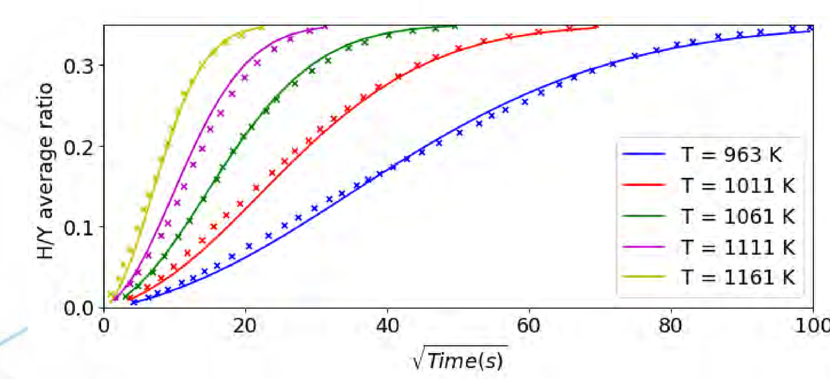
The hydrogen redistributes towards colder zones. The sign of the feedback is negative due to the migration of the hydrogen toward colder axial zones. These axial zones are usually associated with low neutron importance, thus leading to a negative effect on reactivity. The magnitude of the feedback was found to be on the order of −29 pcm on the effective multiplication factor for the SiMBA reactor.

Dissociation

Experimental set-up: Pure yttrium samples (0.142 cm x 1.27 cm x 1.3 cm) are inserted into a reaction tube with fix temperature (no gradient of temperature) and pressure. Adsorption of hydrogen into the yttrium is measured.



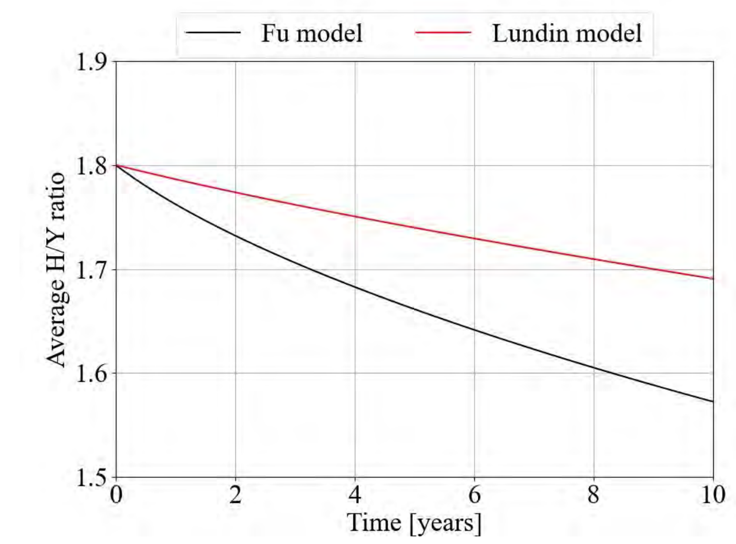
Models for hydrogen dissociation of hydrogen at the yttrium hydride surface, including adsorption and desorption, were implemented in Bison and the results obtained were compared to the experimental values.



The solid line are Bison and the crosses are experimental values.

Leakage

The leakage through 500-µm thick SS-3316 clad was simulated using the permeability-based equation in Bison. Two different PCT curves were used to implement the hydrogen leakage in Bison.

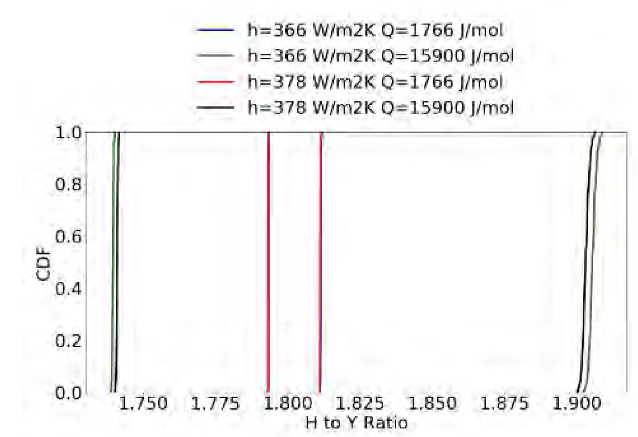


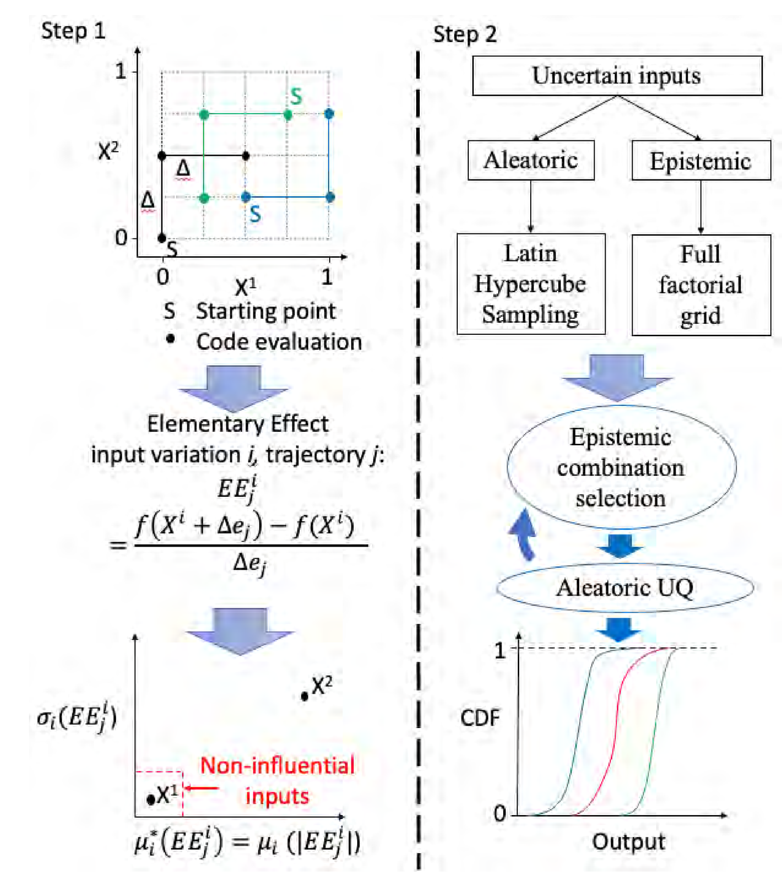
Average hydrogen stoichiometric ratio for the yttrium hydride pins in the SiMBA problem were calculated against time for 10 years operation at 870 K, showing the non-negligible decrease in hydrogen content over the MR lifetime. Additionally, the leakage is strongly dependent upon the model used for the PCT curves.

UQ

To obtain information on the impact of uncertain inputs on the temperature and H/Y ratio distribution, we rely on the two-step approach. The methodology allows to consider the different nature of the uncertainties (epistemic vs. aleatoric).

It was found that the magnitude of the epistemic uncertainty of the heat of transport shadows the influence of the aleatoric uncertainties.





Conclusions

(1) The hydrogen redistribution equation was solved in Bison. The effect of the hydrogen redistribution on the power density, eigenvalue, and temperature was then obtained by coupling the Bison inputs with full core neutronic and heat transfer models developed within the Direwolf software driver.. It was found that the feedback is negative due to the redistribution of hydrogen towards colder zones, usually associated to lower importance zones.
(2) A model describing hydrogen adsorption-desorption and leakage for yttrium hydride was implemented. It was shown that the results are extremely sensitive to the model used to describe the current at the hydride's boundary. This uncertainty may affect estimations of the MR's lifetime non-negligibly.
(3) The UQ analysis confirmed the importance of obtaining a reliable experimental value for the heat of transport in order to accurately quantify the effect of hydrogen redistribution in yttrium hydride on neutronics.

Publications

[1] Terlizzi S., Labouré, V., and DeHart M. (2022). *Preliminary Observations on the Hydrogen Redistribution Feedback in YH-Moderated Monolithic Microreactors*. 2022 ANS Annual Meeting.
[2] Terlizzi S., Labouré, V., and DeHart M. (2022). *Selected results from full-core hydrogen redistribution asymptotic analysis in YH-moderated heat-pipe cooled microreactor*. 2022 ANS Winter Meeting.
[3] Terlizzi S. and Labouré, V.(2023) Asymptotic Hydrogen Redistribution Analysis in Yttrium Hydride Moderated Heat-pipe-cooled Microreactors using DireWolf, *Annals of Nuclear Energy.*
[4] Faure Q., Labouré, V., and Terlizzi S. (2023) Preliminary Results for Uncertainty Quantification on Asymptotic Hydrogen Redistribution in a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor, ANS Winter Meeting, Washington DC, USA, November 2023.
[5] Faure Q., Labouré, V. Terlizzi S. (Expected Submission Date: 20 November 2023). Multi-Physics Uncertainties Quantification on Neutronics Response for a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor, Annals of Nuclear Energy
[6] Terlizzi S., Faure Q., (Expected Submission Date: 30 October 2023) On the effect of hydrogen dissociation on the lifetime of hydride-moderated nuclear microreactors, Physor 2024, April 2024.

Project Number: 21P1056-010FP LRS Number:

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

www.inl.gov

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

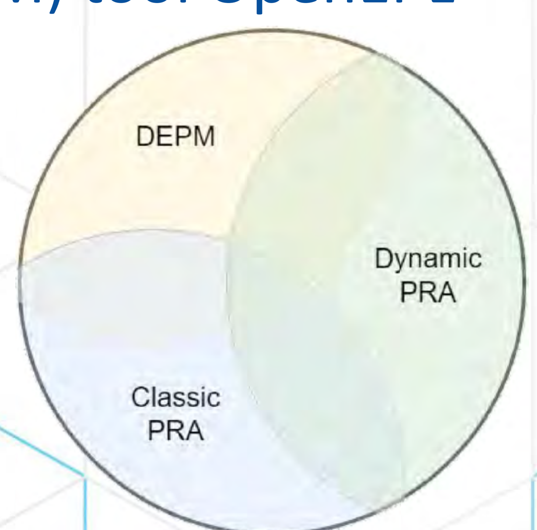
Quantitative Reliability Analysis for Unattended Operation of Fission Batteries

PRESENTER:
Steve Prescott

BACKGROUND: Autonomous controlled, “Plug & Play” fission battery concepts are difficult to model and analyze. These highly Cyber-Physical system need more than classical risk analysis to handle the desired safety and business cases. Dynamic probabilistic risk assessment (PRA) is promising but has limitations, many of which can be overcome.

METHODS

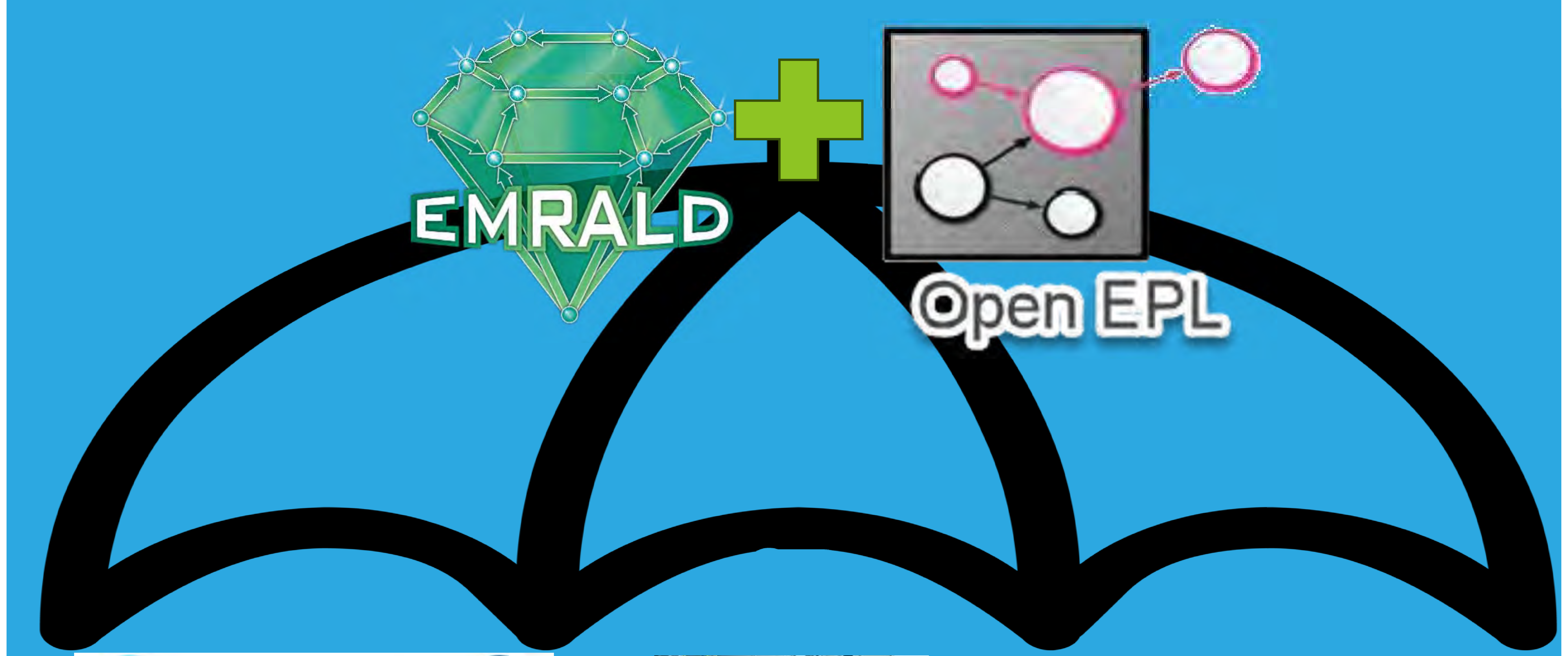
1. Dynamic PRA tool EMRALD
2. Coupled dual-graph error propagation methodology (DEPM) tool OpenEPL



RESULTS

- Cyber protection modeling with reactor behavior
- Complex time scenarios for automated safety control
- Compare operator vs. autonomous

Model and analyze complex Cyber-Physical system interactions



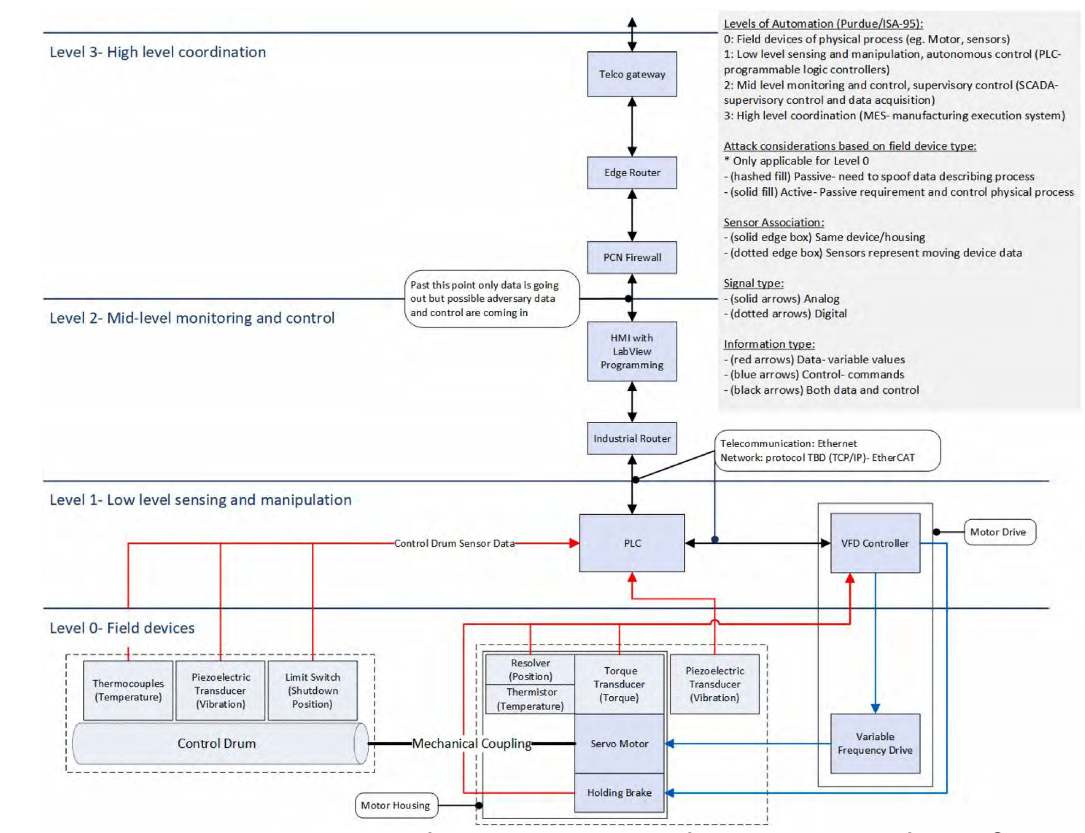
Papers

A combined strategy for dynamic probabilistic risk assessment of fission battery designs using EMRALD and DEPM

Probabilistic Methods for Cyclical and Coupled Systems with Changing Failure Rates

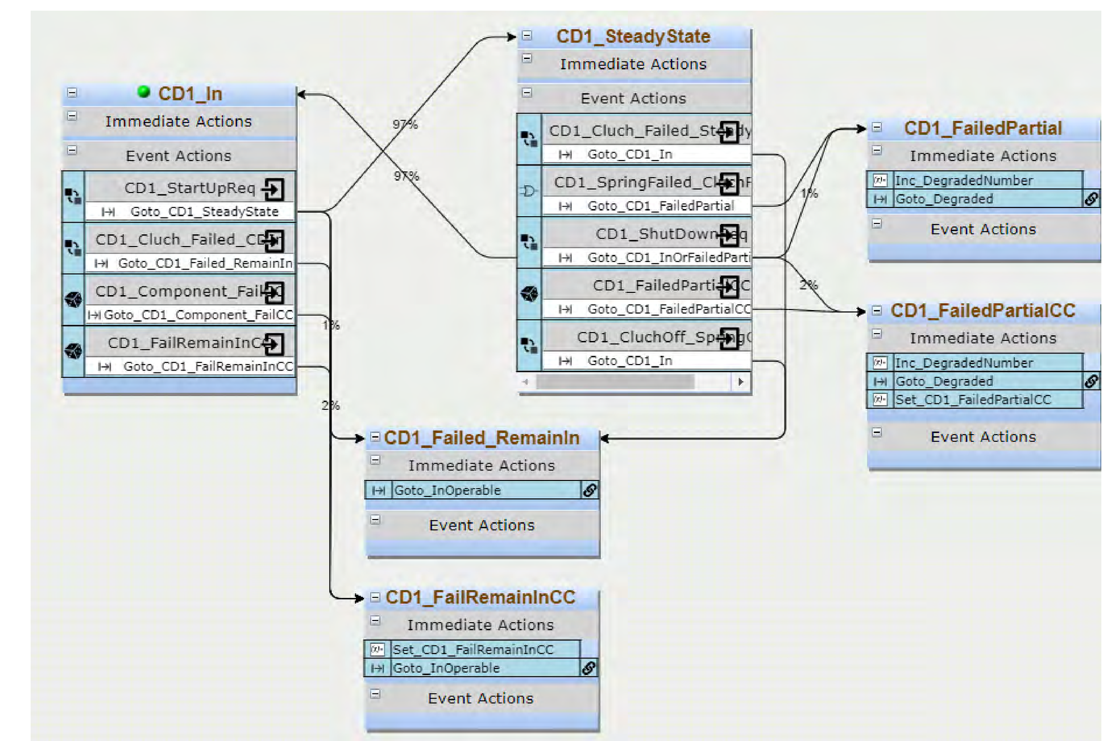
Introducing Multiple Control Paths in the Dual Error Propagation Graph for Stochastic Failure Analysis of Digital Instrumentation and Control Systems

Analyze



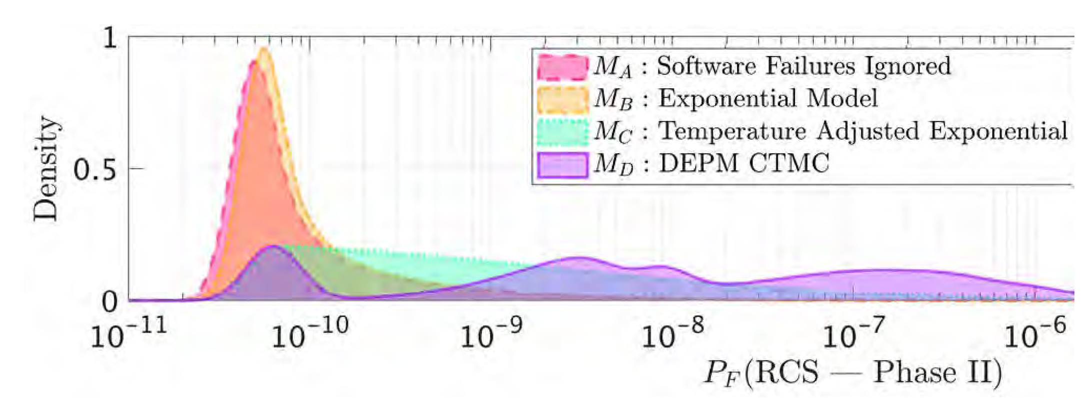
Communication and automation diagram to identify modeling areas and boundaries.

Model

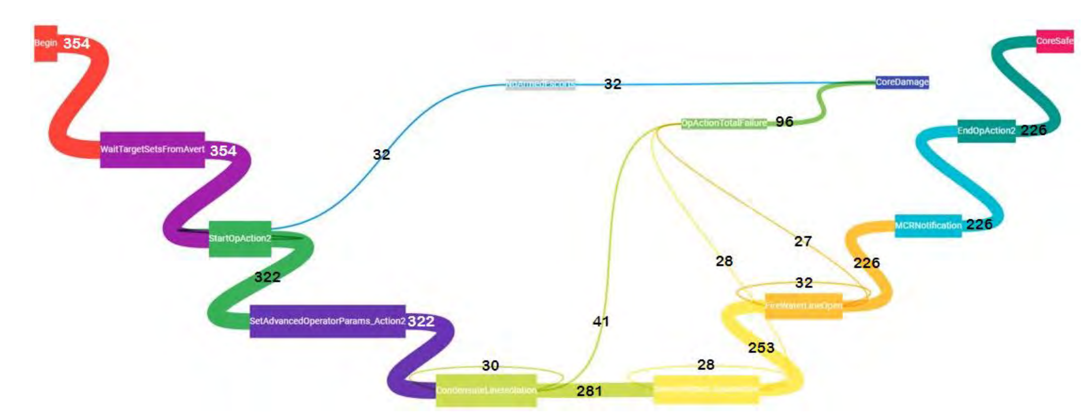


EMRALD model showing the states of a core drum.

Results



Dynamic analysis (purple) vs. standard failure outcomes.



Sankey visualization results for failure paths and timing.

Steven Prescott, Arjun Earthperson, Jooyoung Park, Thomas Ulrich, Mihai Diaconeasa Bri Rolston, Troy Unruh, Jisuk Kim

Project Number: 21A1053-019FP

LRS Number: INL/MIS-23-73993

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy’s Office of Nuclear Energy

Idaho National Laboratory

Characterizing corrosion mechanisms of structural alloys in actinide-based molten chloride salt

Trishelle Copeland-Johnson[1], Michael Woods[1], William C. Chuirazzi[1] ,Ruchi Gakhar[1], Daniel J. Murray[1], Guoping Cao[1]

[1] Idaho National Laboratory, 1955 N. Fremont Ave. Idaho Falls, ID 83415

Motivation

The corrosion performance of structural materials in contact with molten salts for closed fuel cycle applications, such as electrorefining and molten chloride salt fast reactors, are of concern.

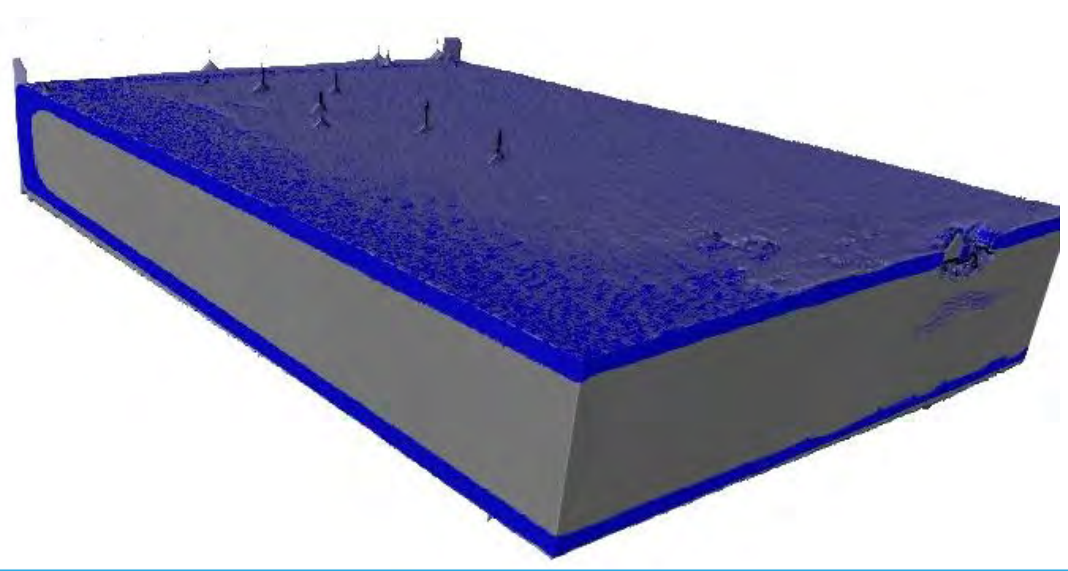
Methodology – Correlated Multi-Modal Advanced Characterization

X-ray computed tomography (XCT) → Scanning electron microscopy (SEM) / Focused ion beam microscopy (FIB) → Transmission electron microscopy (TEM)

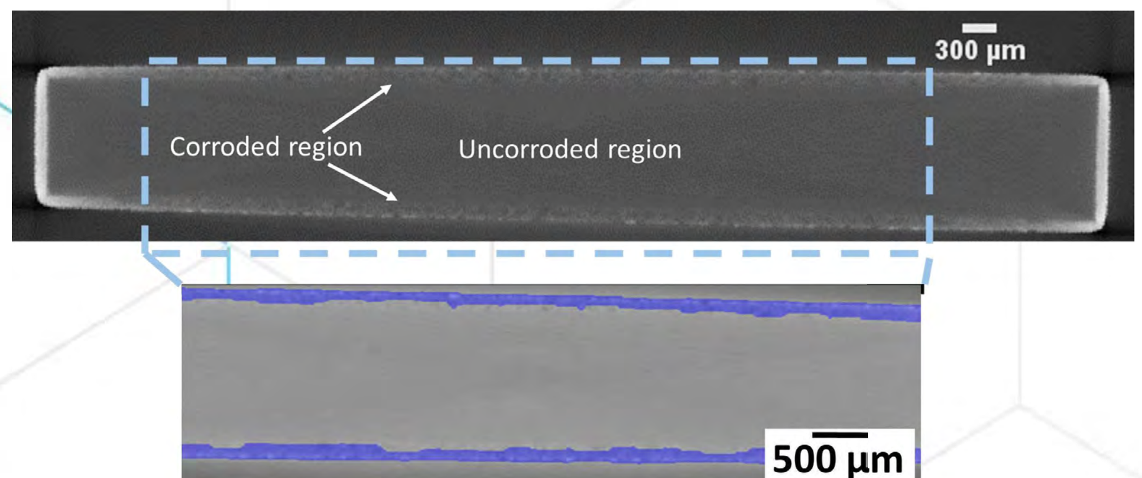
cm —— μm —— nm

Progress-to-Date: Alloy 617 (A617) in $LiCl\text{-}KCl\text{-}UCl_3$ (700 °C for 1000 h)

3D Imaging of Corroded A617 with XCT



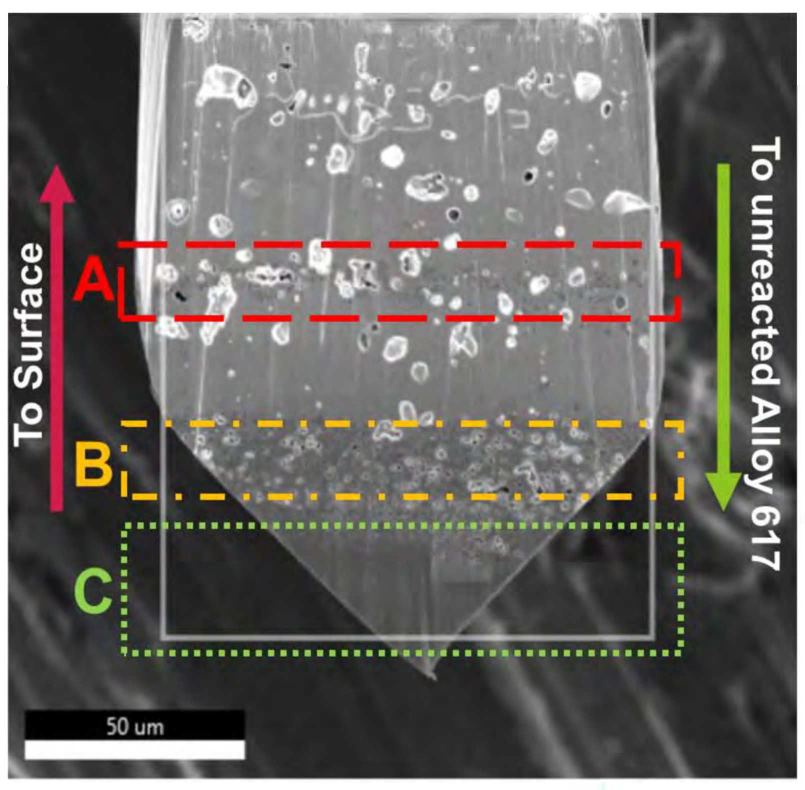
Automated 3D thickness measurement : 123.80 μm ± 15.00 μm



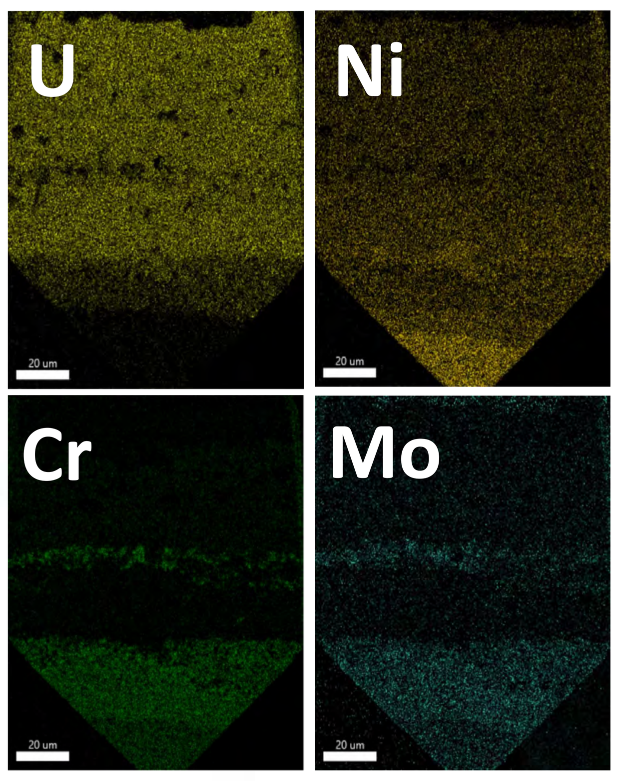
Manual 2D thickness measurement: 118.84 μm ± 17.36 μm

SEM/FIB Microscopy Results

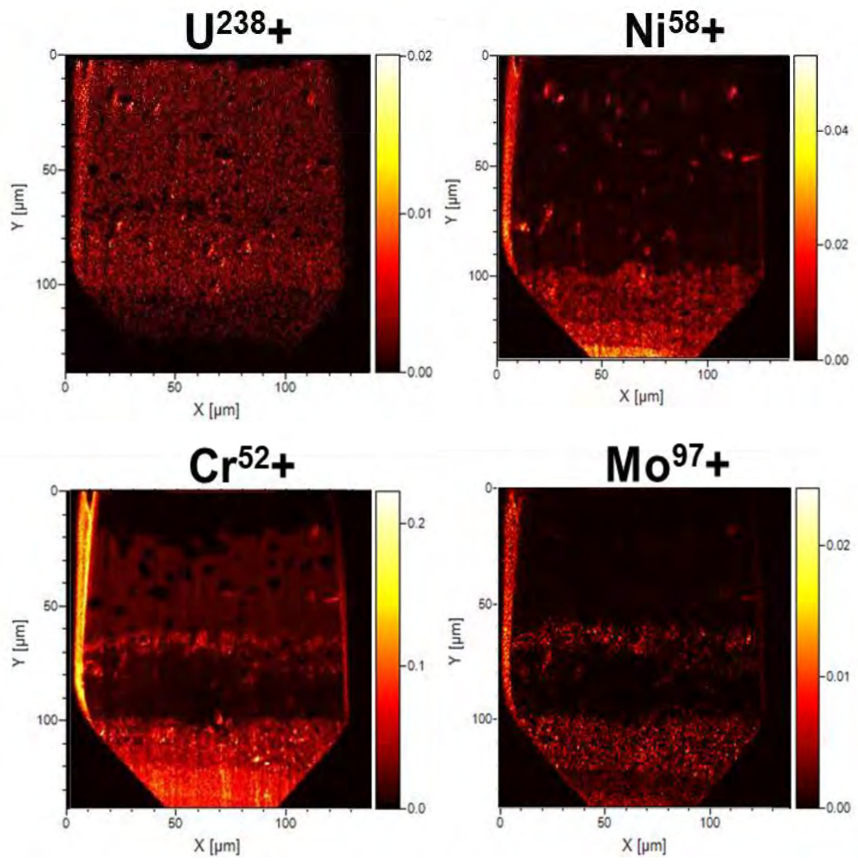
Image of Corroded A617



Elemental Analysis

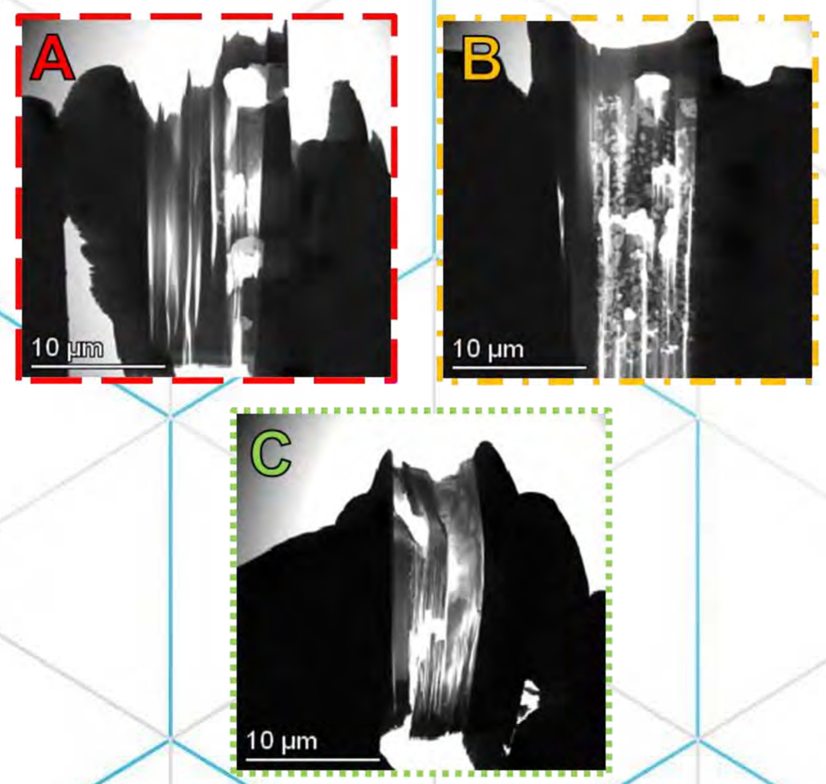


Isotopic Analysis

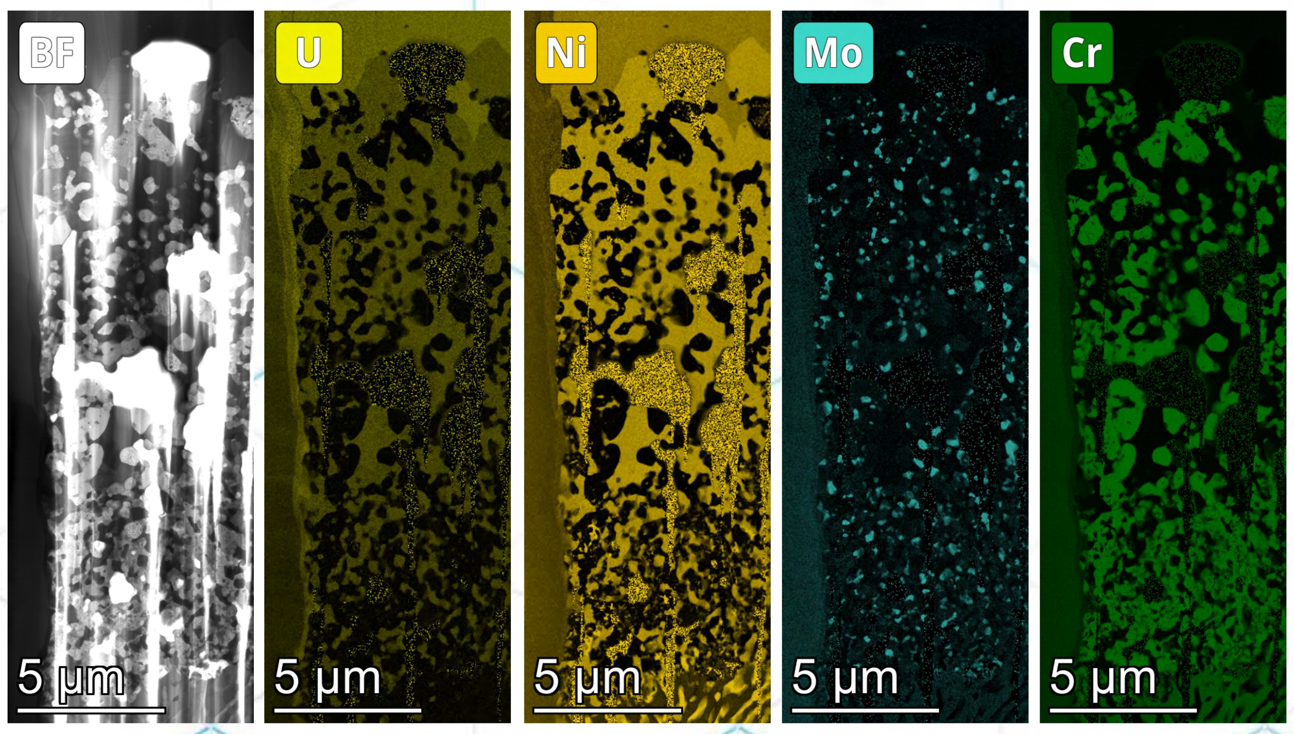


TEM Microscopy Results

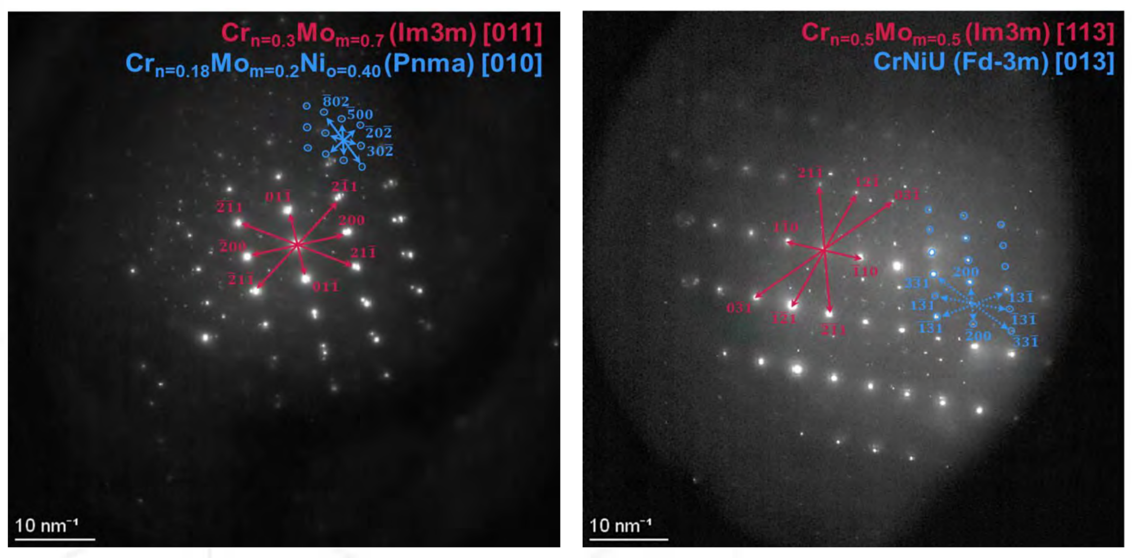
TEM Lamellas from Corroded A617



Site B: Elemental Analysis



Site B: Electron Diffraction



CONCLUSIONS: Non-preferential attack by UCl_3 salt; Diffusion of U into A617

NEXT STEPS: Advanced characterization of Hastelloy C-276 and Hastelloy N before/after corrosion in $NaCl\text{-}UCl_3$ eutectic salt.

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517

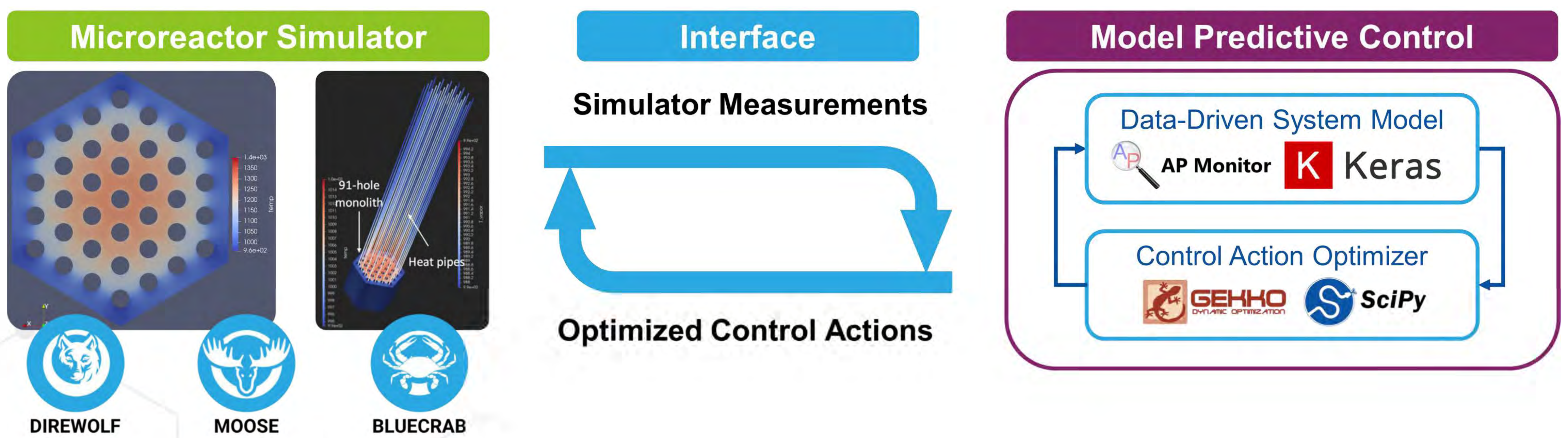
Scalable Framework of Hybrid Modeling with Anticipatory Control Strategy for Autonomous Operation of Modular and Microreactors

Vivek Agarwal (PI), Linyu Lin, Joseph Oncken, Ronald L. Boring, Andrei Gribok, Cody Permann (NS&T); Shannon Eggers (NH&S); and Timothy McJunkin (EES&T)

Objective:

Develop and validate a scalable hybrid modeling and anticipatory control techniques to enable faster than real-time prediction and decision-making capabilities for microreactor control.

Technical Approach:



- Generation of physics-informed simulated data for a heat pipe (HP) based microreactor.
- Development of machine learning (ML) surrogate models.

- Model Predictive Control (MPC) using nonlinear optimization solver.
- ML predictors using neural networks and Sparse Identification of Nonlinear Dynamics with Control

Accomplishments:

Key Innovative Outcomes and Opportunities

Publications

5 journal articles and 8 conference papers and presentations

Talent Pipeline

- 3 Postdocs (Now full-time staffs)
- 2 Summer Graduate Interns

Intellectual Property

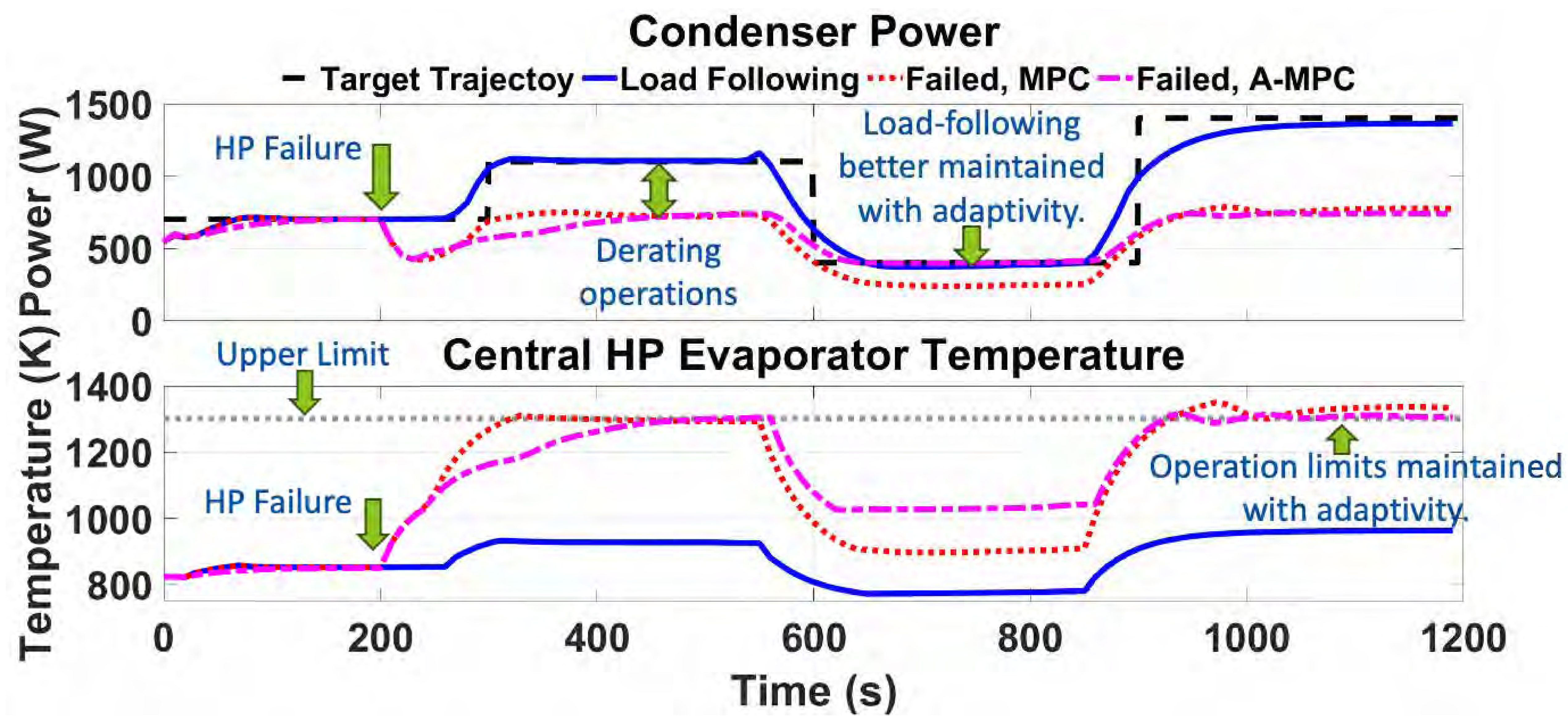
Licensed Software: Autonomous Control fOr Reactor techNologies (ACORN)

Engagement

- National Reactor Innovation Center
- Nuclear Energy Advanced Modeling and Simulation
- Westinghouse, Ultra Safe Nuclear Corporation, Pathfinder Energy Developments

Demonstration Scenarios and Simulation Results:

- Load-following during normal and abnormal conditions.
- Autonomous operations at steady states and power transients.
- Adaptive MPC (A-MPC) configurations based on diagnosis results.



Salient Features of ACORN:

- Situational Awareness – utilize design principals from human factor engineering aspects and regulatory guidance.
- System Stability – robust against sensor drifts/noises, cyber incidents, and failed components.
- Adaptive – utilize artificial intelligent algorithms with transfer learning and online updating.

Path Forward and Impact:

- Demonstrate ACORN to other microreactor stakeholders and quantify uncertainties to build confidence in autonomous controls.
- A first-of-a-kind ability to advance level of autonomy of nuclear reactor operation.

Project Number: 21A1050-067FP

LRS Number: INL/MIS-23-74179

www.inl.gov

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

Accelerate Utilization of Nuclear Fuel Performance Modeling

TEAM:

Yifeng Che, Ryan Stewart, Som Dhulipala, Wen Jiang, James Tompkins (X-energy)

ACKNOWLEDGEMENT:

Mengnan Li, April Novak (ANL), Zachary Prince, Peter German, Casey Jesse, Mohammad Abdo

BACKGROUND:

Nuclear fuels undergo complicated thermo-mechanical-chemical degradation in reactor environment, posing constraints to reactor operation and design. This projects accelerates the utilization of fuel performance modeling by (1) improving the reliability of fuel performance models via inverse uncertainty quantification (UQ), and (2) integrate high-fidelity Bison fuel performance simulation into the multiphysics framework.

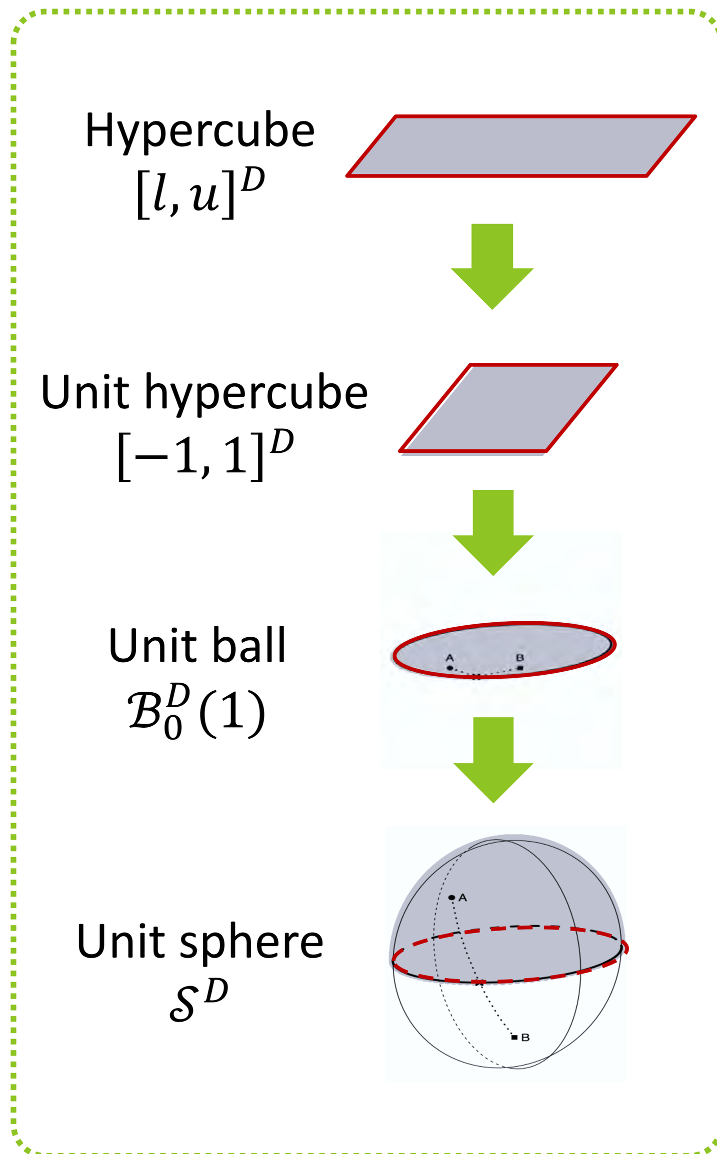
JOURNAL PAPERS UNDER PREPARATION:

- A Review and Outlook for Bayesian Analysis in Modeling and Simulation in Nuclear Engineering
- Coupling high-fidelity fuel performance modeling into the multiphysics simulation of high temperature gas-cooled microreactor

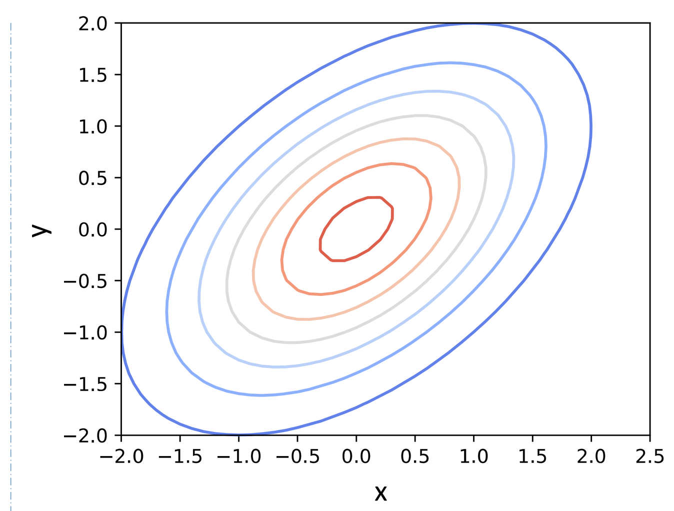
Inverse UQ with Constraints: Spherical Hamiltonian Monte Carlo

- Bayesian inference confined to constrained domains is challenging for commonly used sampling algorithms.
- Boundary conditions handled implicitly via spherical measures in the computational efficient framework Hamiltonian Monte Carlo (HMC).
- Proposed samples are generated on the sphere that remain within boundaries when mapped back to the original space.
- Hamiltonian Neural Networks (HNNs) with HMC and No-U-Turn Sampler (NUTS) are integrated with spherical measures for enhanced efficiency.

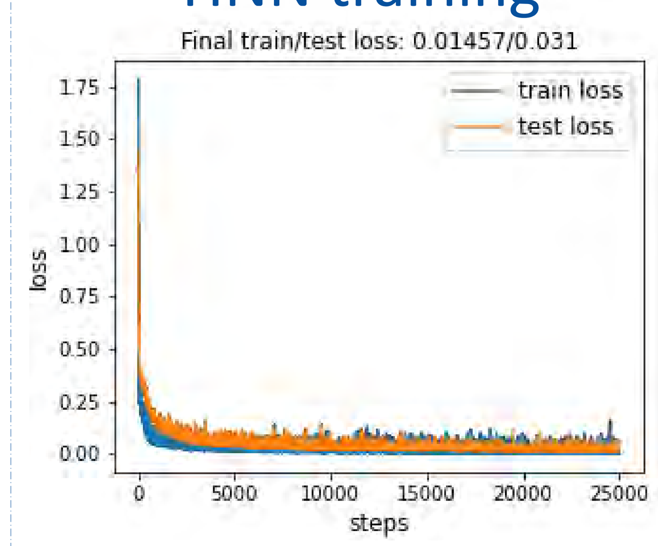
Spherical measure for constrained target distributions



Target distribution: truncated 2D Gaussian



HNN training



Sample quality: cumulative density function (CDF)

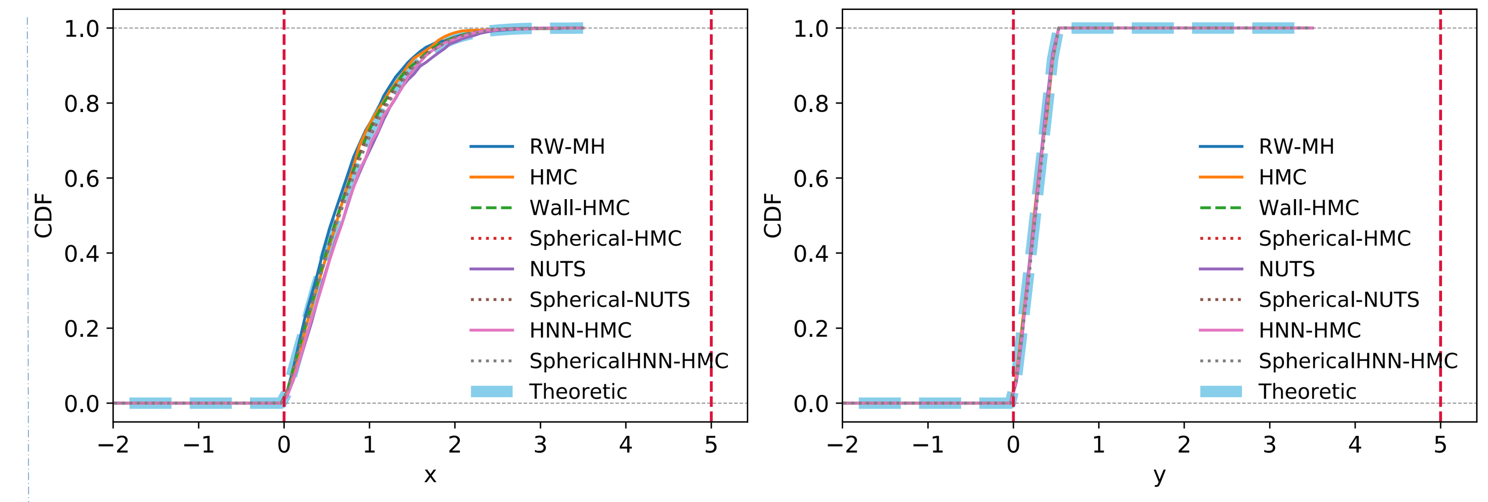
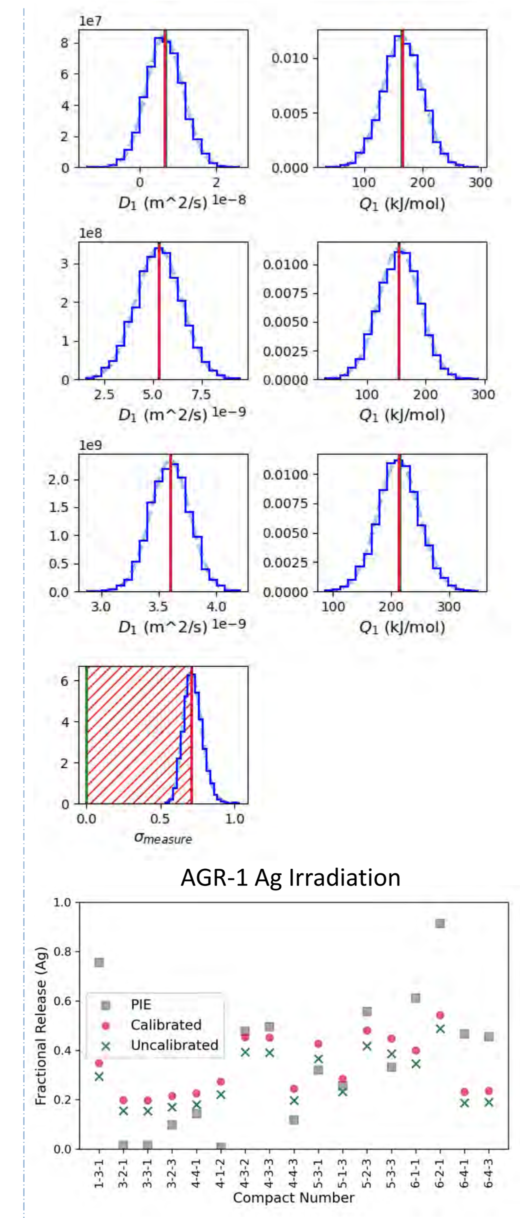


Table 1. Sampling efficiency tested on 2D truncated Gaussian

	Algorithm	Min ESS	Max ESS	Accept Rate	Dimension
Metropolis-Hastings	RWM (discard)	12.64	45.56	0.930	2
Hamiltonian Monte Carlo (HMC)	HMC (discard)	523.56	873.00	0.101	2
	Wall HMC	2715	8293	0.981	2
	Spherical HMC	3079	6692	0.944	2
Nu U-turn Sampler (NUTS)	NUTS (discard)	398.90	931.26	0.214	2
	Spherical NUTS	4543	4700	/	2
Hamiltonian Neural Network (HNN)	HNN (discard)	989	989	0.099	2
	Spherical HNN	5744	7271	0.933	2

*ESS: Effective Sample Size

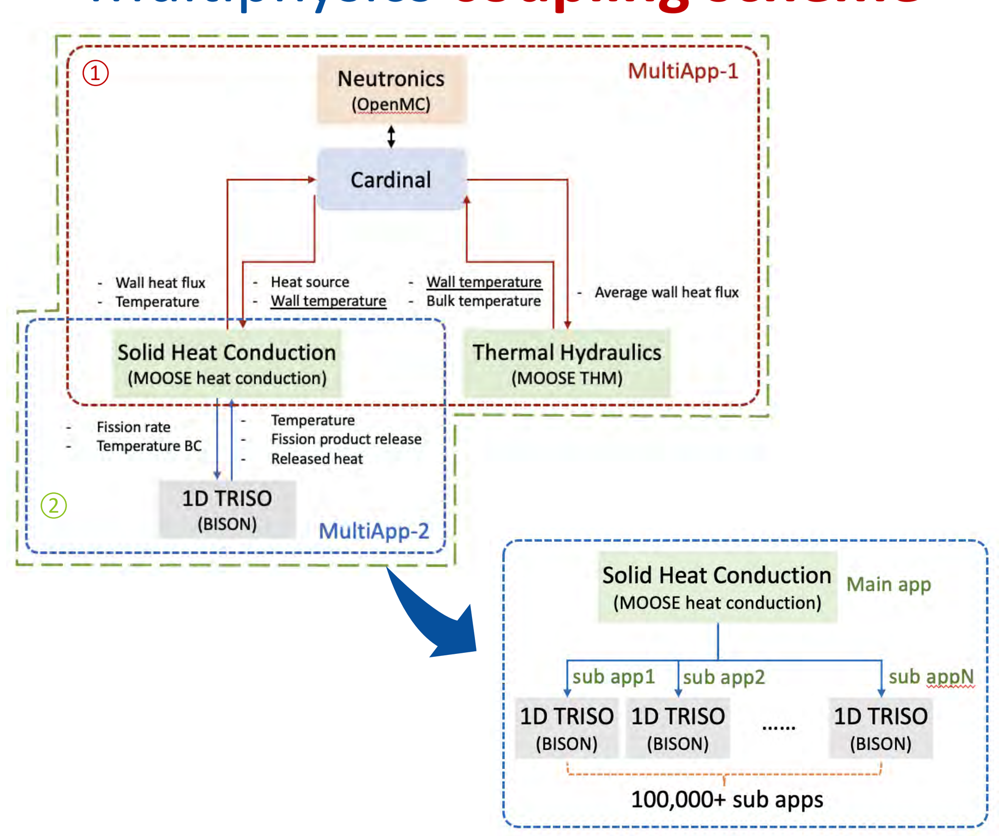
Application: TRISO in AGR-1



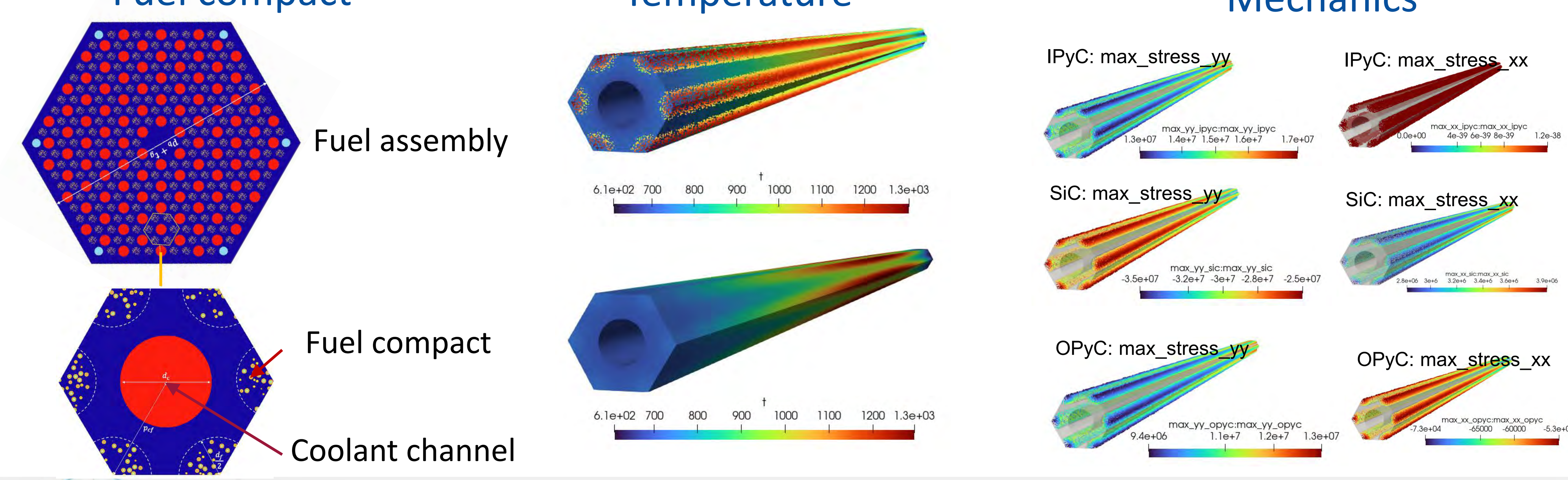
Multiphysics Coupling: TRISO fuel compact in HTGR

- Integrate high-fidelity fuel performance modeling (Bison) into the multiphysics simulation under the MOOSE framework.
- Allows for high-fidelity simulation of fuel mechanics, failure risks and fission product transportation for steady state and long-term transient.

Multiphysics coupling scheme



Fuel compact in a High Temperature Gas-cooled Reactor (HTGR)



Project Number: 22P1066-005FP

LRS Number: INL/EXP-23-74268

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory