INL/MIS-22-69318-Revision-0



# August Nuclear Science & Technology Highlights

August 2022

Addison MArie Arave, Tiffany M Adams

Changing the World's Energy Future

Idaho National Laboratory

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**Addison MArie Arave, Tiffany M Adams**

**August 2022**

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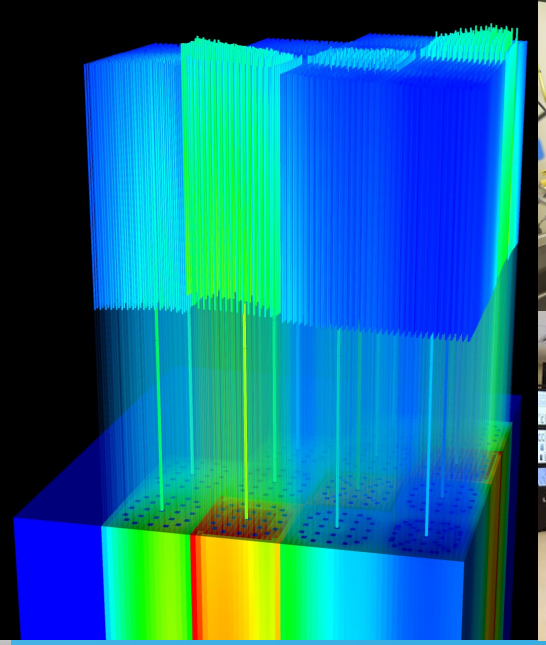


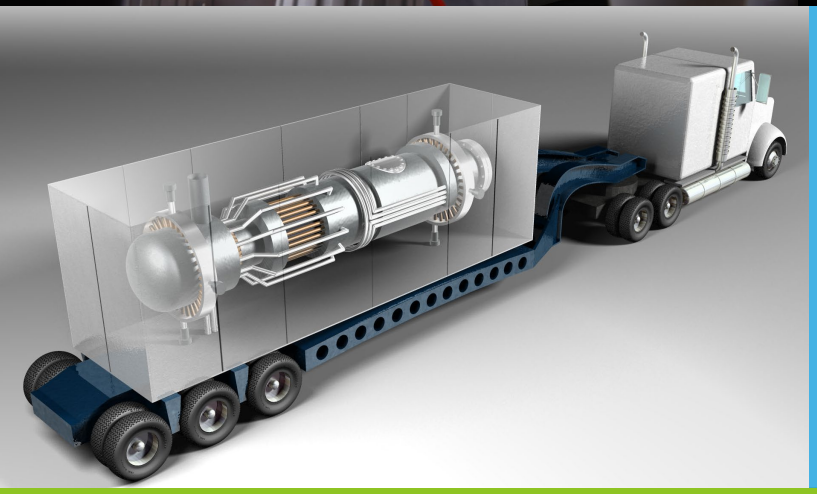

# Nuclear Science & Technology

## August 2022 Highlights

Idaho National Laboratory

# Youssef Shatilla Elected Vice-Chair/Chair-Elect for the Idaho Section of the American Nuclear Society

- ***In May of this year, Youssef Shatilla was elected to the position of vice chair/chair-elect of the Idaho Section of the American Nuclear Society (IANS)***
  - Shatilla is a department manager within the Nuclear Science & Technology (NS&T) directorate at Idaho National Laboratory (INL).
  - Shatilla's first year of service as vice chair of IANS commenced in July.
  - He will serve as chair of IANS beginning in July 2023.
- ***IANS membership information, historical background, and future meeting opportunities are available at the following website:*** https://www.ansidaho.org/home

*Youssef A. Shatilla, manager of the Reactor Physics Methods and Analysis Department at INL and vice chair/chair-elect IANS.*

REACTOR SYSTEMS DESIGN & ANALYSIS | REACTOR PHYSICS METHODS & DEVELOPMENT
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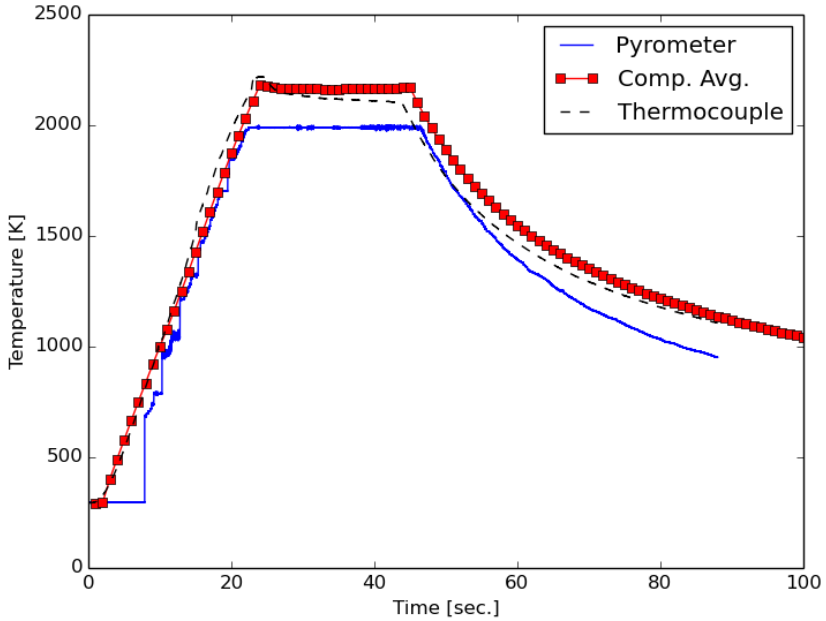
*Space Nuclear Propulsion Project*

# Thermal Modeling and Analysis of the SIRIUS-2 Experiment

- The Scientific International Research in Unique Terrestrial Station (SIRIUS) experiments are being performed to study the nuclear thermal propulsion (NTP) fuel performance subjected to power ramp rates that represent an NTP system startup (i.e., extreme temperatures of ~2200 K).
- This paper presents the status of thermal modeling of a SIRIUS-2 fuel specimen undergoing transient testing in the Transient Reactor Test (TREAT) Facility.
- Simulations were performed using:
  - *Temperature data of the target specimen provided through thermocouples and a pyrometer*
  - *A finite element model of the NTP fuel sample and the local surrounding components*
  - *Precomputed coupling factors and gap heat transfer models in Multiphysics Object Oriented Simulation Environment (MOOSE)*
- The simulated fuel temperatures are compared to the measurements. The comparison validates use of Griffin to simulate NTP engine designs as well as validating the BISON ceramic and metal fuel thermal properties.




Specimen temperature readings from pyrometer and thermocouple instrumentation, with the computed average (Comp. Avg.) specimen temperature for the Griffin simulation. The pyrometer registers the temperature of the top surface, while the thermocouple is placed near the axial center.

**Title**: Thermal Modeling and Analysis of the SIRIUS-2 Experiment
**Authors**: Frederick N. Gleicher, Sebastian Schunert, Ishita Trivedi, and Mark D. DeHart
**Journal**: Transactions of the American Nuclear Society, 2022 Winter Meeting, Phoenix AZ, Nov 2022

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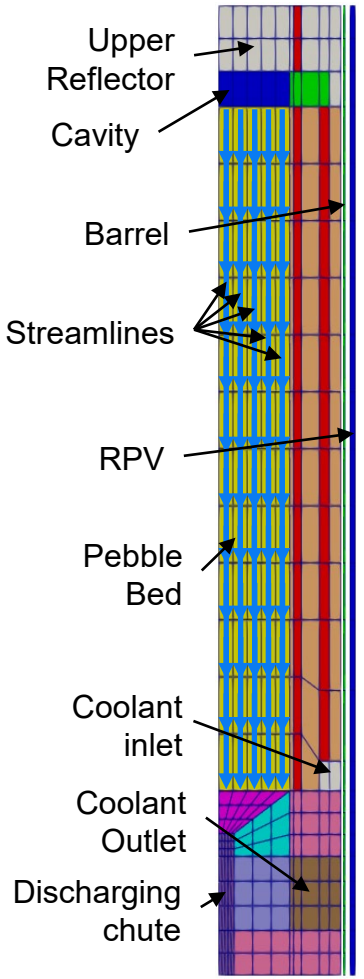
Research Highlight

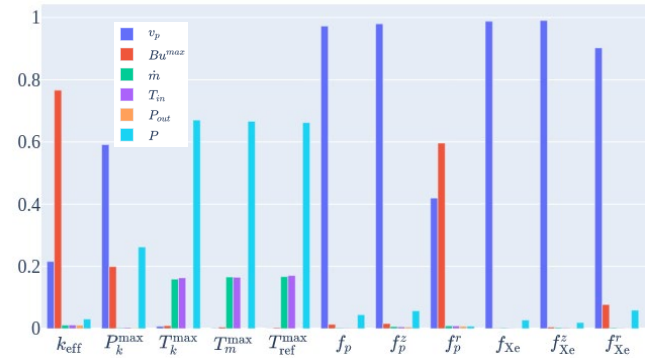
*DOE-NE Advanced Reactor Technologies*

# Initial Study in Reduced Order Model Generation of Pebble-Bed High-Temperature Gas Reactors

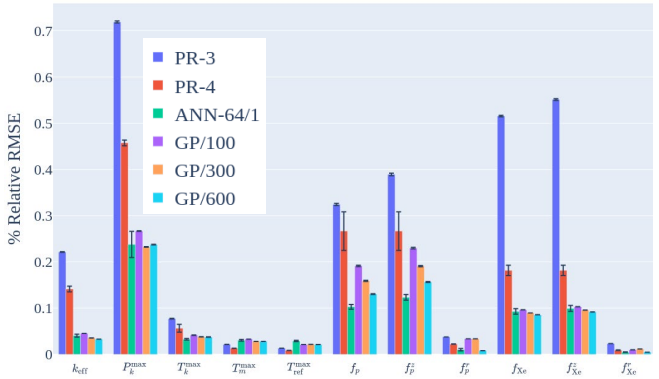
- This project aims at developing a workflow to generate fast-evaluating surrogates of pebble-bed high-temperature gas-cooled reactor models for the purposes of design optimization.
- The project utilizes a multiphysics equilibrium-core Blue-Comprehensive Reactor Analysis Bundle (BlueCRAB) model coupling four physics: neutronics (Griffin), streamline depletion (Griffin), porous flow thermal hydraulics (Pronghorn), and pebble-tristructural isotropic (TRISO) kernel heat conduction (BISON).
- The initial study identified relevant design parameters and quantities of interest (QoIs), performed sensitivity study to gain insight on which parameters affect which QoIs more, and explored and characterized reduced order model methodologies.
  - Stochastic analysis and Reduced Order Model (ROM) study used stochastic tools module MOOSE, which allows researchers to create precise digital models across multiple scales, materials, and research areas
  - Found thermal hydraulics parameters and QoIs have relatively minor effect on simulation results
  - Using cross-validation techniques, the polynomial regression, Gaussian process, and artificial neural network capabilities in the module were analyzed
- Future projects to include building a transient, running-in model, include more design parameters, and utilize surrogates for optimization.




Pebble-Bed High-Temperature Gas Reactor (HTGR) Model




Sensitivity Analysis




Reduced Order Model Study

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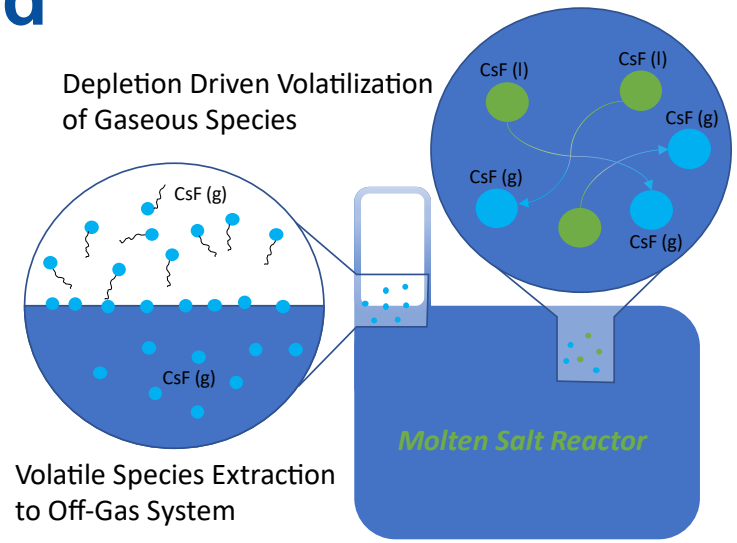
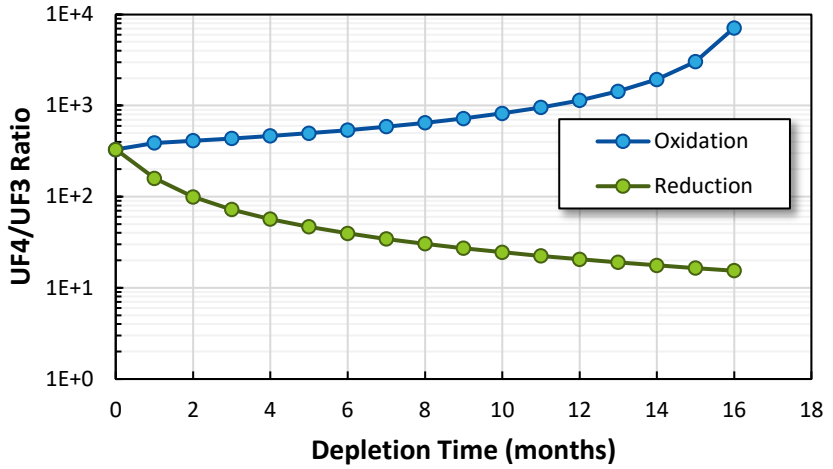
Research Highlight

*DOE-NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program; Molten Salt Reactor campaign*

# New Species Tracking Capability Implemented in Griffin for Molten-Salt Reactor Analysis

- Accurate fuel depletion calculations in molten-salt reactors (MSR) are fundamental to guarantee reactor operability, plan safeguards, and evaluate the radiologic impact of severe accidents.
- In MSRs, depletion calculations simultaneously involve fuel burnup, extraction of gaseous/precipitating species, and online processing.
- A **new capability has been implemented within Griffin** to enable multi-region depletion analysis.
- A **new coupling methodology between Griffin and Thermochimica has been developed**, which enables chemical-informed species depletion analysis.
- The capability was benchmarked and showed good agreement with the Serpent Monte Carlo code, with results to be presented at the 2022 American Nuclear Society (ANS) Winter Meeting.
- INL researchers Olin Calvin, Samuel Walker, Mauricio Tano, Yaqi Wang, and Abdalla Abou-Jaoude worked in collaboration with Sandia National Laboratories (SNL).



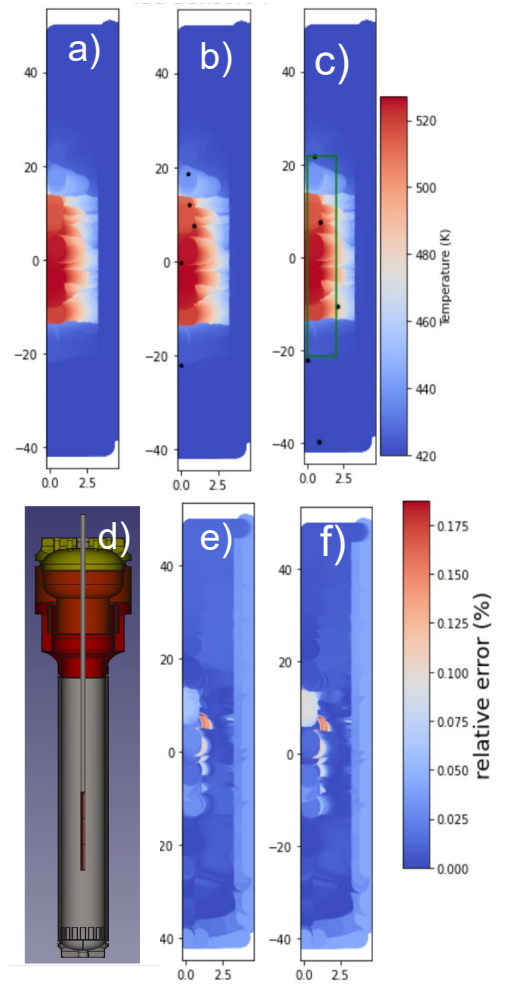

*Evolution of the UF4/UF3 ratio with depletion based on which species is extracted from the salt*

FOR ADDITIONAL INFORMATION: Abdalla.AbouJaoude@inl.gov; Samuel.Walker@inl.gov; Olin.Calvin@inl.gov; Mauricio.TanoRetamales@inl.gov

*Laboratory-Directed Research and Development*

# New Algorithm Developed to Identify Optimal Temperature Sensor Placement in Irradiation Experiment System

- Digital twinning is largely dependent on identifying the minimal set of optimally located sensors needed to replicate the temperature profile.
- An algorithm was developed to incorporate spatial/physical constraints while optimizing sensor placement to predict temperature.
- The algorithm was applied to the Opti-TWIST (Optimal Transient Water Irradiation System) prototype.
- Temperature predictions from computational fluid dynamics (CFD) simulations with StarCCM+ provide training data for the algorithms to reconstruct the temperature profile.
- The max relative errors between CFD and the reconstructed temperature profiles are less than 0.2% for both unconstrained and constrained cases.
- This new capability allows for confidence in designing new experiments and identifying optimal sensor location for accurate temperature prediction.




*a) Temperature prediction from CFD simulations, b)Temperature prediction from five optimized sensor locations, sensors are black dots, c)Temperature prediction from five location-constrained sensors (constrained location within green box), d) Drawing of Opti-Twist showing location of heating element on side, e) Relative error of temperature prediction between CFD and optimized sensor location, f) Relative error of temperature prediction between CFD and location-constrained sensor*

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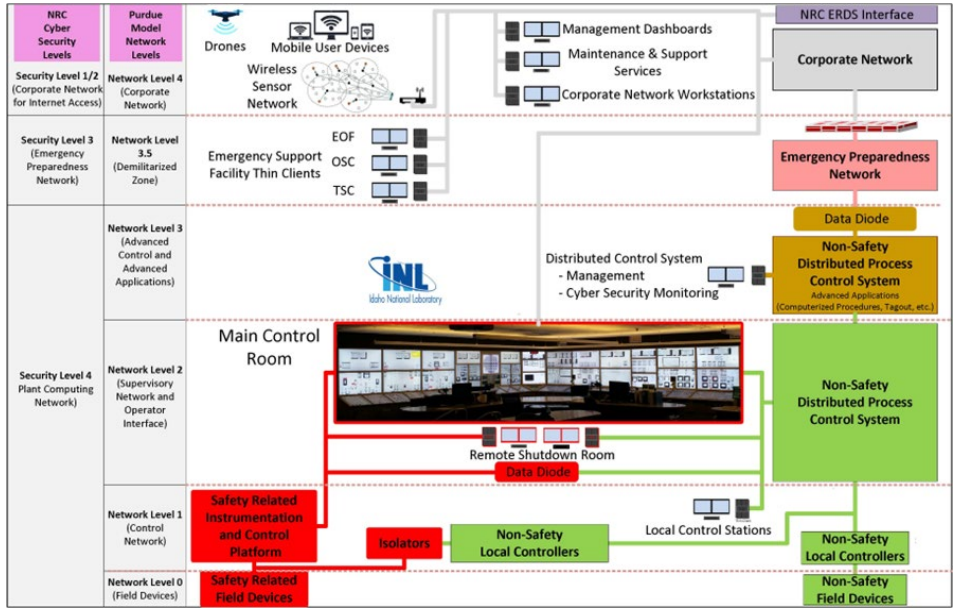
*DOE-NE Light Water Reactor Sustainability Program*

# Plant Modernization Digital Infrastructure Research Highlighted at Industry-Wide Technical Meetings

- On July 17, 2022, Paul Hunton presented Digital Infrastructure Migration Framework Research to the Pressurized Water Reactor Owners Group in Pittsburgh, Pennsylvania.
- On July 19, 2022, Robert England made a similar presentation to at the 48th Annual Nuclear Information Technology Strategic Leadership Conference in Baltimore, Maryland.
- These presentations highlighted the strategic direction to maximize digital modernization benefits. The benefits include reducing plant total cost of ownership and protecting intellectual property investments for 80+ year plant life.




*Simplified digital infrastructure diagram from INL/EXT-21-64590*

**Title**: Digital Infrastructure Migration Framework Report
**Authors**: Paul Joseph Hunton, Robert T. England
**Link**: www.osti.gov/biblio/1822876

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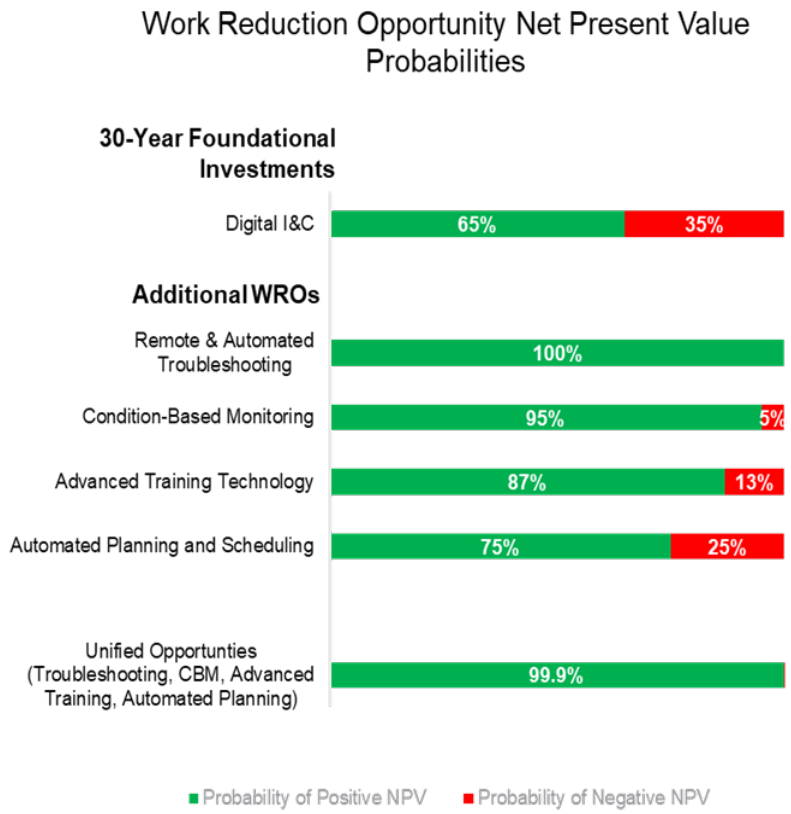
LWRS

*DOE-NE Light Water Reactor Sustainability Program*

# Economic Analysis Confirms Critical Plant Innovation and Upgrades to Reduce Operation and Maintenance Costs for Nuclear Plants

- A business case study was conducted with industry partners that resulted in projections of a positive business case for five innovation areas:
  - Digital Instrumentation and Controls (I&C) for Control and Safety Systems
  - Condition Based Maintenance
  - Remote Plant and Automated Troubleshooting
  - Digital Training Transformation
  - Automated Planning and Scheduling
- Research was conducted in collaboration with five leading utility partners, ScottMadden, and Electric Power Research Institute (EPRI).
- The study collected actual plant data and combined it with the results of previous studies and analyzed using Monte Carlo techniques.
- Each innovation area analyzed separately results in a favorable business case, but when all taken together, results in a 99.9% chance of a positive business case.

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LWRS

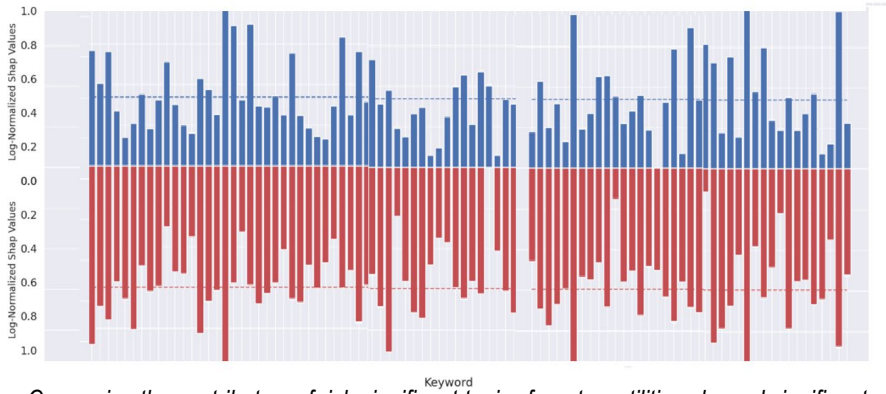
Research Highlight

*DOE-NE Light Water Reactor Sustainability Program*

# A New Approach to Risk-informing Trends Developed to Track Nuclear Power Plants Performance

- The Light Water Reactor Sustainability (LWRS) Program created a new approach to automatically label events in nuclear power plants with themes or topics that can be counted and trended to track plant performance.
- This replaces the current manual and subjective process of performance tracking.
- The approach uses machine learning and a game-theory method to identify the main type of issues or topics that are risk-significant and likely to cause a safety-related event in the plant.
- The generated list of topics was developed using data from 39 reactors and will be shared with the industry to risk-inform the performance tracking process.


*An improving trend of a certain theme of events can be properly prioritized if it is risk-informed.*




*Comparing the contributors of risk-significant topics from two utilities showed significant similarity, indicating topics could be scalable across the industry.*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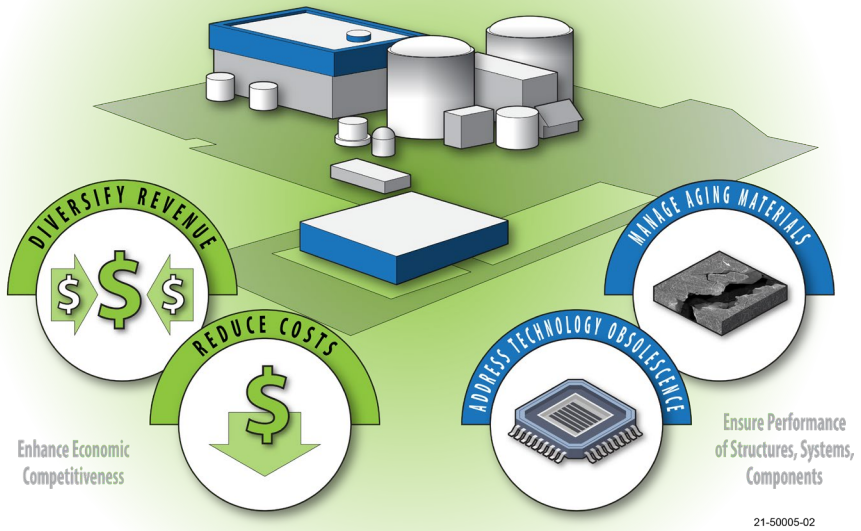
LWRS

IDAHO NATIONAL LABORATORY

*DOE-NE Light Water Reactor Sustainability Program*

# Stakeholder Event Demonstrates Industry Support of LWRS Program

- A virtual kickoff session provided LWRS Program stakeholders an overview of the Plant Modernization Pathway followed the sessions in:
  - Integrated Operations for Nuclear
  - Digital Infrastructure
  - Human & Technology Integration
  - Data Analytics for Nuclear Plant Innovation
- Pathway research projects were presented from our industry collaborators viewpoint. Industry collaborators include Constellation, Xcel Energy, Dominion Energy, Southern Nuclear, PWR Owner's Group, Luminant, Utilities Service Alliance, ScottMadden, and Sargent & Lundy.
- Strong industry support was shown by having over 550 attendees across the five sessions.




*Five Virtual Sessions*
*August 16–18, 2022*

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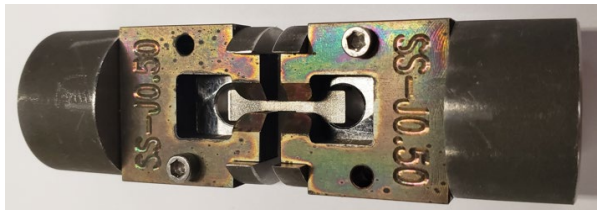
*National Reactor Innovation Center*

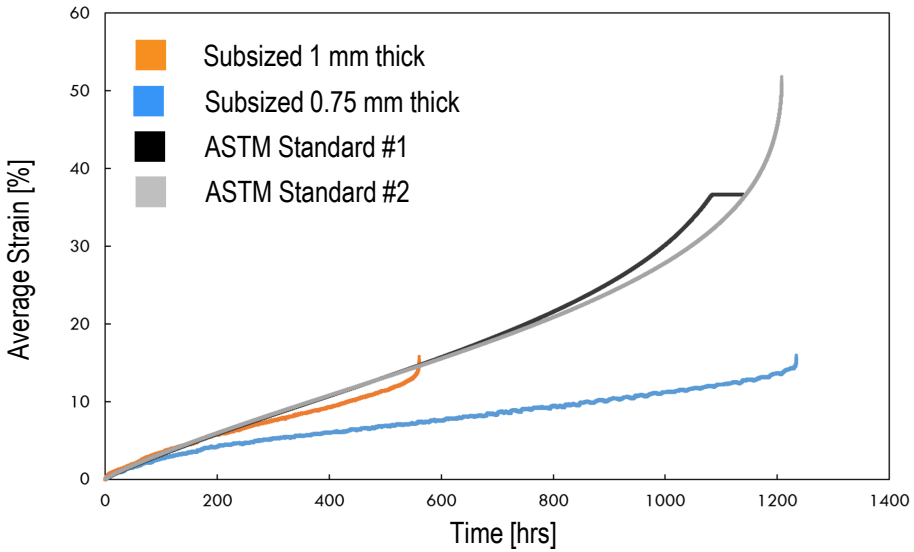
# In-Cell Thermal Creep Frames Fabricated for High-Temperature Mechanical Testing

- Several advanced reactor concepts have potential core temperatures greater than 500°C, requiring long-term thermal mechanical performance data to qualify structural materials.
- Modular creep frames were fabricated to fit within existing hot-cell facilities at the Fuels and Applied Science Building (FASB).
- Special clevises were developed to hold flat tensile specimens for high-temperature creep testing.
- Multiple specimens were tested on existing creep frames at INL and compared to significantly larger sample tests for Alloy 617.
- Calibration and baseline testing of creep frames (performed out-of-cell) is underway.




Clevis for holding subsized samples during high-temperature creep testing.

Fabricated in-cell creep frame.




Comparison of creep rupture time between subsized and American Society for Testing and Materials (ASTM) standard samples.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*Gateway for Accelerated Innovation in Nuclear*

# GAIN and NRIC Partner to Host Forum Highlighting States Hosting Advanced Nuclear Projects

- The Gateway for Accelerated Innovation in Nuclear (GAIN) and the National Reactor Innovation Center (NRIC) joined the United States (U.S.) Department of Energy's Office of Nuclear Energy (DOE-NE) at the Energy Communities Alliance (ECA) Forum in Salt Lake City, Utah, Aug. 3–5 .
- The Forum, "Hosting New Nuclear Development," featured case studies from advanced nuclear energy reactor sites.
- Katy Huff, assistant secretary for Nuclear Energy at DOE, highlighted DOE's efforts to support advanced nuclear projects, including communities transitioning to clean energy.
- NRIC director Ashley Finan and Stakeholder Engagement (SE) team member Wendolyn Holland acted as panel moderators at the event.
- During this event, the communities declared their suitability for hosting advanced reactors, effectively uniting the nuclear energy and environmental management mission spaces, a milestone for ECA.


*GAIN participated in the ECA forum by hosting a booth and moderating a discussion on Oak Ridge, TN.*

*GAIN Director Christine King & NRIC Director Dr. Ashley Finan collaborating in person at the Marriott, University of Utah for the ECA Conference, August 2022.*

GATEWAY FOR ACCELERATED INNOVATION IN NUCLEAR/NATIONAL REACTOR INNOVATION CENTER
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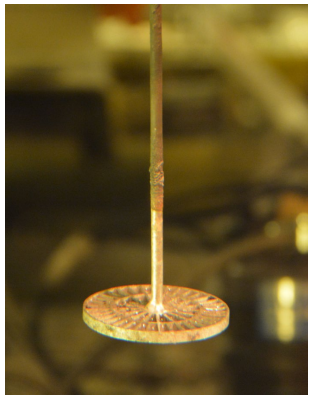
*DOE-NE Joint Fuel Cycle Studies*

# INL Demonstrates First Ever Iridium Anode at Engineering Scale for Deployment in Extreme Environments

- Traditional platinum anodes have been used in the pyrochemical treatment of used oxide nuclear fuels, but they are highly prone to extensive degradation.
- An alternative to platinum electrodes has been the focus of studies to provide reliable and stable electrodes for the reprocessing of used oxide fuels.
- Research within DOE's Joint Fuel Cycle Studies program and a collaborative effort between U.S. national laboratories and international partners resulted in the development of a monolithic iridium anode as a robust alternative to platinum.

- The successful outcomes of this development effort have resulted in the following deliverables:
  - A U.S. Patent
  - A peer-reviewed publication
  - An exclusive licensing partner: Caltrode Inc. (Tuscan, Arizona)
  - A 2022 R&D 100 award finalist

**(A)**



**(B)**

*Robust iridium anode (A) and degraded platinum anode (B)*

PYROCHEMISTRY AND MOLTEN SALT SYSTEMS DEPARTMENT
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*DOE Office of Science Basic Energy Sciences*

# Clean Energy Technology and Manufacturing Program Receives Funding to Investigate the Radiation-Induced Fate of Iodine in Molten Salts

- The chemical behavior of the radioactive fission product, iodine, within advanced reactor fuels is complex. Understanding its behavior is of essential importance to the operation of these reactors.
- The **INL Center for Radiation Chemistry Research**, in collaboration with **Brookhaven National Laboratory** (BNL), was awarded $3.8M over 3 years in response to the *Chemical and Materials Sciences to Advance Clean Energy Technologies and Low-Carbon Manufacturing* initiative supported by the DOE Office of Science Basic Energy Sciences.
- The goal of this program is to "*Understand and Predict Radiation-Induced Iodine Speciation, Chemistry, and Transport in High-Temperature Molten Salts*" over multiple time and distance arrangements.
- These studies will leverage state-of-the-art irradiation facilities, multimodal characterization techniques, and high-performance computing at both laboratories.

*Program principal investigators (PIs) from top left to bottom right:* ***Gregory P. Horne*** *(director, INL),* ***Ruchi Gakhar*** *(INL),* ***Simerjeet Gill*** *(BNL),* ***Jacy K. Conrad*** *(INL), and* ***Trishelle M. Copeland-Johnson*** *(INL).*

NUCLEAR SCIENCE & TECHNOLOGY | AQUEOUS SEPARATIONS & RADIOCHEMIISTRY
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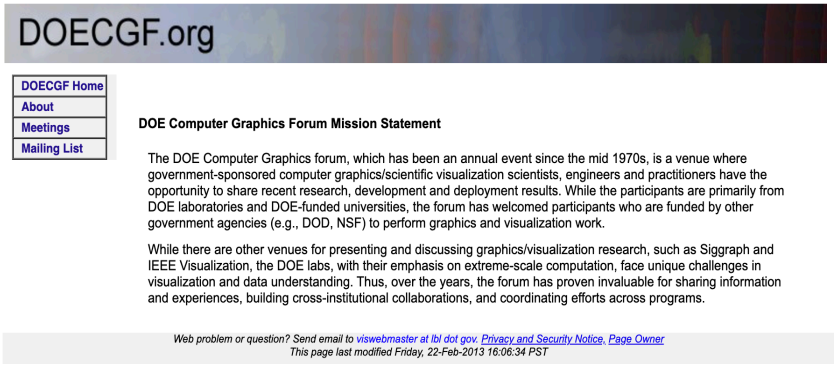
# INL Visualization Capabilities Presented to the Department of Energy Computer Graphics Forum

- The Department of Energy Computer Graphics Forum has been around for decades and held its first annual meeting in the 1970s.
- The community is made up of government-sponsored computer graphics/scientific visualization scientists, engineers, and practitioners.
- The impetus of the forum is to allow DOE labs to connect and discuss the unique challenges of visualization for extreme scale computation.
- Nathan Woods represented INL at the 2022 annual conference, held virtually August 30–September 1.
- A site report highlighting current INL visualization capabilities, including equipment and skillsets, was presented. Highlights touched on augmented, virtual, and mixed reality equipment and capabilities, High Performance Computing Graphics Processing Unit specifications, and Scientific Visualization capabilities.




*DOE-CGF Organization Web Page*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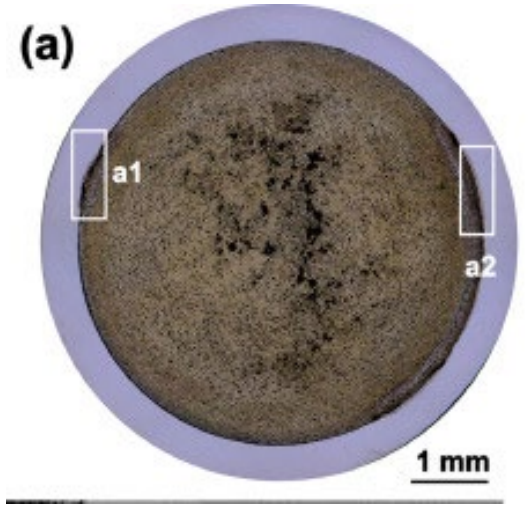
Research Highlight

*DOE-NE Nuclear Science User Facilities*

# Characterization of Fuel Cladding Interaction Contributes to Next Generation Reactor Development

- Interaction between nuclear fuel and the cladding surrounding it, or fuel cladding chemical interaction (FCCI), is the primary cause of cladding wastage, weakening mechanical integrity of the cladding, and placing fuel and cladding at risk.
- Studies of the effect of FCCI on mechanical properties are difficult due to the limited reaction volume.
- Researchers from INL and Oak Ridge National Laboratory combined advanced electron microscopy characterization and small-scale mechanical testing techniques to investigate the microscale mechanical properties of the FCCI region of HT9-clad U-based metallic fuel.
- Results show significant hardening and embrittlement in the FCCI region.
- This data is of particular significance due to the high cladding temperature achieved during irradiation, enabling the continued development of multiscale mechanical behavior models of HT9 cladding for next generation reactors.
- Nuclear Science User Facilities (NSUF) provided access to the Advanced Test Reactor at INL.




*A microscopic image of the irradiated fuel with HT9 cladding.*

**Title**: Small-scale mechanical testing and characterization of fuel cladding chemical interaction between HT9 cladding and advanced U-based metallic fuel alloy
**Authors**: Yachun Wang, David M. Frazer, Fabiola Cappia, Fei Teng, Daniel J. Murray, Tiankai Yao, Colin D. Judge, Luca Capriottia (Idaho National Laboratory), Jason M. Harp (Oak Ridge National Laboratory)
**Journal:** Journal of Nuclear Materials
**Link**: doi.org/j.jnucmat.2022.153754

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NSUF Nuclear Science User Facilities

IDAHO NATIONAL LABORATORY

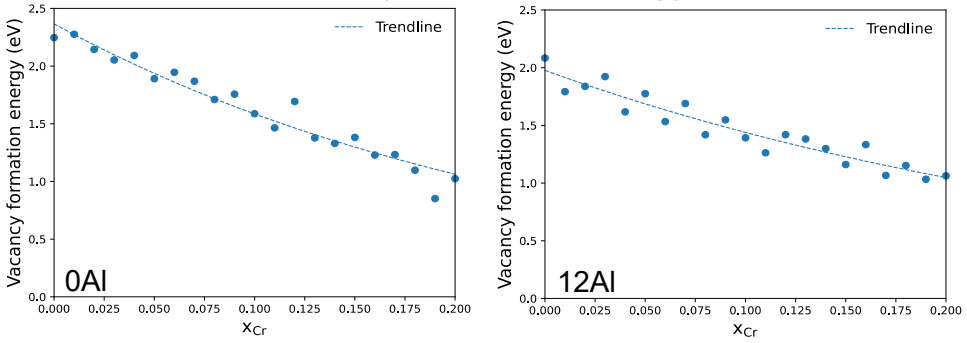
Research Highlight

*DOE-NE Advanced Materials and Manufacturing Technologies (AMMT) program*

# Machine Learning Pipeline to Predict Defect Behavior and Phase Stability in Metallic Alloy Systems

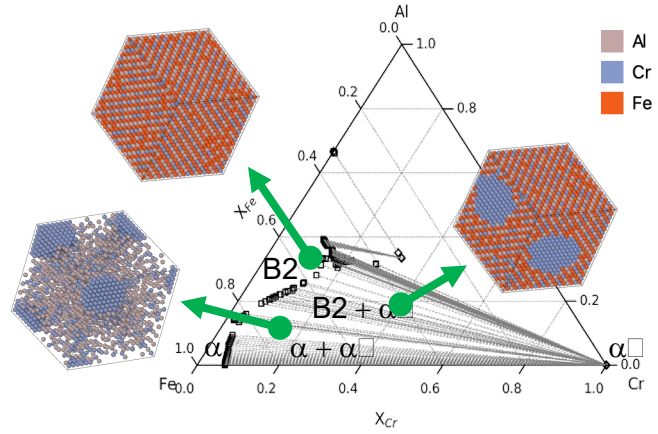
- The interaction between solute elements and defects is critical to understand the defect and thermo-kinetic properties of metallic alloys for nuclear energy applications.
- The science underlying the solute-defect interactions is of significant challenge due to the complexities involving a wide possibility of atomic configurations and environments.
- INL researchers have successfully employed a pipeline of machine learning regression and cluster approaches to predict the energy of any atomic configuration in FeCrAlMo system from *ab initio* data.
- The predicted properties include the vacancy formation energies, mixing enthalpy, phase diagrams, as well as phase transformations involving clustering and ordering.
- This generic pipeline demonstrates important applications to study solute and irradiation effects in multicomponent nuclear materials, which will benefit both multiscale modeling and qualification of new alloys.

Vacancy formation energy




Multicomponent phase diagram

600 K




NUCLEAR FUELS & MATERIALS | COMPUTATIONAL MECHANICS & MATERIALS
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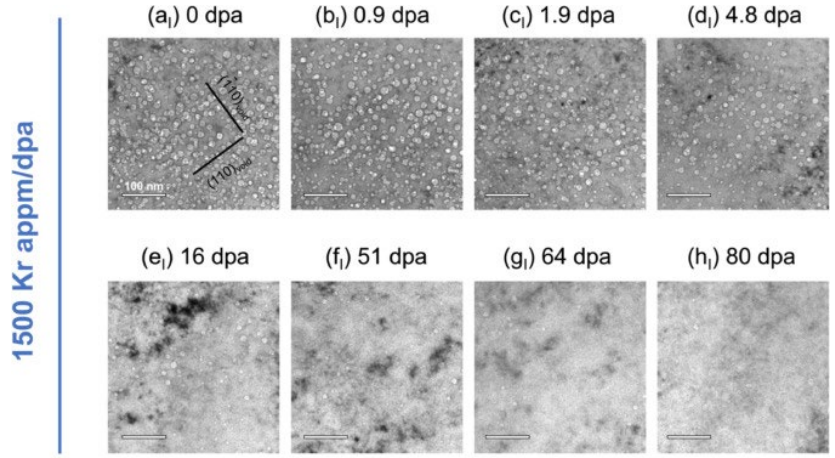
Research Highlight

*DOE-NE Nuclear Science User Facilities, DOE Office of Basic Energy Science, Materials Sciences and Engineering Division*

# Research Provides Understanding of Microstructural Evolution, Aids in Developing Advanced Materials

- While voids are often considered detrimental defects, the patterning of nanoscale voids provides a highly efficient mechanism for gas storage in irradiated materials.
- How these voids degrade under irradiation is unclear and understanding the degradation mechanisms is essential to designing radiation damage tolerant materials.
- Material specimens were subjected to *in situ* ion irradiation and studied using a transmission electron microscope. Under irradiation, the void shrinkage rate is rapid initially but decreases as the applied dose increases.
- Transforming irradiation damage from a liability to an asset is a paradigm shift that could help develop advanced materials with exceptional properties.
- Researchers can employ this knowledge to develop advanced materials that utilize irradiation to improve performance.



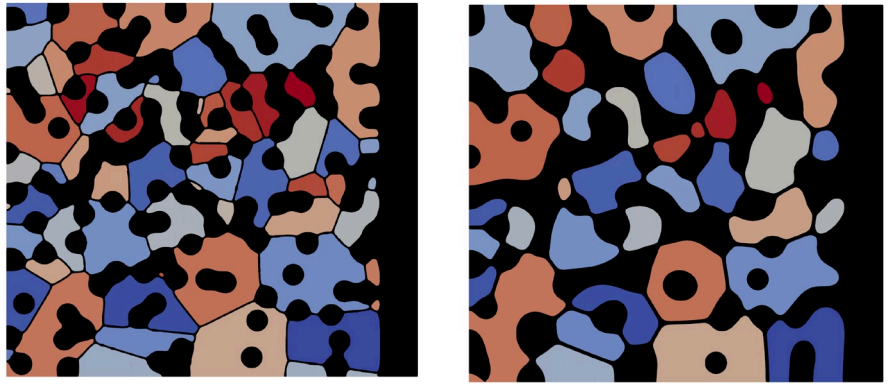

*TEM micrographs showing the decrease in void size and density as the dose increases.*

**Title**: Unveiling the interaction of nanopatterned void superlattices with irradiation cascades
**Authors**: Cheng Sun, Chao Jiang, Yifeng Che, Andrea M. Jokisaari, Larry K. Aagesen, Jian Gan (Idaho National Laboratory), Wei-Ying Chen (Argonne National Laboratory) Yongfeng Zhang (University of Wisconsin, Madison) Lin Shao (Texas A&M University).
**Journal:** Acta Materialia
**Link:**
https://doi.org/10.1016/j.sciencedirect.com/science/article/pii/S1359645422006620

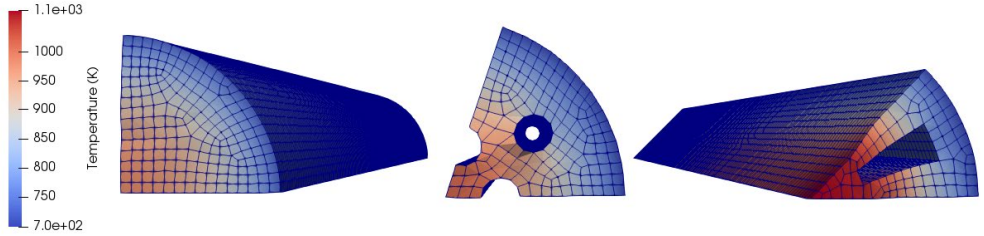
*Advanced Research Projects Agency–Energy*

# Oklo to Use BISON to Design Novel Fuels for Fast Reactors

- INL collaborated with Rensselaer Polytechnic Institute, University of Wisconsin-Madison, Oregon State University, and Oklo to manufacture and evaluate the performance of a novel porous metallic fuel for fast reactors. The objective of this new fuel is to facilitate removal of sodium layer between the fuel and the cladding.
- Advanced manufacturing techniques were used to fabricate surrogate fuels with different level of microscopic pores and macroscopic slots/holes.
- Multiscale modeling approach was used to evaluate the material properties, microstructural evolution, and performance of the new fuel designs in reactor conditions.
- Phase-field modeling was employed to model the densification of the microscopic pores at the mesoscale, which provided the porosity evolution model for the engineering-scale analysis.
- Improvement in terms of swelling and heat transfer at the engineering scale was evaluated using BISON, a nuclear fuel performance code.
- It was concluded that microscopic inter-connected pores provide the optimal performance.
- Updated codes and input files are made available to Oklo, which will be used for their continued fuel design.



*Mesoscale modeling provide evolution of microscopic pores in reactor conditions.*




*BISON evaluates performance of various surrogate fuel designs with macroscopic holes/slots.*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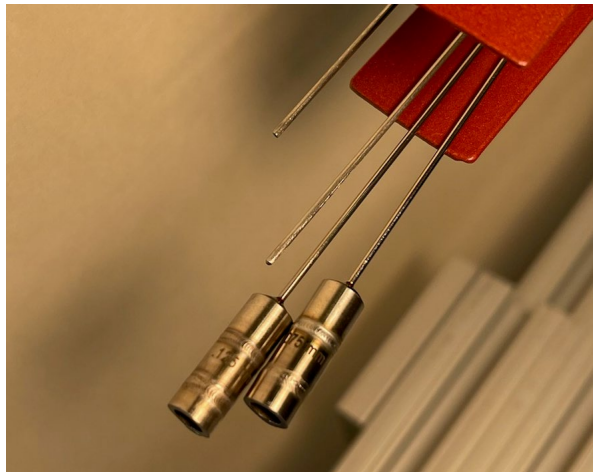
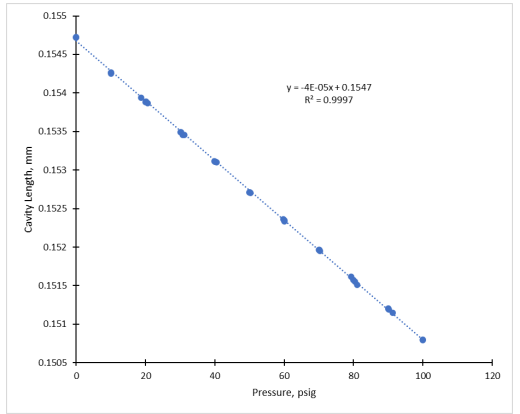
*DOE-NE Advanced Sensors and Instrumentation (ASI) program*

# Measurement Science Laboratory Developed Fiber Optic Pressure Sensors Deployed in TREAT Experiment HERA Series

- New fiber optic-based pressure sensor designed and developed by the Measurement Science Laboratory was deployed for the first time in the High-burnup Experiments in Reactivity Initiated Accidents (HERA) Transient Reactor Test (TREAT) experiment.
- HERA is a Joint Experimental Program designed to understand light water reactor fuel performance under reactivity-initiated accidents.
- Measuring pressure with commercially available products in the nuclear research environments is challenging due to the combination of physical size, radiation, temperature, and gas environments.
- This new compact pressure sensor saves space but can also withstand high radiation fields, high temperatures, and can work in water and gaseous environments.
- This design will be deployed in other TREAT experiments requiring a robust, fast response pressure sensor including the TWIST for TREAT.

*(right) Fiber Optic Pressure Sensors Protected with Stainless Steel for Deployment within HERA-Calibration experiment Capsule.*






*(left) Example of a calibration curve of a pressure sensor fabricated for use in HERA.*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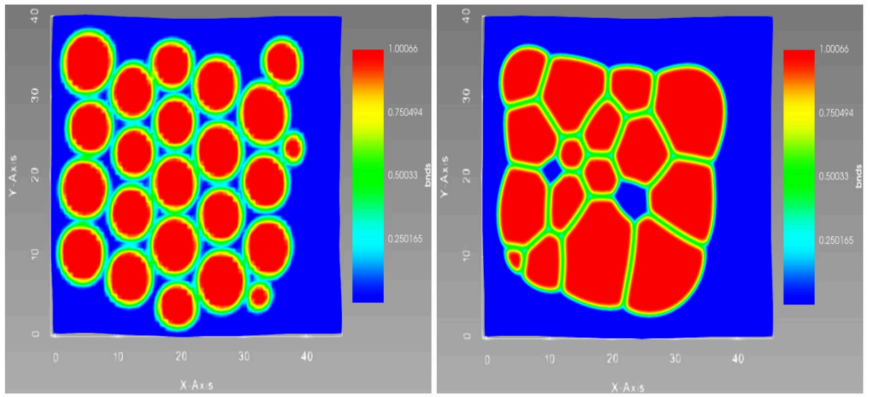
*National Aeronautics and Space Administration*

# INL Participates in NASA Collaboration, Utilizes Advanced Manufacturing Modeling System

- The National Aeronautics and Space Administration (NASA) has become the first external user for the MOOSE Application Library for Advanced Manufacturing UTilitiEs (MALAMUTE).
- MALAMUTE builds on the MOOSE, which allows researchers to create precise digital models across multiple scales, materials, and research areas.
- A Government Use Agreement is established between NASA Ames Research Center and INL for use of MALAMUTE.
- NASA will be using MOOSE and MALAMUTE for their In-space Manufacturing Program, regarding modeling and simulation for advanced manufacturing techniques.
- Recent collaborative publication demonstrates microstructural evolution during sintering at zero gravity using MOOSE-based sintering model.



*Microstructural evolution of particles during sintering at zero gravity, simulated using MOOSE-based phase-field model for sintering.*

**Title:** Multiscale Modeling of the Bound Metal Deposition Manufacturing of Ti6Al4V
**Authors:** Dmitry G Luchinsky (LU, KBR), Vasyl Hafiychuck (KBR), Kevin R Wheeler (NASA), Sudipta Biswas (INL), Christopher E Roberts (NASA), Ian M Hanson (NASA), Tracie J Prater (NASA), Peter VE McClintock (LU)
**Journal: Thermo**
**Link:** https://doi.org/10.3390/thermo2030011

MOOSE

MALAMUTE

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