INL/RPT-22-66427

Nuclear Science User Facilities High Performance Computing

March 2022

FY 2021 Annual Report

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Nuclear Science User Facilities High Performance Computing

FY 2021 Annual Report

EXECUTIVE SUMMARY

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities (NSUF), provides access to supercomputer systems and data storage along with support staff for system management, software installation, cybersecurity, and user support to the broader DOE-NE user community. Users include individuals at universities, industry, and government laboratories, enabling a wide range of research and development and mission-supporting activities. The availability of high-performance computing (HPC) capabilities is a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL staff directly support the mission and objectives of DOE-NE.

In fiscal year (FY) 2021, INL HPC delivered 1 billion core hours in support of modeling and simulation. Requests for INL HPC accounts increased significantly with the launch of the Nuclear Computational Resource Center (NCRC) website and user portal. In addition, improvements and additions were made to the INL HPC web interface, and authentication system, and training was developed for artificial intelligence and machine learning software. In support of digital engineering and digital twin work, HPC resources were integrated with the Deep Lynx data platforms.

During FY-21, INL HPC capabilities were utilized by a diverse set of 795 computing and applied researchers. The majority came from national laboratories (444) with university researchers (as a group), making up the second largest group of users (199), while industry partners accounted for a substantial number of users (152). In addition, INL also supported users from nuclear regulatory agencies, demonstrating our commitment to foster relationships between research and regulatory personnel.

INL HPC capabilities were instrumental enablers for a wide range of research and engineering activities in FY-21, with summaries of a number of these activities presented as user-provided project reports (see Appendices A through E). A large portion of HPC use was geared towards nuclear energy, with numerous computational studies on important topics relevant in nuclear energy. The subset of projects presented in this report give a clear indication of the high value and strong utilization of the INL HPC capabilities supported by DOE-NE. Though most of the projects focus on the challenges facing nuclear energy, the breadth of scope of the investigations supported is a clear indication of the multidisciplinary nature of the INL HPC usage.

CONTENTS

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ACRONYMS

AI	Artificial Intelligence
AIMD	ab initio molecular dynamics
AKMC	Atomic Kinetic Monte Carlo
ALD	Atomic Layer Disposition
ANL	Argonne National Laboratory
ARPA-E	Advanced Research Projects Agency - Energy
ASC	Advanced Scientific Computing
ATF	Accident Tolerant Fuel
ATR	Advanced Test Reactor
bcc	body-centered-cubic
BlueCRAB	Comprehensive Reactor Analysis Bundle
BWR	Boiling-Water Reactor
C3	Collaborative Computing Center
CASL	Consortium for Advanced Simulation of Light Water Reactors
CFD	Computational Fluid Dynamics
CNN	Convolutional Neural Network
CNT	carbon nanotubes
CPU	central processing unit
CSAP	Core Safety Assurance Package
DEM	Discrete Element Modeling
DFT	Density Functional Theory
DNB	Departure from Nucleate Boiling
DOE-NE	Department of Energy Office of Nuclear Energy
EBSD	Electron Backscatter Diffraction
EERE	Office of Energy Efficiency and Renewable Energy
EM	Office of Environmental Management
EXAFS	Extended X-ray Absorption Fine Structure
FCCI	Fuel-cladding Chemical Interface
FCU	Fan Coil Unit
FGR	Fission Gas Release
FPoliAAP	FPoli Agile Application Platform
FPoliDON	test data management
FPoliDOX	document management

FPoliSIM	simulation management
GAIN	Gateway for Accelerated Innovation in Nuclear
HEU	highly enriched uranium
HFIR	High-Flux Isotope Reactor
HPC	High-Performance Computing
HPGe	High-Purity Germanium
HTGR	High-Temperature Gas Reactor
IES	Integrated Energy Systems
IHX	intermediate heat exchanger
INL	Idaho National Laboratory
ISRU	in situ resource utilization
IUC	Idaho University Consortium
KTH	Kungliga Tekniska högskolan (Royal Institute of Technology)
LaRomance	Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations
LDRD	Laboratory Directed Research and Development
LWR	Light-Water Reactor
LWRS	Light Water Reactor Sustainability
MATHAM	Mars Active Tracer High-Resolution Atmospheric Model
MCNP	Monte Carlo N-Particle
MCO	Moisture Carryover
ML	Machine Learning
MOOSE	Multiphysics Object-Oriented Simulation Environment
MPCMIV	multiphysics pellet-cladding mechanical interaction validation
MQM	modified quasichemical
MSTDB	Molten Salt Thermodynamic Database
NCRC	Nuclear Computational Resource Center
NE	Nuclear Energy
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NEGF	nonequilibrium Green's functions
NEUP	Nuclear Energy University Program
NF	nanofiber
NRAD	Neutron Radiography Reactor
NRC	Nuclear Regulatory Commission
NRIC	National Reactor Innovation Center
NRS	North Radiography Station

NSUF	Nuclear Science User Facilities
OS	Office of Science
PBR	Pebble-Bed Reactor
RAVEN	Risk Analysis Virtual ENvironment
RCCS	Reactor Cavity Cooling System
RE	Reactor Engineering
RELAP5	Reactor Excursion and Leak Analysis Program
RIS	Radiation-Induced Segregation
RISE	risk-informed system engineering
RPV	Reactor Pressure Vessel
SQS	Special Quasi-Random
TAPE	Transient Analysis PackagE
TES	Thermal Energy Storage
TREAT	Transient Reactor Test
UIUC	University of Illinois at Urbana-Champaign
VASP	Vienna ab initio Simulation Package
VBMC	Variational Bayesian Monte Carlo
vdW	van der Waals
VERA	Virtual Environment for Reactor Analysis
VTT	Valtion Teknillinen Tutkimuskeskus (Technical Research Centre [of Finland])

1. INTRODUCTION

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities (NSUF), provides access to supercomputer systems and data storage along with support staff for system management, software installation, cybersecurity, and user support to the broader DOE-NE user community. Users include individuals at universities, industry, and government laboratories enabling a wide range of research and development and mission-supporting activities. The availability of high-performance computing (HPC) capabilities is a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL directly support the mission and objectives of DOE-NE.

Due to continuous and rapid transformation developments in the field of scientific computing, INL continues to look for new and innovative ways to expand our computational research capabilities through:

- Investments in scientific computing capacity
- Development and validation of innovative modeling tools
- Expansion of expertise in deep machine learning, artificial intelligence, advanced visualization, and large-scale data processing and analytics.

Fiscal Year (FY) 2021 was one that saw many significant accomplishments associated with HPC at INL. For the first time ever, INL HPC delivered one billion core hours in support of modeling and simulation. This level of compute core hours is challenging to deliver and an important accomplishment. Requests for INL HPC accounts increased significantly with the launch of the Nuclear Computational Resource Center (NCRC) website and portal. Also, improvements and additions were made to the INL HPC web interface, and authentication system, and training was developed for artificial intelligence and machine learning software. In support of digital engineering and digital twin work, HPC resources were integrated with the Deep Lynx data platforms.

In FY-21, INL HPC systems delivered more than 1,026 million core hours of compute time. This is an increase of 396 million core hours from the previous year, largely due to the 5.6 petaFLOPS Sawtooth system, which was deployed in FY-20.

A total of 129 user-supplied HPC usage summaries are included as appendices to this report. These summaries are submitted as part of a newly implemented process for user account renewals. While the breadth and depth of the user reports vary, they serve to document and demonstrate the types of work being conducted on INL HPC resources. The vast majority support nuclear energy research and development.

The following discussion expands on these topics and serves to demonstrate INL's commitment to expanding its HPC capabilities and resources.

2. MAJOR ACCOMPLISHMENTS

INL recognizes the importance of HPC in all areas of science and, as such, is strongly committed to growing its capabilities and enhancing its ability to support DOE-NE's computational science programs. Major accomplishments for INL HPC in FY-21 are listed below and discussed in the following subsections:

- Delivered one billion core hours in FY-21
- Developed artificial intelligence and machine learning software training
- Simplified user access through an improved INL HPC web interface
- Updated HPC user authentication system
- Streamlined processing of HPC accounts
- Integrated HPC resources with Deep Lynx Data Platforms.

2.1 One Billion Core Hours in FY-21

INL HPC delivered one billion core hours in support of modeling and simulation in FY-21, a first time ever in INL history. This threshold was achieved in the early hours of September 19, 2021. A desktop computer with single core would have to run continuously for over 114,155 years to achieve this.

Figure 1. HPC Data Center at C3.

2.2 Artificial Intelligence and Machine Learning Software Training

The availability of artificial intelligence (AI) and machine learning (ML) capabilities is a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL staff directly support the mission and objectives of DOE-NE.

In January 2021, INL launched a ML and AI software training course based on interactive Jupyter notebooks and labs designed to assist researchers in gaining experience and fluency with ML frameworks and techniques. Researchers can interactively learn and experiment with the latest ML frameworks and software on advanced graphics processing unit (GPU) hardware without having to resort to using the unsecured cloud-based platforms that are typically used for this type of training. These hands-on tutorials are self-guided and cover a wide variety of topics and software with curated datasets and all needed software preinstalled. It functions in a similar way to Google Colab, but on INL's HPC systems and with all appropriate security controls in place. Since the launch of the tutorial training series, the course has been launched 119 times and consumed over 800 cores hours.

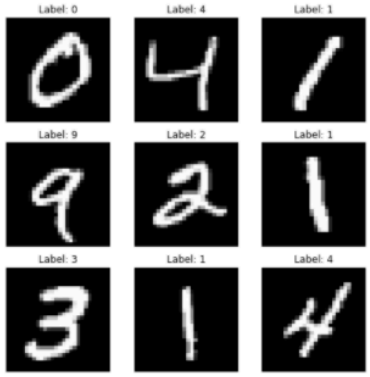
Visualizing the Dataset

After we import `pyplot` from `matplotlib` to help us plot the images in our dataset, let's see what some of our data looks like!

In [6]:
```
import matplotlib.pyplot as plt

figure = plt.figure(figsize=(8, 8))
cols, rows = 3, 3

for i in range(1, cols * rows + 1):
    img, label = train_data[i]
    figure.add_subplot(rows, cols, i)
    plt.title("Label: " + str(label))
    plt.axis("off")
    plt.imshow(img.squeeze(), cmap="gray")
plt.show()
```



Preparing our data for training and testing with DataLoaders

To prepare our data for the ML process, we are going to use `DataLoader`, which wraps an iterable around the dataset allowing us to access our dataset in "batches" while shuffling the data which can be very essential to the efficiency of the learning process.

We will begin with a batch size of 64. But, feel free to come back and change this value to see how it effects the learning process.

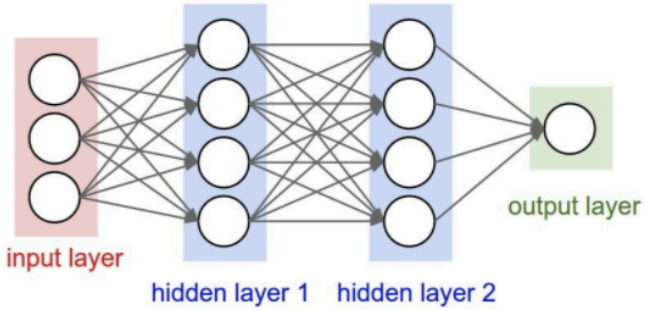
In [7]:
```
from torch.utils.data import Dataset, DataLoader

BATCH_SIZE = 64 # This value is completely up to you! Feel free to change it!

train_dataloader = DataLoader(train_data, batch_size=BATCH_SIZE, shuffle=True)
test_dataloader = DataLoader(test_data, batch_size=BATCH_SIZE, shuffle=True)
```

Creating an ANN Model

Aritifical Neural Networks (ANNs) are just your typical fully-connected neural networks with an input layer, some hidden layers, and an output layer.



The `nn` models in PyTorch helps us the creation and training of neural network models:

In [8]:
```
import torch.nn as nn
```

Figure 2. Excerpt from the tutorial "Introduction to Image Classification (PyTorch)."

2.3 Increased Capabilities to INL HPC Web Interface

In FY-21, multiple commonly used applications were added to the internal and external HPC user interface, OnDemand. OnDemand is a browser based "one-stop-shop" HPC solution, allowing users to create virtual Linux desktops, Jupyter Notebooks, transfer files, and connect to clusters with an SSH session all within their browser. Newly added applications to OnDemand systems in FY-21 consisted of:

- Visual Studio Code
- MOOSE applications and MOOSE Training Videos
- BarracudaVR
- AI/ML Tutorial Series.

These applications simplify the process, lower barriers of adoption, and decrease the amount of time required to perform scientific tasks. Overall, OnDemand had a 304.48% increase of core hours, with an overall total of 7.042 million core hours and 686 unique users in FY-21.

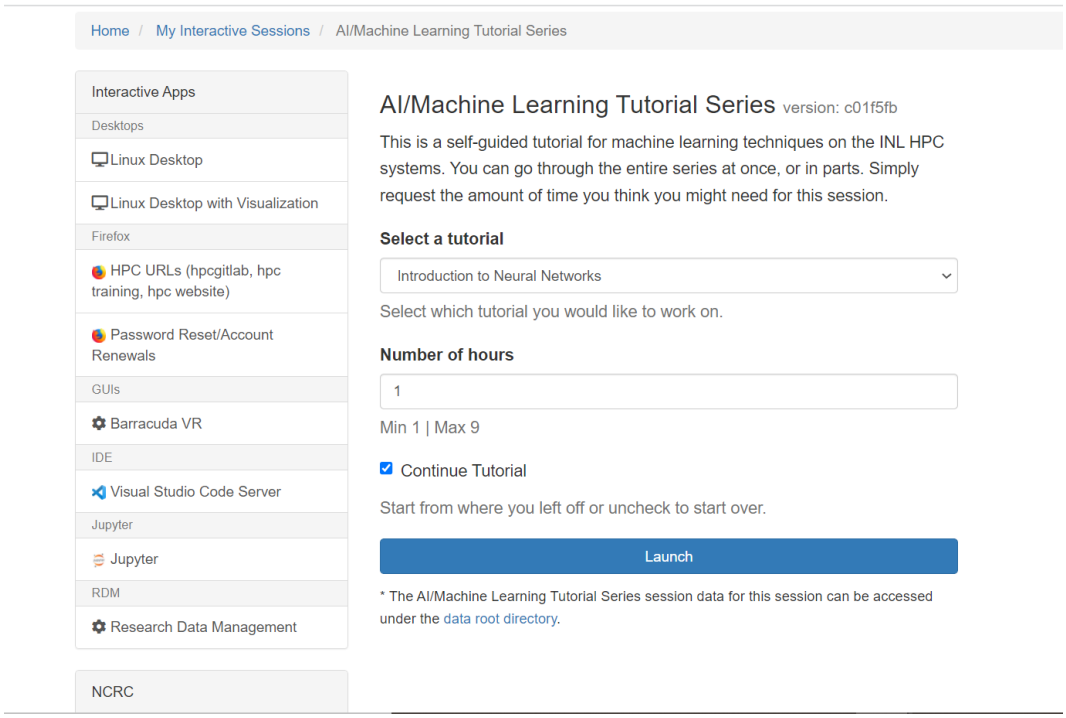


Figure 3. AI/ML Tutorial Series Session on OnDemand.

2.4 HPC User Authentication System Updated

Red Hat Identity Manager, also known as IPA, is designed to provide an integrated identity management service. In FY-21, HPC deployed a new cluster of four IPA servers to provide a modern robust user authentication and authorization system. The system is utilized by 4500+ HPC nodes for all authentication and authorization. It provides a standard web interface, programming interface, and command line to support user, group, and resource management. Development of internal tools and the NCRC are simplifying and standardizing code by using the new IPA application programming interface (API).

2.5 Change in Processing of HPC Accounts

On June 24, 2021, requests for HPC accounts started being processed via the NCRC). The NCRC was established at INL to provide secure access to NEAMS computational tools and HPC resources and training. The NCRC system is used by all requesters, including INL employees, interns, and external collaborators. The target audience includes users from the private sector, national laboratories, universities, and federal agencies.

Since HPC accounts started being processed via NCRC in June 2021, INL has experienced a 4-fold increase in the number of HPC account requests compared to the same period in 2020. Selected metrics for the NCRC HPC account requests are shown in Table 1. A total of 236 HPC account requests were received between the launch date for the NCRC website (6/24/21) and near the end of FY-21 (9/8/21).

Table 1. HPC account metrics for NCRC portal in FY-21.

HPC Account Requests via NCRC	
Timeframe: 6/24/2021–9/8/2021	
Stats	**Count**
Total number of HPC account requests received via NCRC	236
Total number of New HPC accounts approved and created	147
Total number of HPC users already having HPC accounts, but accessing NCRC portal	17
Total number of HPC account requests pending action (user started but not submitted, sponsor approval, FV&A plan, etc.)	67
Total number of HPC account requests denied or withdrawn	5
Total number of HPC account requests submitted via NCRC for foreign nationals	95
Total number of HPC account requests submitted via NCRC for U.S. citizens	141
Total number of HPC account requests submitted via NCRC for INL employees	61
Total number of HPC account requests submitted via NCRC for external users	175

2.6 Integration of HPC Resources with Deep Lynx Data Platforms

In FY-21, the HPC Team has been planning and coordinating with the the Department of Energy National Nuclear Security Administration's (DOE-NNSA) digital twin effort to enable integration of HPC resources with the Deep Lynx data warehouse and research platform. This effort will soon enable users to run Serpent Monte Carlo simulations and other computationally demanding tasks on supercomputing resources from within the Deep Lynx interface, significantly reducing the amount of time researchers will need to spend transferring data and manually submitting jobs. The input files are validated on both the Deep Lynx and HPC sides, and results are uploaded back to Deep Lynx when the analyses are complete.

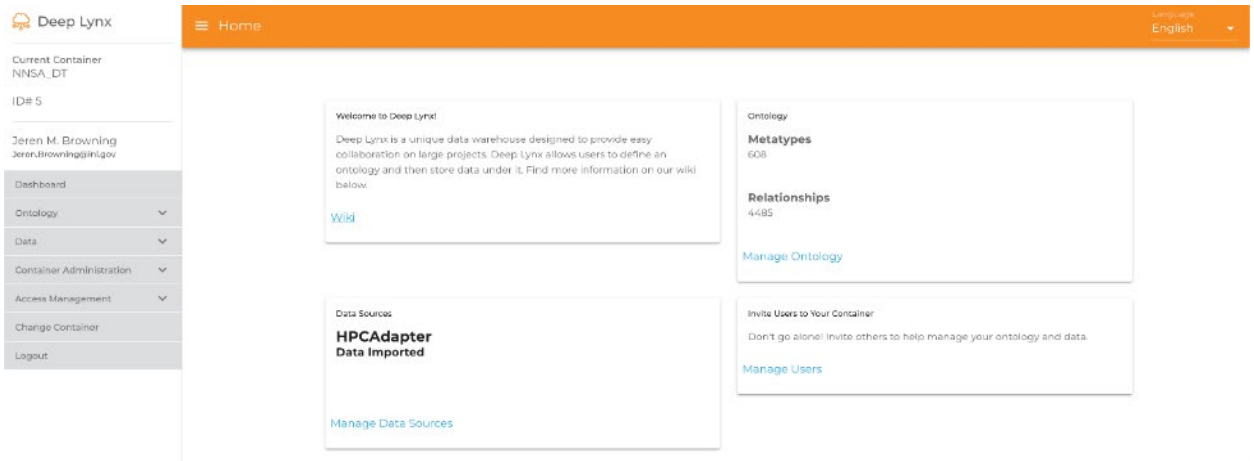


Figure 4. Deep Lynx Dashboard.

3. UTILIZATION

The Sawtooth, Falcon, and Lemhi systems combined delivered more than 1,026 million core hours of compute time in FY-21. This is an increase of 396 million core hours from FY-20. This level of compute time exceeded our operational goals.

The average queue size is an important measure of demand for computational resources. The systems were all fully utilized; oversubscription is a ratio of the average queue and computational demand relative to total system capacity. In FY-21, the average oversubscription of Sawtooth was 3.24 (meaning the average queue was 323, 425 processor cores for the year). The average oversubscription of Lemhi was 2.12 (queue was 42,747 processor cores). The average oversubscription of Falcon was 1.52 (queue was 53, 102 processor cores).

The HPC job scheduler utilizes fair-share metrics along with other considerations for prioritizing work. Given a specific need, users may request higher priority. The scheduler maintains very high overall system utilization while assuring that the most critical work runs first. Total utilization has increased by a factor of ten over the past few years. Figure 5 shows the increase of HPC usage from April 2011 to September 2021.

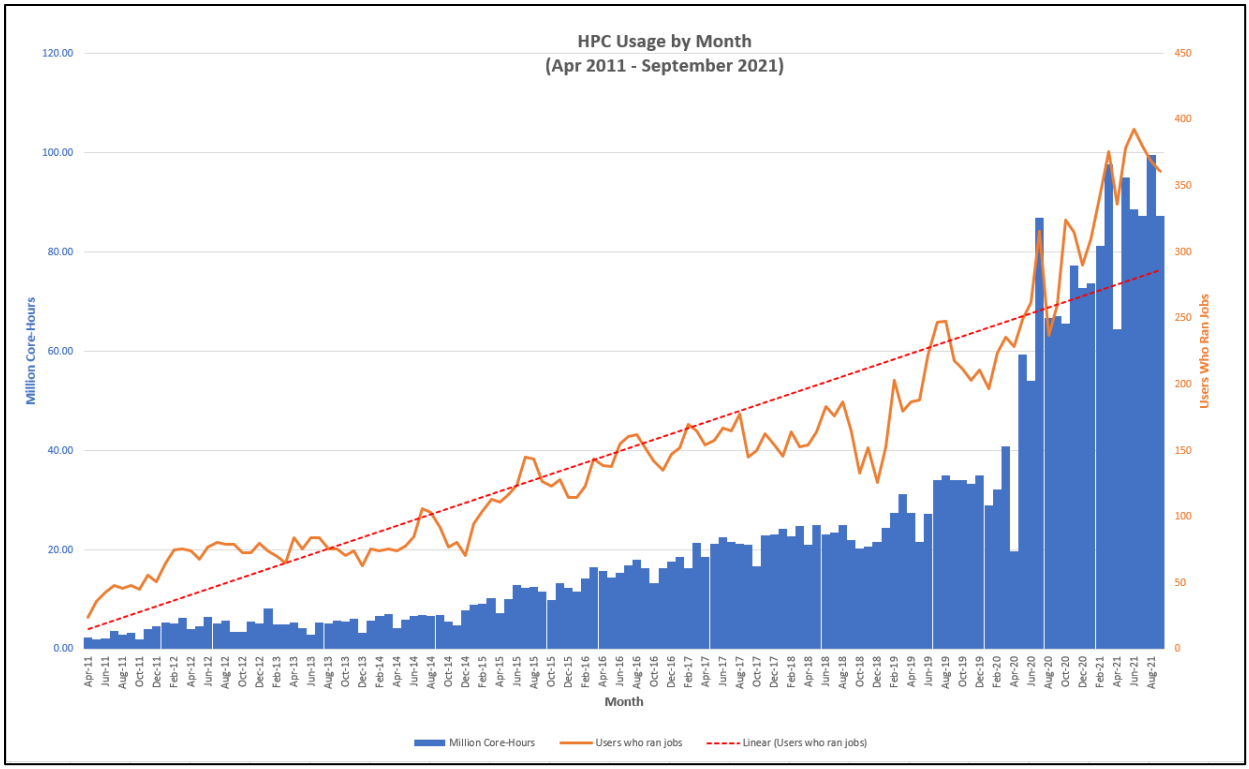


Figure 5. HPC utilization for April 2011–September 2021.

4. USER INSTITUTIONS

The following pages present a summary of institutions utilizing INL's HPC resources in FY-21. As shown in Figure 6, INL HPC capabilities were utilized by 795 researchers during FY-21, with the majority coming from national laboratories (444) using 553.46 million core hours. University researchers/students, as a group, made up the second largest group of users (199) utilizing 314.60 million core hours, while industry partners also accounted for a substantial number of users (152) with 157.78 million more hours.

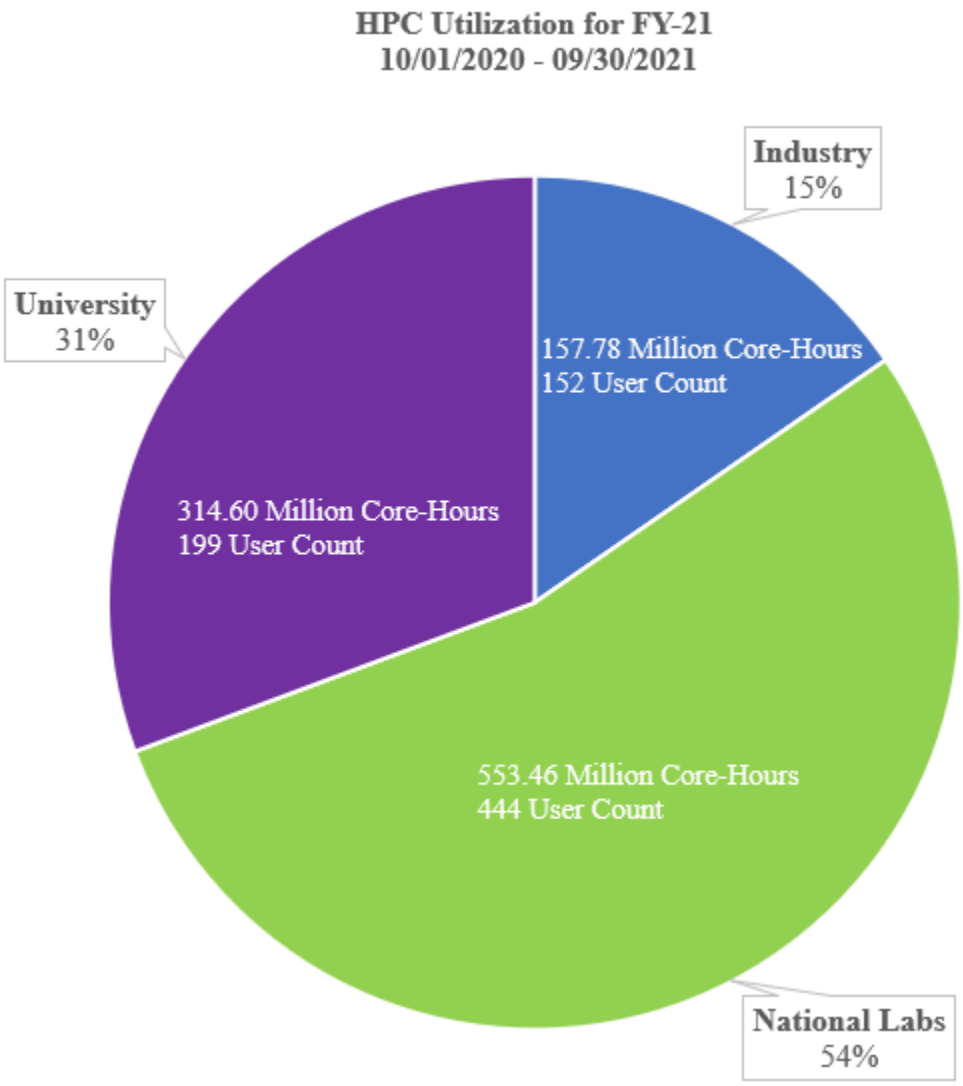


Figure 6. HPC utilization for FY-21.

Table 2 lists the top 29 institutions with largest user count utilizing INL HPC systems as of September 30, 2021. The majority of users coming from the INL (547), followed by the second largest from Naval Nuclear Laboratory (85). The remaining top 29 organizations include a mix of universities (263), industry partners (140), other national laboratories (95), and Nuclear Regulatory Commission (20).

Table 2. Top 29 institutions with largest user count utilizing INL HPC systems as of September 30, 2021.

Institution	User Count
Idaho National Laboratory	547
Naval Nuclear Laboratory	85
Argonne National Laboratory	46
Idaho State University	36
Oak Ridge National Laboratory	34
Framatome	34
University of Idaho	33
TerraPower	33
Boise State University	30
North Carolina State University	30
MPR Associates	27
Westinghouse Electric Company	25
University of Tennessee Knoxville	22
Nuclear Regulatory Commission	20
Texas A&M University	16
Los Alamos National Laboratory	15
Massachusetts Institute of Technology	11
Pennsylvania State University	11
University of Illinois at Urbana-Champaign	11
University of Wisconsin	11
University of Michigan	10
University of South Carolina	10
University of Utah	10
Oregon State University	9
Radiant Industries Incorporated	8
Lehigh University	7
FPoliSolutions LLC	7
Purdue University	6
BWX Technologies, Inc	6

A total of 129 reports were submitted by researchers for this FY-21 Annual Report. Reports were grouped by project reporting categories for the research.

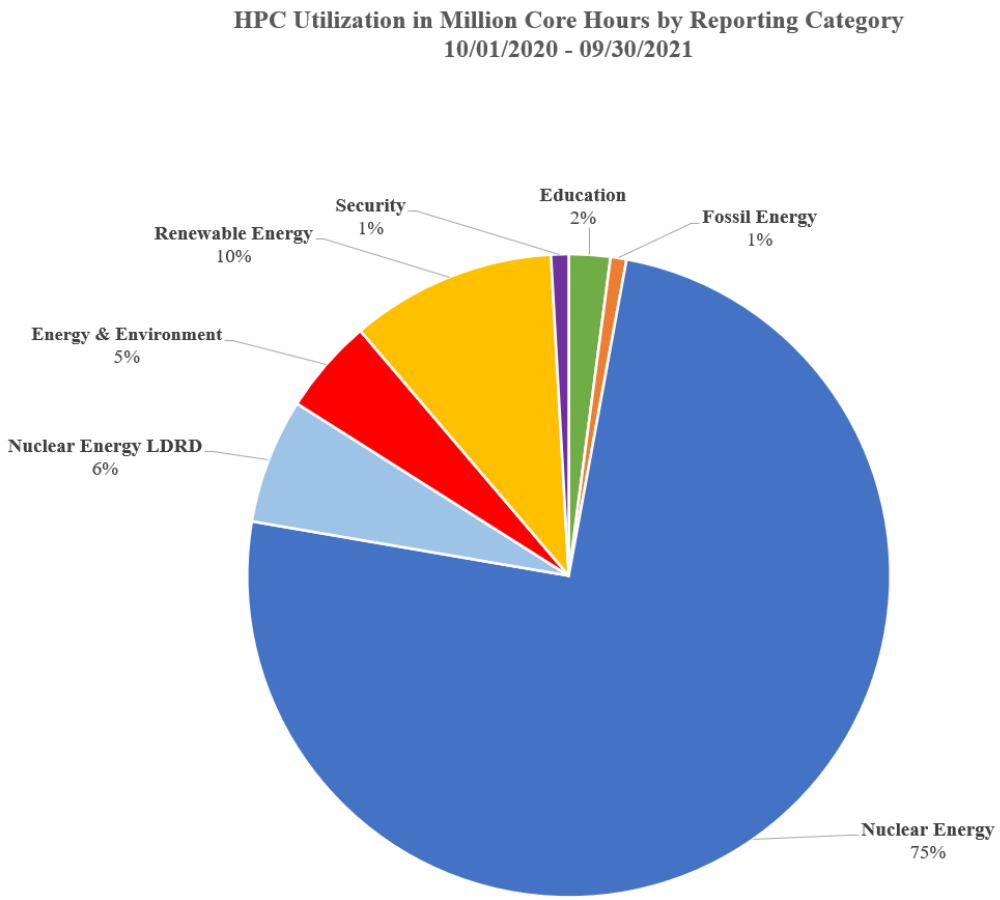


Figure 7. FY-21 HPC Utilization in Million Core Hours by Reporting Category.

Figure 7 shows compute utilization in million core hours for all project categories and systems from October 1, 2020, through September 30, 2021 for a total of 1,026 million core hours. The majority of utilization (81%, 828.6 million core hours) was from nuclear energy related projects.

The following appendices highlight a subset of projects that were completed in FY-21 by researchers using INL's HPC resources, grouped in specified project reporting categories for the research. All reports were user-provided.

Users are required to include attribution to NSUF as follows: "This research made use of the resources of the HPC INL 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."

Appendix A

NUCLEAR ENERGY

Table of Contents

A.1. Acceleration of Multigroup Cross-Section Generation Using Generation Using Many-Core Architectures

Report Participants

Steven Douglass[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The generation of multigroup cross sections typically involves the implementation of algorithms for resonance self-shielding, nuclide mixing, and energy group collapse. For large problems with hundreds of thousands or millions of individual materials, this can become a significant fraction of the runtime of a deterministic transport solver, even when parallelized across large HPC processor domains. This project considers this as a software optimization problem and explores the vectorization of the resonance self-shielding, nuclide mixing, and group collapse algorithms. Vectorization involves converting from a "material-based parallelism" where cross sections for each material are solved in their entirety before moving on, to a task-based parallelism where individual reactions are added to every material for which they are needed before moving on. The primary goal of this vectorization is to optimize the software for memory access and determine the feasibility of using GPUs to accelerate cross-section calculations for problems with large numbers of unique materials.

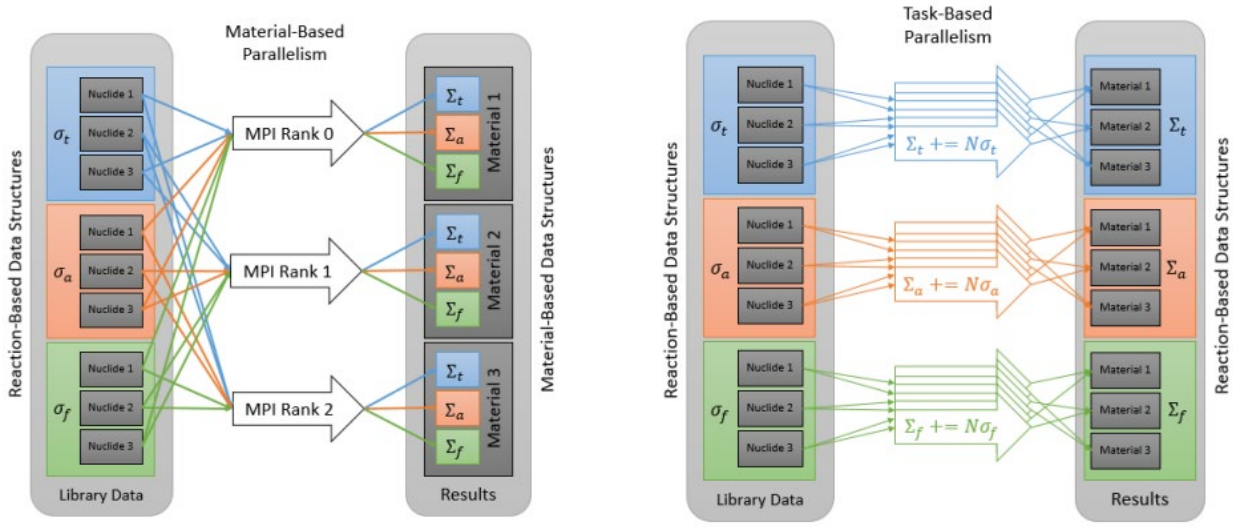


Figure 1. Graphical representation of algorithmic differences between material-based and task-based cross-section generation.

Significance

Using material-based parallelism, cross-section generation accounts for a significant fraction of the runtime when performing deterministic transport simulations for problems with a large number of materials. In addition, the type of parallelism can also create memory access bottlenecks which result in poor or inconsistent scaling even for a relatively small number of MPI processors. Using tasked-based parallelism has resulted in significant performance improvements (~80% reduction in runtime) even without use of GPUs. With GPUs, additional performance improvement has been shown to be possible (~98% reduction in run time over materials-based parallelism). Because of the high cost of cross-section generation, realizing the performance benefit demonstrated by this project can result in significantly faster analysis for large-scale deterministic transport problems.

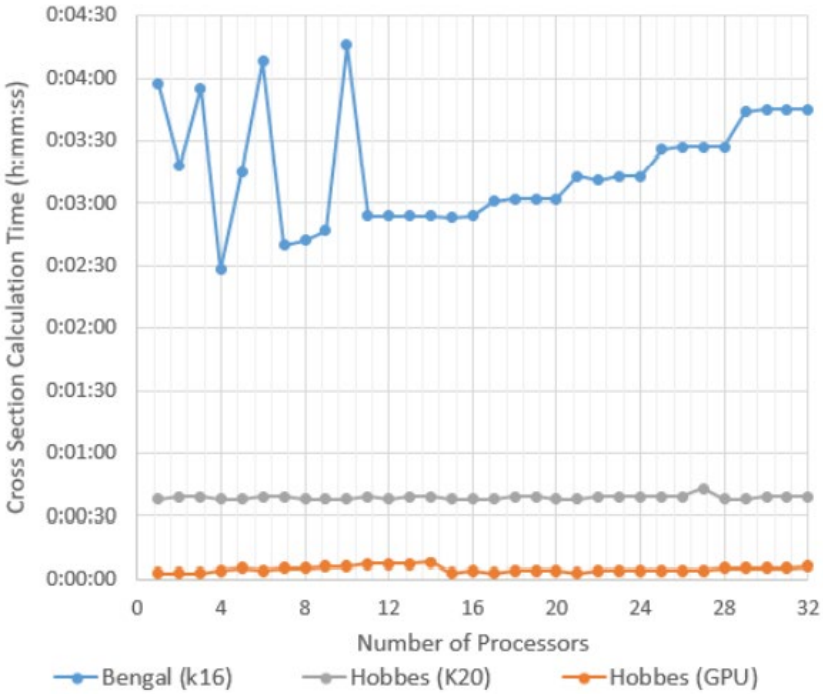


Figure 2. Weak-scaling study generating cross sections for approximately 2,000 materials per MPI process using an existing materials-based code, Bengal, and a new vectorized code, Hobbes. Results are also included for Hobbes deployed on a GPU using the same number of total materials as the other calculations.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.2. Achieving Exceptional Radiation Tolerance with Crystalline-Amorphous Nanocrystalline Structures

Report Participants

Miaomiao Jin,[1] Penghui Cao,[1,2] Michael P. Short[1]

1 Massachusetts Institute of Technology

2 University of California

Scientific Achievement

We developed a radiation collision cascade model, studied radiation defects generation, growth, and evolution in nanocrystalline metals and alloys, and found that the amorphous interfaces-engineered alloys hold promises as highly radiation tolerant materials with strong structural stability and self-healing capability under radiation damage.

Significance

Nanostructured materials with amorphous intergranular films (AIFs) have demonstrated superior strength and ductility. Their radiation tolerance is expected to be high as the large fraction of interfacial volume efficiently sinks radiation-induced defects. Here we demonstrate how a crystalline-amorphous system (nanocrystalline Cu with Zr-doped AIFs) responds to continuous irradiation with molecular dynamics simulations.We propose a diffusion model that characterizes the cascade-drivenmixing process and reveal that the spread of Zr distribution scales linearly with the damage level. The exceptional radiation resistance is attributed to the interfaces acting as sustainable defect sinks, Zr mixing into the bulk to enhance local defect annihilation due to solute-interstitial dragging, and Zr impeding radiation-enhanced grain growth by restraining AIFs from migration and maintaining interface stiffness.

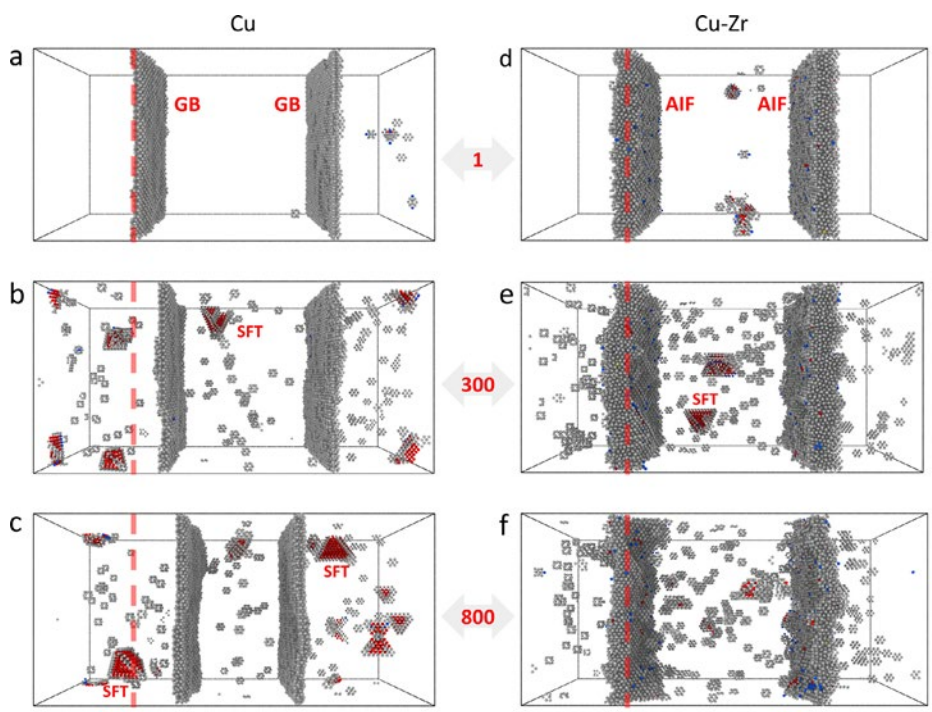


Figure 1. Comparison of radiation response between bicrystal systems containing GBs (a–c) and AIFs (d-f). Non-FCC atoms are shown after 1,300, and 800 damage cascades for each system at an ambient temperature of 800 K, which suggest the defect locations and sizes. The dashed red line marks the

original position of the left interface. Multiple SFTs are recognized. The initial spacing between the interfaces is 11.6 nm, and the AIF thickness is 12 Å. Grain stabilization and reduced defect cluster size have been observed in the AIF system. Atoms are colored by structure type from common neighbor analysis (gray: unstructured atoms, red: hexagonal close packed atoms, and blue: body-centered-cubic atoms; FCC atoms are removed for clarity).

Key Publications

- Jin, M., P. Cao, and M. P. Short. 2020. "Achieving exceptional radiation tolerance with crystalline-amorphous nanocrystalline structures," *Acta Materialia* 186:587–596.

Sponsor/Program

Laboratory Directed Research and Development (LDRD)

A.3. Advanced Materials Simulation Engineering Tool

Report Participants

Jonathan Wormald,[1] Richard Smith,[1] Michael Zerkle,[1] Thomas Webb[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The Advanced Materials Simulation Engineering Tool (AMSET) project is a multi-institutional effort to develop a module in the MedeA simulation environment (TMMaterials Design Inc.) that generates machine learning interatomic potentials (MLPs) trained to ab initio calculations. A key part of this project is the validation of MLPs. Currently, a Zr-H MLP is being tested for the lattice expansion and the associated ε to δ phase transition of ZrH2 using the LAMMPS molecular dynamics software. Present results have demonstrated the novel ability to predict the phase transition in ZrH2 associated with lattice expansion using the newly developed Zr-H MLP.

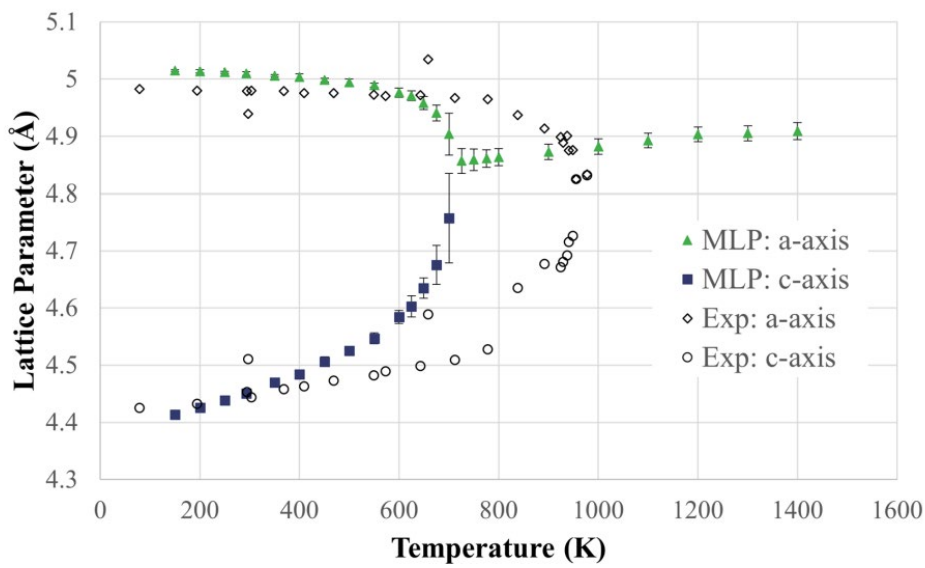


Figure 1. Lattice Expansion of ZrH2 predicted with a Zr-H MLP and compared to experiment (E. Zuzek et al. 1990. Bulletin of Alloy Phase Diagrams, 111(4) 385-395). The tetragonal ε to cubic δ phase transition and associated behavior of the lattice is observed with a transition temperature of 725 K for the MLP, compared to experimental value of more than 900 K.

Significance

Atomistic simulations are the first stage of constructing multiscale models of materials behavior. Due to their predictive accuracy, ab initio calculations are the ideal technique to quantitatively inform multiscale materials models; however, computational restrictions limit the applicabilty of these calculations to systems too small to study materials degradation. Despite their success in modeling sufficiently large systems, conventional interatomic potentials are often limited in accuracy and lack transferability to a broad range of chemistries, stoichiometries and crystal structures needed to provide flexibility for studying complex phenomena. MLPs are a new form of interatomic potential that provides the quantitative accuray of ab initio calculations at a length-scale sufficient for materials degradation but with the flexibility in chemistry, stoichiometry, and crystal structure lacking in conventional potentials. As a first step in AMSET, a Zr-H MLP was generated to study corrosion effects in Zr-based materials as well as the thermal neutron scattering law of Zirconium Hydride (ZrHx) used in TRIGA reactors. The

initial validation of the MLP was the study of the lattice expansion of ZrH2 and the associated tetragonal ε to cubic δ phase transition. The validation of the lattice expansion and phase transition will help determine the fitness of the MLP for modeling the δ phase corrosion product in Zr-based materials and its ability to model the material behavior of TRIGA reactor fuel elements.

Key Publications

- Materials Design Inc. 2020. "The Advanced Materials Simulation Engineering Tool (AMSET) Project: Ushering in a new age of atomic potentials with engineering accuracy," https://www.materialsdesign.com/post/2020/05/06/the-advanced-materials-simulation-engineering-tool-amset-project.

Sponsor/Program

Nuclear Science and Technology

A.4. Advancements in Fundamental Modeling of Hydrides in Zirconium-Based Alloys

Report Participants

Jesse Carter[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Hydride precipitation and dissolution can be modeled using physically based free energy sources and material properties using combined phase-field and mechanics modeling. The work was done using the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework.

Significance

It was shown that the needle-like hydride shape that is reported from characterization of zirconium-based alloys can be reproduced only if anisotropy of growth strains is included in mechanical modeling. This makes the MOOSE framework a prime candidate for performing such modeling since it allows for a full strain tensor to be specified. Performing 2D and 3D finite element modeling at typical hydrogen concentrations can require very large problems, so the use of INL HPC is crucial for performing such applications in a timely manner.

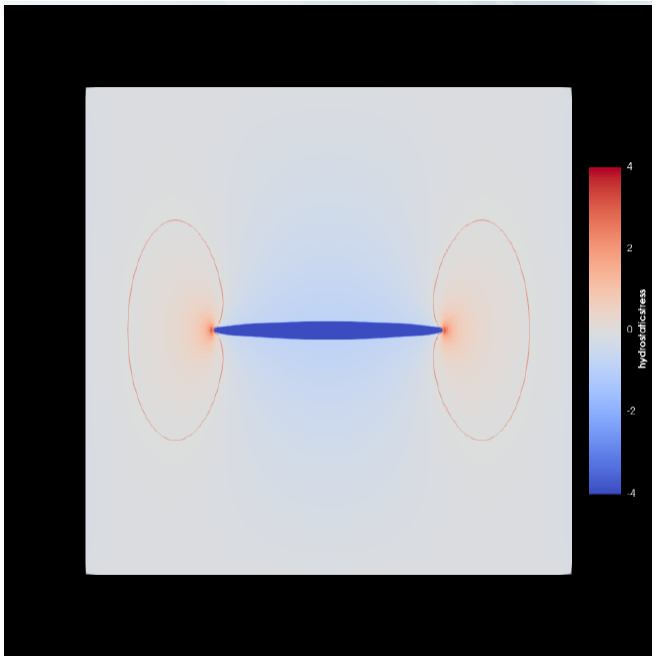


Figure 1. Hydrostatic stress near a 2D model of a delta hydride growing in zirconium. Blue represents compressive stress, and red represents tension. Contour lines represent border between compressive and tensile regions.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.5. A Molecular Dynamics Survey of Grain Boundary Energy in Uranium Dioxide and Cerium Dioxide

Report Participants

Yongfeng Zhang,[1,2] Evan Hansen,[3] Tim Harbison,[3] Sean Masengale,[1] Jarin French,[4] Larry Aagesen[2]

1 University of Wisconsin-Madison

2 Idaho National Laboratory

3 Brigham Young University-Idaho

4 Virginia Polytechnic Institute and State University

Scientific Achievement

Uranium dioxide (UO2) is the primary fuel material that is used in current nuclear reactors. As one of the most fundamental material parameters, grain boundary (GB) energy strongly influences many fuel properties including grain size evolution, fission gas bubble swelling, gas release, and fracture, and the influences depend on the characters and properties of individual GBs. As such, accurate data for GB energy in UO2 and its dependence on the GB character are critical for accurate prediction of fuel performance using modeling tools. However, such data are not yet available. To make up for the scarcity of data, molecular dynamics (MD) simulations adopting the LAMMPS simulation package were performed to obtain the energy for 230 UO2 GBs, for the purpose of elucidating the roles of GB geometry such as misorientation and inclination, as well as the bonding nature of UO2, in affecting GB energy. Four different interatomic potentials are adopted to explore the dependence on potential. The results show significant GB energy anisotropy that is associated with the cubic fluorite symmetry and the ionic bonding nature of UO2. The data from MD simulations are used to construct to 5D model for predicting GB energies in UO2 for usage in upper scale modeling.

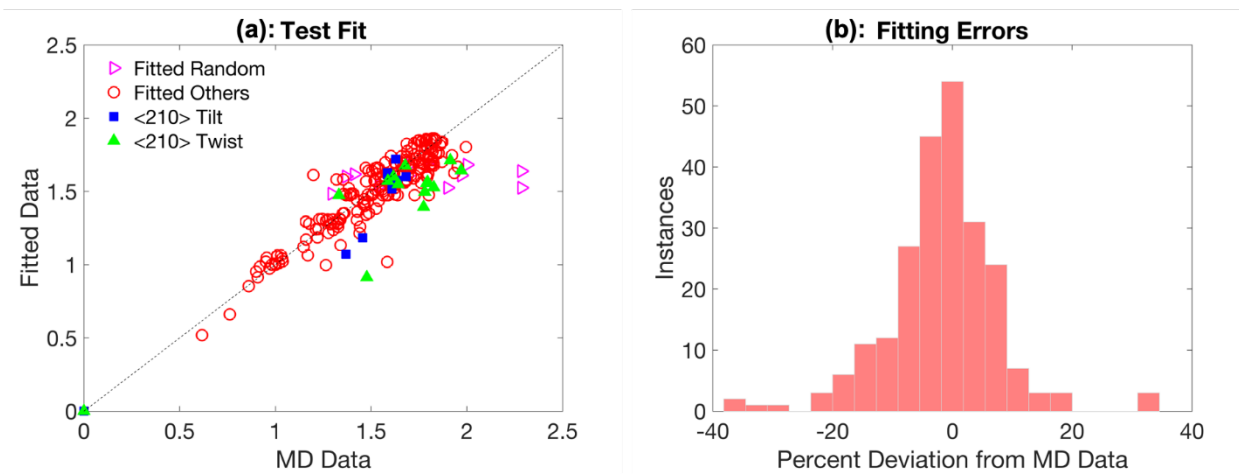


Figure 1. (a) GB energies in UO2 predicted by the fitted 5D model versus MD data and (b) the fitting errors shown by distribution of percent deviation of fitted GB energies from MD data. In (a), the GB energies used in the fitting are shown by open symbols, and a dash line y=x is added to help visualization. As shown in (b), most fitting errors are within 20%.

Significance

Comprehensive MD calculations are carried out to survey the GB energies in UO¬2 and CeO2 for the purpose of elucidating the roles of crystal structure and bonding nature in affecting GB energy. It is found that the GB energy anisotropy in UO2 resembles the trends in fcc metals, implying the primary influence of the fcc U-sublattice on GB energy. However, it is also found that <111> twist GBs are of higher energy than <100> twist GBs, different from in fcc metals, likely caused by the strong repulsion between ions of the same charge, implying the influence of the bonding nature. The GB energy anisotropy observed in UO2 may be general for oxide with the fluorite structure by comparing the results with that in CeO2. The results elucidate the GB anisotropy in fluorite phase ceramics such as UO2 and CeO2. The data and the 5D GB energy model will be useful in upper scale fuel performance modeling.

Key Publications

- Zhang, Y., E. D. Hansen, T. Harbison, S. Masengale, J. French, and L. Aagesen. ND. "A Molecular Dynamics Survey of Grain Boundary Energy in Uranium Dioxide and Cerium Dioxide," under INL export review and will be submitted soon.

Sponsor/Program

NEAMS and INL joint appointment

A.6. An Asynchronous GPU-Enabled Cross-Section Lookup Algorithm for Monte Carlo Transport Simulations

Report Participants

Alicia Klinvex,[1] Paul Burke,[2] Kyle Remley,[1] Neale Petrillo,[1] David Griesheimer,[1] Adam Bird[3]

1 Naval Nuclear Laboratory

2 Georgia Institute of Technology

3 ANSWERS Software Service, Jacobs

Scientific Achievement

In this study, we consider a novel algorithm to asynchronously offload cross-section lookup operations to a graphics processing unit (GPU) during Monte Carlo transport. A theoretical model for the proposed algorithm suggests that improvements in overall transport runtime can be achieved by overlapping execution of cross-section lookups on the GPU and geometry (i.e., ray tracing) work on the central processing unit (CPU). Additional performance improvements are realized by allowing parallel threads to collect cross-section lookup requests from multiple concurrent particles in order to reduce the CPU-GPU communication overhead by minimizing the number of GPU kernel launches. The proposed asynchronous lookup algorithm was prototyped in a mini-application using a GPU-implementation of a traditional bisection search cross-section lookup algorithm coupled with spin-wait routines to simulate kinematics and geometry work on the CPU. The prototype mini-application was used to perform timing studies for the proposed (CPU-GPU) and traditional (CPU-only) lookup algorithms under a wide range of execution strategies and realistic transport conditions.

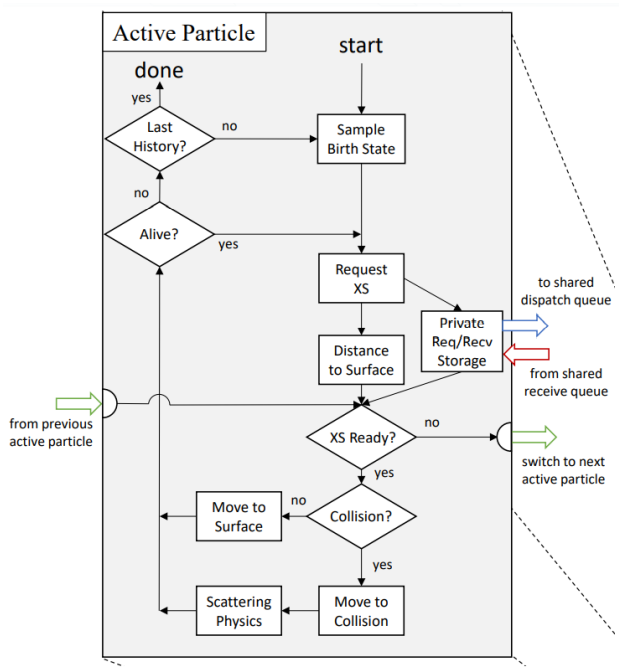


Figure 1. Illustration of asynchronous CPU/GPU Monte Carlo cross section lookup algorithm.

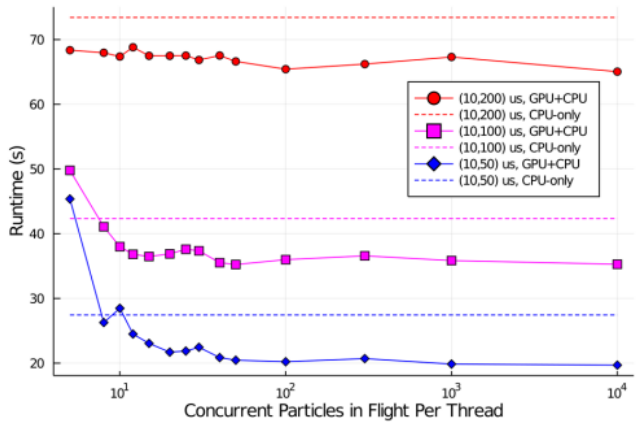


Figure 2. Plot of runtime behavior with respect to available particle concurrency.

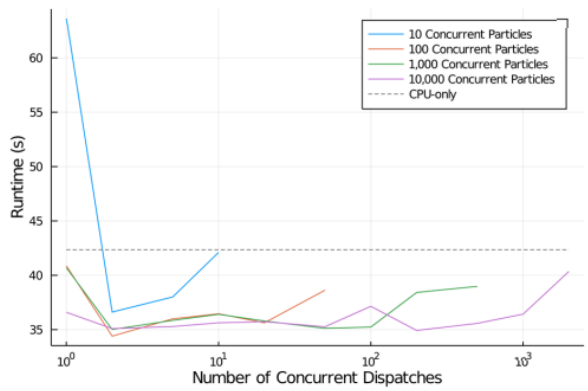


Figure 3. Plot of runtime behavior with respect to the dispatch threshold.

Significance

Numerical results demonstrated that the proposed algorithm was more efficient than the traditional (CPU-only) algorithm in simulations where the number of concurrent particles in flight per thread was ≥ 12. In the case where cross-section lookups accounted for ~36% of the total transport time, the asynchronous GPU lookup algorithm produced a 28% decrease in runtime relative to the reference CPU-only run when using ≥ 100 concurrent particles in flight per thread. This improvement is close to the theoretical maximum and suggests that the implementation is able to fully overlap execution of the cross-section lookup kernel on the GPU in parallel with ray tracing work on the CPU. The proposed algorithm successfully demonstrates that using a combination of traditional CPU kernels in conjunction with GPU kernels can result in improved performance with minimal disruption to existing Monte Carlo codes.

Key Publications

- Klinvex, A., P. Burke, K. Remley, N. Petrillo, D. Griesheimer, and A. Bird. 2021. "An Asynchronous GPU-Enabled Cross-Section Lookup Algorithm for Monte Carlo Transport Simulations," ANS M&C 2021, Raleigh, North Carolina, October 3–7, 2021.

Sponsor/Program

Nuclear Science and Technology

A.7. An Atomistic Study of Defect Energetics and Diffusion with Respect to Composition and Temperature in γU and γU-Mo Alloys

Report Participants

Gyuchul Park,[1] Benjamin Beeler,[2,3] Maria A. Okuniewski[1]

1 Purdue University

2 North Carolina State University

3 Idaho National Laboratory

Scientific Achievement

The point defect formation energies in γU and γU-xMo (x= 7, 10, 12 wt.%) alloys were calculated at the temperature ranges from 400 K to 1200 K using MD simulations. Self-diffusion and interdiffusion coefficients in U-xMo alloys are also calculated using the defect energetics at the equivalent temperature ranges.

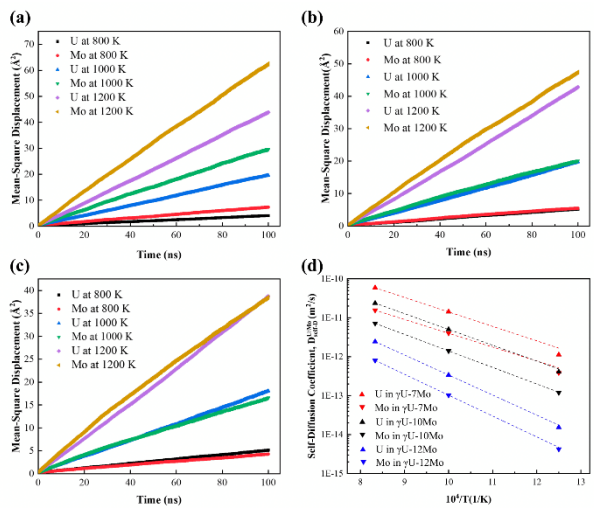


Figure 1. The mean-square displacements of U and Mo atoms with respect to time in (a) U-7Mo, (b) U-10Mo, and (c) U-12Mo containing a self-interstitial. Note the differences in y-scales. (d) The self-diffusion coefficients of U and Mo atoms in U-Mo with respect to temperature and composition. The self-diffusion coefficients in each composition were plotted to the Arrhenius equation.

Significance

In both γU and γU-xMo (x= 7, 10, 12 wt.%) alloys, the vacancy formation energy was greater than the self-interstitial formation energy at the temperature ranges from 400 K to 1200 K. This implies that diffusion will primarily occur through interstitials rather than vacancies. In γU-xMo, as the Mo concentration increased, the vacancy formation energy increased, whereas the self-interstitial formation energy decreased in the temperature range between 400 K and 1200 K. Subsequently, as Mo concentration increased, the self-diffusion coefficients decreased, and the diffusion activation energies increased, which qualitatively agreed with previous experimental results. Point defect formation energies and self-diffusion coefficients in the γU-xMo alloys obtained in this work can be used as input parameters in both microscale and mesoscale nuclear fuel modeling codes.

Key Publications

- Park, G., B. Beeler, and M. A. Okuniewski. 2021. "An atomistic study of defect energetics and diffusion with respect to composition and temperature in γU and γU-Mo alloys," *Journal of Nuclear Materials*, 552:152970.

Sponsor/Program

U.S. High Performance Research Reactor (USHPRR)

A.8. Analyzing the Risk of PCI Failure for PWR Fuel Cycles Featuring Mid-Cycle Power Maneuvers

Report Participants

Dylan Wray,[1] Brenden Mervin,[2] Kevin Clarno[3]

1 University of Texas, Austin

2 Electric Power Research Institute

3 University of Texas, Austin

Scientific Achievement

Used Virtual Environment for Reactor Applications (VERA) and Falcon software to analyze cladding stress in a pressuried-water reactor (PWR) for a set of various power cycles with different "mid-cycle maneuvers," where there is a period within the power cycle that the reactor operates at lower than full power. Table 1 shows some top line results for the four cases analyzed.

Table 1. PCI failure margin decreases in midcycle maneuvers relative to initial ramp margins.

Case	Time into Cycle (GWd/MTU)	Reduced Power Level During Maneuver (% Full Power)	Duration of Operation at Low Power (days)	Rod Burnup (GWd/MTU)	Mean Margin Percent Decrease with Standard Deviation	Minimum Margin Percent Decrease	Maximum Margin Percent Decrease	Minimum Margin Remaining (MPa)
1	2	20	28	30.9 ± 0.6	56% ± 2.8%	52%	61%	106
2	2	20	14	30.9 ± 0.6	43% ± 10%	24%	53%	149
3	2	60	28	30.9 ± 0.6	57% ± 3.3%	49%	63%	116
4	12	60	28	42.5 ± 0.7	53% ± 10%	40%	74%	125

Significance

For the cases that have been completed, this analysis found that the cases with mid-cycle maneuvers attained a higher peak cladding hoop stress during the power ramp at the end of the maneuver than at the start of the power cycle, meaning that the cases all demonstrated a higher risk of PCI failure than the case with no maneuver.

Key Publications

Still in progress, work to be presented at Top Fuel conference in October 2021.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors (CASL)

A.9. Atomistic Simulations of the Effects of Additives on Radiation-Induced Segregation in FeNiCr Alloys

Report Participants

Yongfeng Zhang,[1,2] Anus Manzoor,[3] Dilpuneet Aidhy,[3] Chao Jiang,[2] Daniel Schwen[2]

1 University of Wisconsin-Madison

2 Idaho National Laboratory

3 University of Wyoming

Scientific Achievement

Radiation-induced segregation (RIS) in austenitic steels causes redistribution of alloying elements such as depletion of Cr from grain boundaries (GBs) and degrades the corrosion resistance, potentially facilitating irradiation assisted stress corrosion cracking (IASCC). This project focuses on the effect of additives on RIS in stainless steels based on FeNiCr. In the computation side, first principle based density functional theory calculations are carried out and coupled with statistical mechanics theories to obtain the vacancy formation energy distribution in Fe-10Ni-20Cr alloy, which is used as a model alloy for austenitic steels. In addition, atomic kinetic Monte Carlo simulations are performed to elucidate the role of additives in affecting RIS. It is found that additives such as Hf can strongly trap point defects, leading to reduced RIS and swelling. However, its beneficial effect is limited by its solubility. New simulations suggest a possibility of adding secondary additives that attract Hf, such as Ti, to promote the solubility of Hf in steels and to maximize the beneficial effect of Hf.

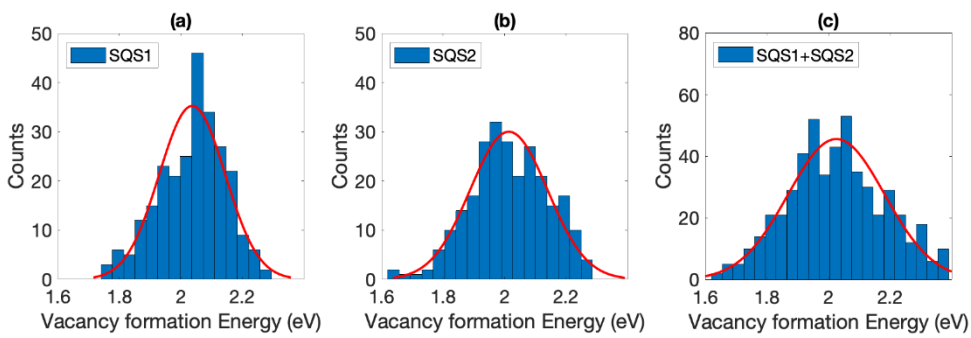


Figure 1. Distribution of vacancy formation energy in Fe-10Ni-20Cr alloy obtained with three different special quasi-random structures.

Significance

The obtained results significantly enhanced our understanding on the thermodynamics of vacancies in random concentrated alloys. A new statistical approach has been proposed for more accurate and convenient calculations of point defect energies using atomistic simulations. In addition, the AKMC simulation results can provide recommendations on additives to be added to modify austenitic steels for improved resistance to irradiation-induced change in microstructure and microchemistry. More importantly, the simulation results suggest a new approach of modifying steels by introducing combinations of additives to improve the performance of steels under irradiation. The combination of modeling and experiments may accelerate the development of modified autenitic steels with additives that are resistant to RIS, thereby mitigating the detrimental effect of IASCC.

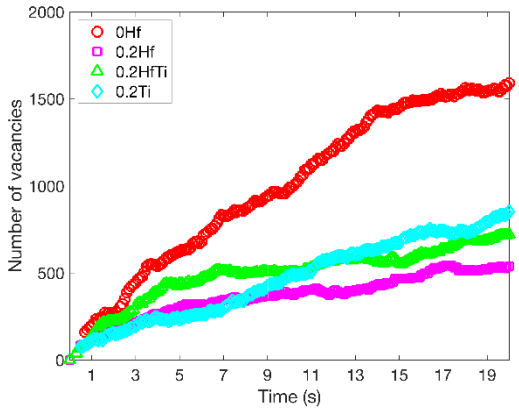


Figure 2. Amount of vacancy as a function of irradiation time showing adding additives reduced vacancy accumulation.

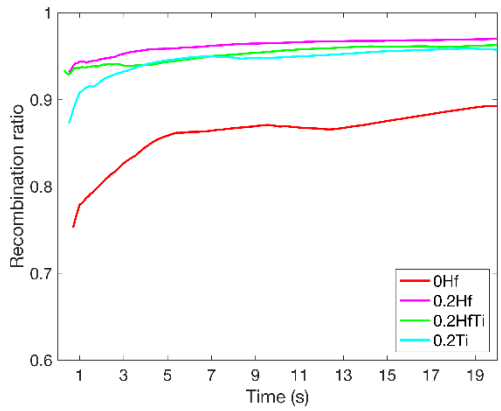


Figure 3. Fraction of recombined defects as a function of irradiation time showing additives promote defect recombination.

Key Publications

- Zhang, Y., A. Manzoor, C. Jiang, D. Aidhy, and D. Schwen. 2021. "A statistical approach for atomistic calculations of vacancy formation energy and chemical potentials in concentrated solid-solution alloys," *Comput. Mater. Sci.* 190:110308. https://doi.org/10.1016/j.commatsci.2021.110308.
- Morgan, D. and Y. Zhang. 2020. Comment on "Thermal vacancies in random alloys in the single-site mean-field approximation," *Physical Review B* 101(13):136101. https://doi.org/10.1103/PhysRevB.93.134115.
- Manzoor, A., Y. Zhang, and D. Aidhy. 2021. "Factors affecting vacancy formation energy in Fe70Ni10Cr20 random concentrated alloy," *Comput. Mater. Sci.* 198:110669. https://doi.org/10.1016/j.commatsci.2021.110669.

Sponsor/Program

INL LDRD 19A39-071FP: Mitigating irradiation assisted stress corrosion cracking by rapid alloy design

A.10. Atomistic Spin Dynamics for Magnetic Material Simulation

Report Participants

Brian McDermott,[1] Jonathan Wormald[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Atomistic spin dynamics methods with input from density functional theory calculations are being developed to examine the correlations between spin waves and magnetic material properties. Calculations are performed using the UppASD code to simulate the temperature-dependent magnetization and dynamic spin structure factor ( ). $S(\boldsymbol{Q},\omega)$Subsequently, these properties are used to derive the Curie temperature and thermal neutron scattering kernel.

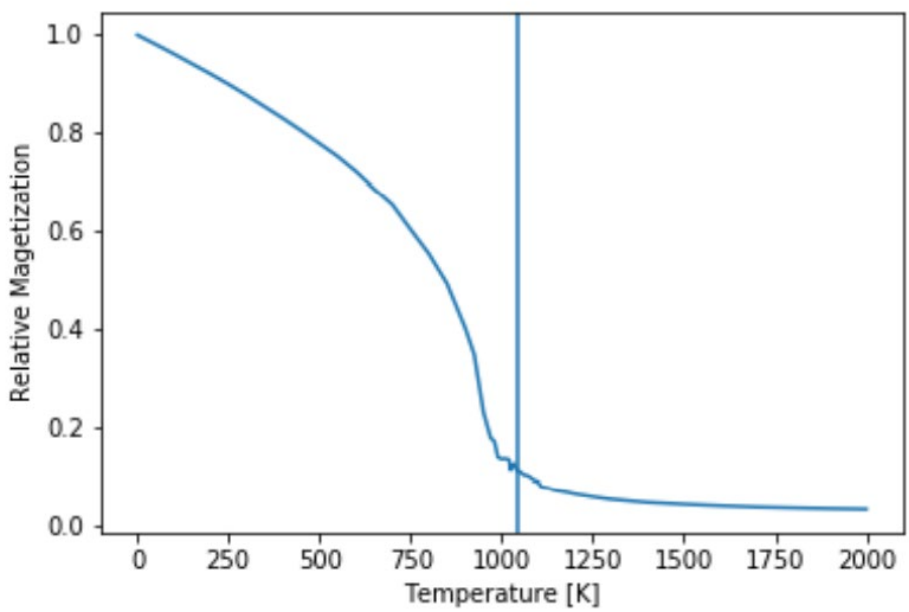


Figure 1. Exemplar magnetization temperature dependence of BCC iron calculated with the UppASD atomistic spin dynamics code. The vertical line is the approximate Curie temperature.

Significance

Elementary magnetic excitations of crystals (i.e., spin waves) influence the macroscopic magnetic behavior of materials and are integral to the operation emerging quantumtechnologies. Accurate modeling of spin waves enables improved engineering models of magnetic materials. Atomistic spin dynamic simulation—the magnetic analogue of molecular dynamics—may be used to model the correlation between spin waves and macroscopic magnetic material properties, such as the temperature dependence of the magnetic succeptibility across the ferromagnetic to paramagnetic transition. Additionally, spin dynamics informed by density functional theory may be used to directly evaluate the dynamic spin structure factor to assist in the interpretation of inelastic neutron spectroscopy of magnetism in crystalline materials.

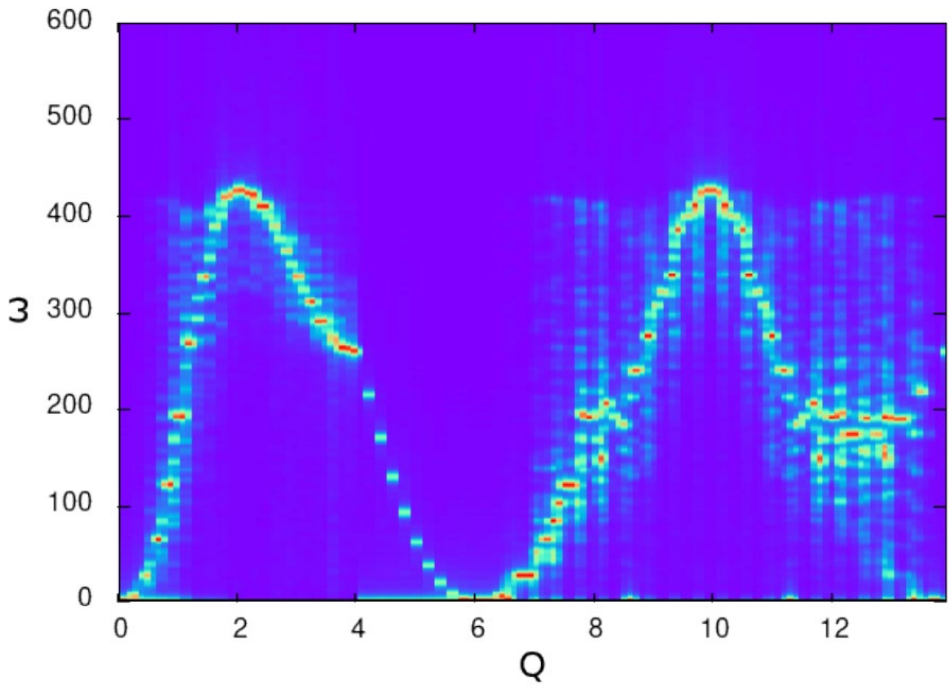


Figure 2. Magnon dispersion curve of BCC iron extracted from calculated with the $\boldsymbol{S}(\boldsymbol{Q},\boldsymbol{\omega})$UppASD atomistic spin dynamics code. The calculation is an example of the use of spin dynamics to evaluate observables from inelastic neutron scattering spectroscopy.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.11. Atomistic Study on Fundamental Properties and Anisotropic Elastic Response of Defects in Alpha-Uranium

Report Participants

Yuhao Wang,[1] Khadija Mahbuba,[2] Benjamin Beeler,[2] Andrea Jokisaari[3]

1 University of Michigan

2 North Carolina State University

3 Idaho National Laboratory

Scientific Achievement

This research is part of a larger project that focuses on the investigation of irradiation-induced microstructure and property changes in alpha-uranium via a combination of modeling and experimental techniques. The goal of this research subset is to use atomistic simulations to access and characterize a series of bulk properties of alpha-uranium as well as thermodynamic and mechanical properties of atomistic defects in the material. Single vacancies and interstitials as well as di-vacancies and di-interstitials are investigated over the temperature range of 400 K–750 K. Utilizing the LAMMPS code, bulk properties, such as thermal expansion and heat capacity, defect properties, such as formation energy and directionally-dependent diffusion coefficients, and elastic response properties, such as elastic stiffness tensors and elastic dipole tensors have been calculated. The result of thermal expansion and defect formation energy has been compared to previously published ab initio MD simulations and shows good consistency, providing a strong indicator that the other values calculated by standard molecular dynamics, which are too computationally demanding for ab initio methods, are physically significant. From our result, the defect formation energies for single self-interstitial atom (SIA), single vacancy, di-SIA, and di-vacancy increases with increasing temperature. In addition, the calculated thermal expansion, defect diffusivity, and the elastic dipole tensor for all defect types investigated show significantly different variation and magnitude as the function of temperature in different crystallographical directions (anisotropy).

Significance

Alpha-uranium plays an important role in the performance and structure evolution of metallic fuels under irradiation. It is a highly anisotropic material that demostrates a wide variety of phenomena under irradiation depending on the temperature, such as swelling and deformation, and the mechanisms that control this behavior are not well-understood. It is hypothesized that the interaction behavior of defects introduced into the material via irradiation changes with temperature, controlling the macroscopic observed behavior. One major macroscopic behavior is the overall shape change of an alpha-uranium single crystal under irradiation, which is thought to be driven by defect motion. In a polycrystal, this can cause swelling and deformation. The variation in defect formation energy with temperature may explain the change in irradiation behavior with temperature. This project aims to provide a comprehensive atomistic understanding of defect structural and transport properties in alpha-uranium, especially at non-zero temperatures. These results can also be used as input for modeling at longer length scales to study mesoscale and macroscale behavior (e.g., swelling).

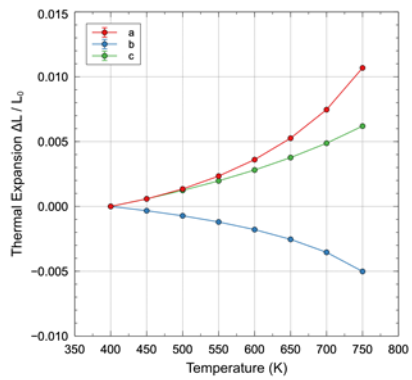


Figure 1. Calculated thermal expansion for each crystallographical direction as a function of temperature, which agrees well with empirical data (not shown).

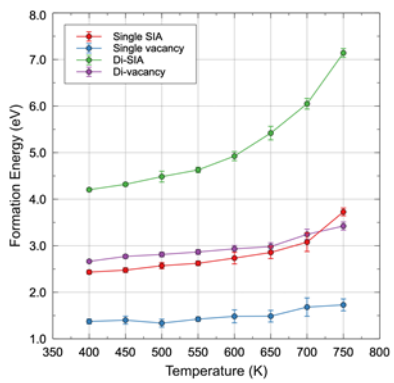


Figure 2. Defect formation energy for single SIA, single vacancy, di-SIA, and di-vacancy as a function of temperature.

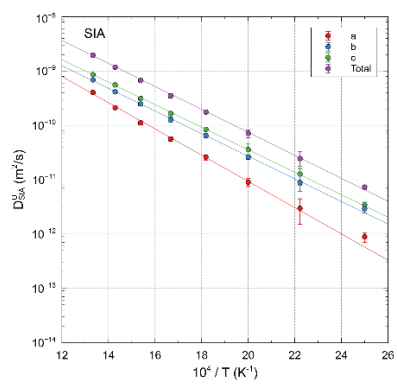


Figure 3. Atomic diffusivity of single SIA as a function of temperature.

Key Publications

- Wang, Y., B. Beeler, A. Jokisaari. "An atomistic study of fundamental bulk and defect thermodynamic properties in α-uranium," (in progress, targeted journal: Journal of Nuclear Materials).
- Wang, Y., B. Beeler, A. Jokisaari. "Atomic assessment of anisotropic elastic response for defects in α-uranium," (in progress, targeted journal: Journal of Nuclear Materials).
- Beeler, B., K. Mahbuba., Y. Wang, and A. Jokisaari. 2021. "Determination of thermal expansion, defect formation energy, and defect-induced strain of α-U via ab initio molecular dynamics," *Frontiers in Materials* 8:188. https://doi.org/10.3389/fmats.2021.661387.

Sponsor/Program

This work is supported through the INL LDRD program under DOE Idaho Operations Office Contract DE-AC07-05ID14517 under the LDRD 20A44-121, "Modeling and characterization of alpha-U to accelerate metallic fuel development."

A.12. ATR LEU Conversion

Report Participants

Michael Saitta[1]

1 MPR Associates, Inc.

Scientific Achievement

DOE-NNSA's Office of Material Management and Minimization's (M3's) mission is to convert, remove, and dispose of vulnerable nuclear material located at civilian sites worldwide. As part of its mission, M3's Office of Conversion works around the world to convert research reactors and isotope production facilities to non-weapon usable nuclear material both domestically and abroad. In support of this effort, the Office of Conversion's United States High Performance Research Reactor (USHPRR) Conversion Program is working with the INL to develop and qualify new low-enriched uranium (LEU) fuels and technologies for use in the Advanced Test Reactor (ATR), the Advanced Test Reactor Critical (ATRC) facility, High Flux Isotope Reactor (HFIR), Nation Bureau of Standards Reactor, Massachusetts Institute of Technology Reactor, and University of Missouri Research Reactor.

The USHPRR program has selected a monolithic U-Mo fuel plate design consisting of uranium-10 wt% molybdenum alloy (U-10Mo) foils clad in aluminum alloy 6061 as the best candidate for the USHPRR LEU fuel plates. The Fuel Qualification Pillar at the INL is responsible for the development and qualification of the new U-10Mo LEU fuel plates. Major fuel development activities include the demonstration, thorough testing and analysis, of the new fuel that meets the operational safety, dimensional stability, thermal stability, performance, and other requirements for the reactors.

The work required to design, evaluate, and qualify a new LEU fuel element using the U-10Mo fuel plates for use in the ATR and ATRC is directed by the ATR LEU fuel project at the INL. The ATR LEU fuel element design (referred to as the LOWE element) has been selected as the best performing LEU fuel element design to use in place of the present highly enriched uranium (HEU) fuel element in the ATR. Therefore, the LOWE fuel element design will be moved forward for further testing and evaluation to determine if the monolithic U-10Mo fuel plates are safe for use in the ATR and ATRC.

To support qualification of the LEU fuel, a series of three irradiation tests is planned with full-size LOWE elements in ATR core driver positions. To place LOWE elements in ATR core driver positions, a core safety assurance package (CSAP) must be completed.

Significance

The ongoing work has so far demonstrated several of the required safety margins, reactor control limits, and other quantities of interest for the first of three element tests. Further work will continue to demonstrate the acceptability of thermal hydraulic accidents, reactivity controls and excursions, and reactor performance for the remaining element tests and the unrestricted use of LEU fuels.

Key Publications

None.

Sponsor/Program

ATR, NNSA's M3

A.13. ATR LEU Fuel System Design

Report Participants

Rachel Romano[1]

1 MPR Associates, Inc.

Scientific Achievement

Develop the design basis for LEU fuel system in the ATR. Analyses develop the design basis for calculating various neutronics parameters such as local power uncertainties, critical positions, power profiles, kinetics parameters, etc. Analyses use the Monte Carlo MC21 particle transport code developed by Naval Nuclear Laboratory (NNL).

Significance

These analyses calculate reactor neutronics parameters for the new LEU fuel system being designed for the ATR. Previous analyses performed for the HEU fuel system used a different software and method. Therefore, these analyses for the new fuel system develop the design basis for use in the ATR.

Key Publications

MC21 requires all information to go through NNL's public utterance process. No publications made it through the public utterance process.

Sponsor/Program

ATR

A.14. Automated X-Ray Spectroscopy Analysis Using Genetic Algorithms

Report Participants

Min Long,[1] Miu Lun (Andy) Lau,[1] Donna P. Guillen,[2] Jeff Terry,[3] Shlomo Argamon[3]

1 Boise State University

2 Idaho National Laboratory

3 Illinois Institute of Technology

Scientific Achievement

We developed a ML system for automated analysis of extended X-ray absorption fine structure (EXAFS) spectroscopy measurements and demonstrated its effectiveness on measurements collected at powerful, third generation synchrotron radiation facilities. Specifically, the system uses a genetic algorithm to efficiently find sets of structural parameters that lead to high-quality fits of the experimental spectra. A human analyst suggests a set of chemical compounds potentially present in the sample, used as theoretical standards. The algorithm then searches the large multidimensional space of combinations of these materials to determine the set of structural paths using the theoretical standards that best reproduces the experimental data. The algorithm further calculates a goodness-of-fit value from the suggested standards that can be used to identify the chemical moieties present in the measured sample.

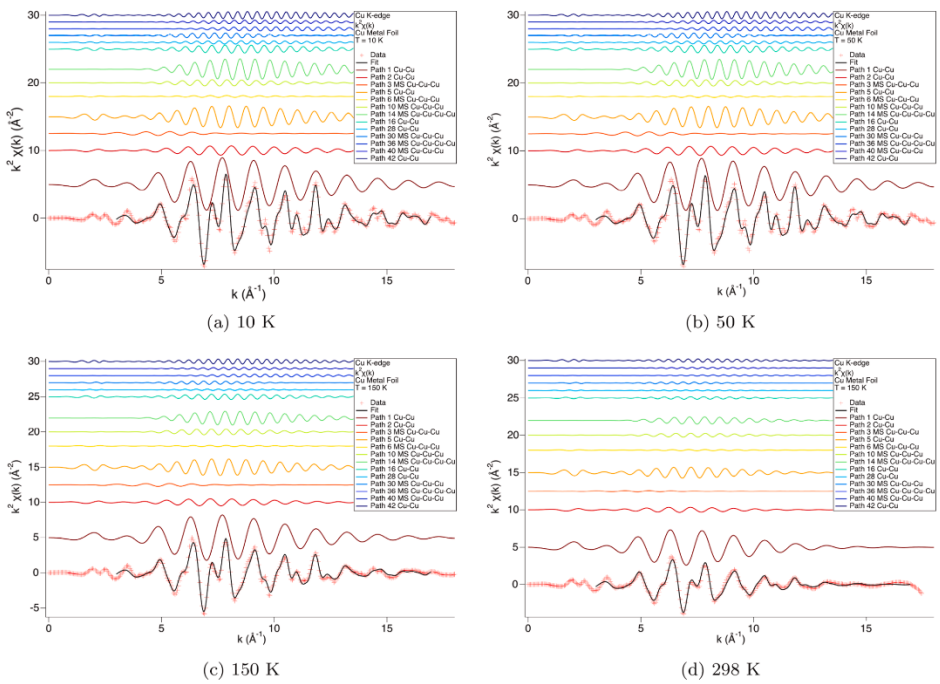


Figure 1. Cu K-edge EXAFS from a metallic copper foil as a function of temperature has been refined with the genetic algorithm. The best fits (black) are shown with the experimental data (+). The individual paths that combine to make up the measured spectra are also shown. See details in the paper listed in "Key Publications."

Significance

It is a well-known issue of improper and unreliable analysis of materials characterization data by developing an artificial-intelligence-based methodology that can reliably and more efficiently analyze experimental results from EXAFS measurements. Such methods help address growing reproducibility problems that are slowing research progress, discouraging the quest for research excellence, and inhibiting effective technology transfer and manufacturing innovation.

Key Publications

- Terry, J., M. L. Lau, J. Sun, C. Xu, B. Hendricks, J. Kise, M. Lnu, S. Bagade, S. Shah, P. Makhijani, A. Karantha, T. Boltz, M. Oellien, M. Adas, S. Argamon, M. Long, and D. P. Guillen. 2021. "Analysis of Extended X-ray Absorption Fine Structure (EXAFS) Data Using Artificial Intelligence Techniques," *Applied Surface Science*, 547:149059. https://doi.org/10.1016/j.apsusc.2021.149059.

Sponsor/Program

INL LDRD program under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

A.15. Benchmarking MC21 Through the Use of ICSBEP Evaluations

Report Participants

Kyle Neumann,[1] Michael Elo,[1] Corey Schmitzer,[1] David Spengler[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Through the modeling of various International Criticality Safety Benchmark Evaluation Project (ICSBEP) benchmarks, engineers were better able to assess the ability of the MC21 Monte Carlo code with various cross-section sets to predict the eigenvalue of a critical configuration. ICSBEP models were used to benchmark the validity and accuracy of MC21 models of known critical solutions and assemblies. An example of an ICSBEP model developed in the Physics Unified Modeling and Analysis system (PUMA) for MC21 is provided in Figure 1. Utilizing the computing resources of the INL HPC allowed for the rapid development of over 100 ICSBEP model cases to benchmark the capabilities of MC21.

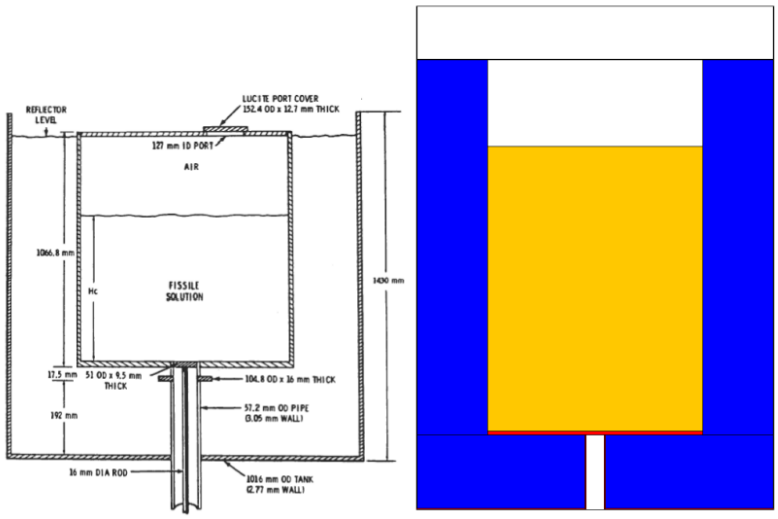


Figure 1. Example of a simplified ICSBEP evaluation, modeled via PUMA.

Significance

A perfect Monte Carlo code and perfect cross-section set should predict a critical eigenvalue for a known critical assembly. With approximations in the transport solution or cross-section set, Monte Carlo codes may demonstrate a reactivity bias with a number of parameters (e.g., neutron spectrum or spatial distribution). Modeling known critical configurations from the ICSBEP database allows for an evaluation of reactivity trends for MC21 with a given cross-section set.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.16. Cardinal: A Lower-Length-Scale Multiphysics Simulator for High-Resolution Analysis

Report Participants

A. Novak,[1] P. Shriwise,[1] R. Rahaman,[1] P. Romano,[1] E. Merzari,[2] D. Gaston[3]

1 Argonne National Laboratory

2 Pennsylvania State University

3 Idaho National Laboratory

Scientific Achievement

Cardinal is a multiphysics solver that leverages the MOOSE to couple NekRS (computational fluid dynamics) and OpenMC (Monte Carlo particle transport). Cardinal is intended to provide lower-length-scale simulation of wide classes of nuclear reactor concepts, with initial applications to pebble-bed reactors, sodium-fast reactors, and thermal striping. All physics domains are tightly coupled using advances in the MOOSE framework such as the MultiApp system and MOOSE-wrapped applications.

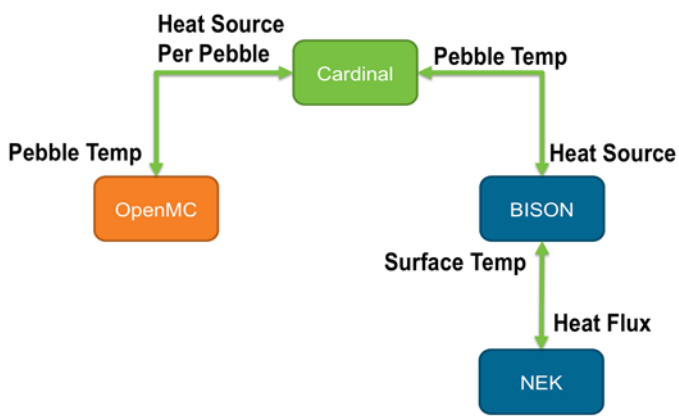


Figure 1. MOOSE-enabled MultiApp coupling scheme used in Cardinal for pebble-bed reactor applications.

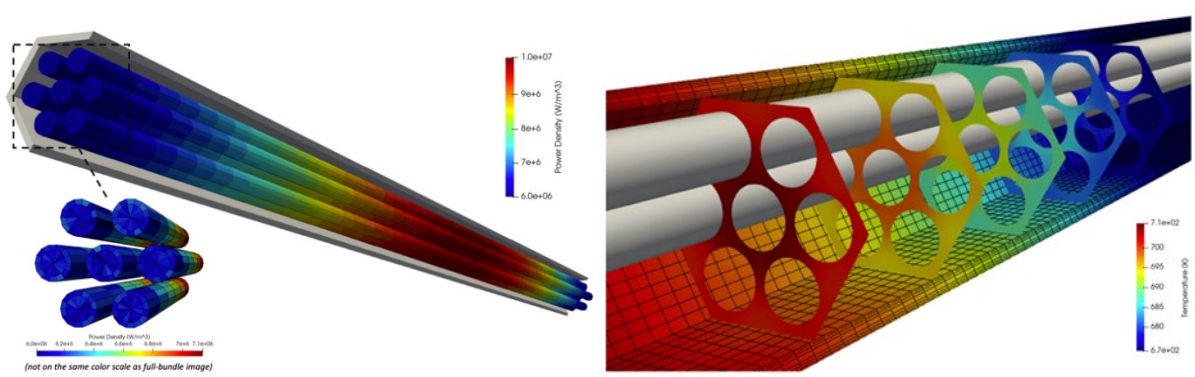


Figure 2. NekRS fluid temperature (left), BISON duct temperatures (left), and OpenMC fission energy distribution (right) for a tightly coupled model of a sodium-fast reactor.

Significance

Cardinal provides detailed modeling of reactor systems with continuous field transfers of conjugate heat transfer boundary conditions and volumetric source terms, allowing general high-fidelity modeling of arbitrary geometries. Cardinal is able to leverage heterogeneous architectures, where NekRS runs on the graphics processing units (GPUs) and OpenMC/MOOSE on CPU. Asynchronous execution of solutions is being explored. Extension to include online mesh deformation for core radial expansion calculations is on the Cardinal development roadmap.

Key Publications

- Novak, A. J., P. Shriwise, R. Rahaman, et al. 2022. "Coupled Monte Carlo Transport and Conjugate Heat Transfer for Wire-Wrapped Bundles within the MOOSE Framework," Proceedings of NURETH (submitted).
- Merzari, E., H. Yuan, M. Min, D. Shaver, et. al. 2021. "Cardinal: A Lower-Length-Scale Multiphysics Simulator for Pebble Bed Reactors," *Nuclear Technology* 7:1118–1141. https://doi.org/10.1080/00295450.2020.1824471.

Sponsor/Program

NEAMS-TH-COE, ANL LDRD

A.17. Cardinal: A Lower-Length-Scale Multiphysics Simulator for Pebble-Bed Reactors

Report Participants

E. Merzari,[1] H. Yuan,[2] M. Min,[2] D. Shaver,[2] R. Rahaman,[2] P. Shriwise,[2] P. Romano,[2] A. Talamo,[2] Y. Lan,[2] D. Gaston,[3] R. Martineau,[3] P. Fischer,[4] Y. Hassan[5]

1 Pennsylvania State University

2 Argonne National Laboratory

3 Idaho National Laboratory

4 University of Illinois, Urbana-Champaign

5 Texas A&M University

Scientific Achievement

Cardinal is a multiphysics solver that leverages the MOOSE for pebble-bed reactors, in particular, for Berkeley's pebble-bed fluoride salt-cooled high-temperature reactor (PB-FHR) Mark I design. Cardinal is intended to provide lower-length-scale simulation of pebble-bed designs by coupling three physics domains: neutronics (OpenMC), thermal fluids (Nek500/NekRS), and fuel performance (BISON). All three domains are tightly coupled using advances in the MOOSE framework such as the MultiApp system and MOOSE-wrapped applications.

Significance

Cardinal provides detailed modeling of pebble-bed reactors with explicit representation of each pebble in the reactor in both the neutronics and thermal hydraulics domains. It is able to leverage heterogeneous architectures, where NekRS runs on the graphics processing units (GPUs) and OpenMC/BISON on CPU. Asynchronous execution of solutions is being explored. Extension to gas reactor pebble-bed simulations is also on the Cardinal development roadmap via coupling of radiative heat transfer by leveraging MOOSE's newly added ray tracing module.

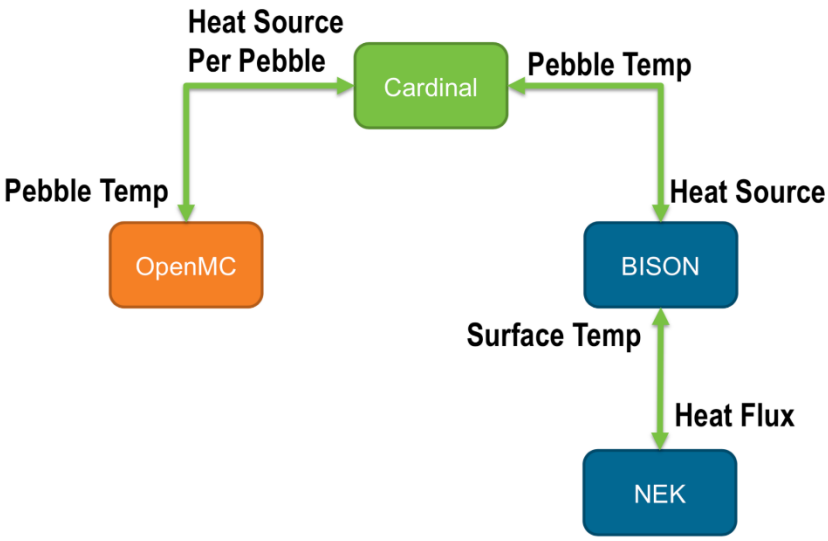


Figure 1. MOOSE-enabled MultiApp coupling scheme used in Cardinal.

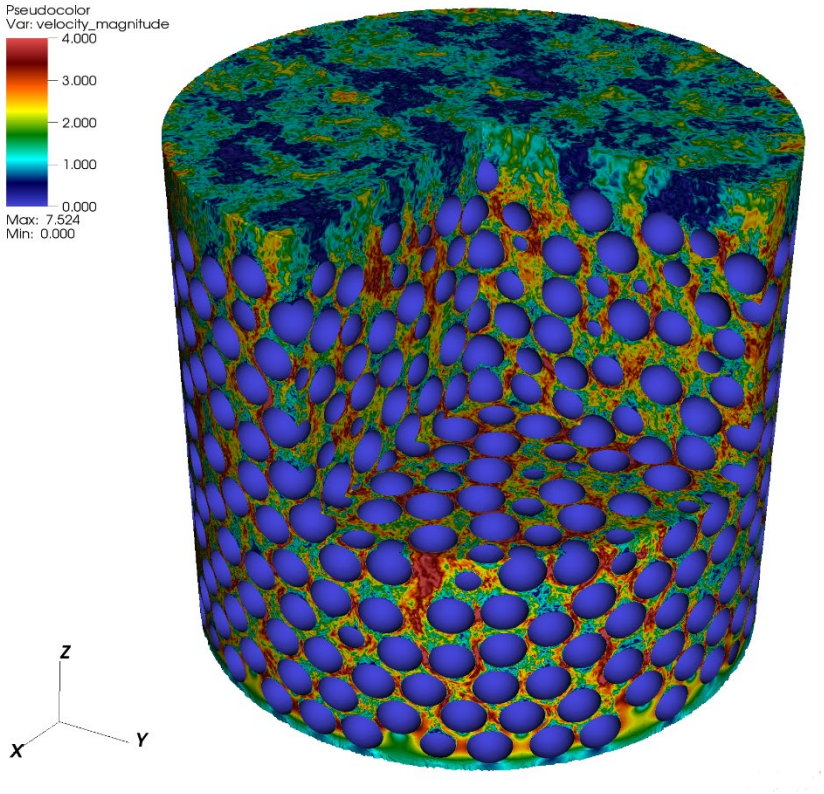


Figure 2. NekRS velocity profile of a test model with 1,568 pebbles.

Key Publications

- Merzari, E., H. Yuan, M. Min, D. Shaver, et. al. 2021. "Cardinal: A Lower-Length-Scale Multiphysics Simulator for Pebble Bed Reactors," *Nuclear Technology* 7:1118–1141. https://doi.org/10.1080/00295450.2020.1824471.
- Merzari, E., D. Gaston, R. Rahaman, A. Talamo, H. Yuan, P. Romano, and R. Martineau. 2019. "Cardinal: A Lower Length-scale Simulator for Flouride Cooled High Temperature Reactors," ANL/MCS-TM-383, Argonne National Laboratory. https://doi.org/10.2172/1755934.

Sponsor/Program

NEAMS-TH-COE

A.18. Common Monte Carlo Design Tool Unclassified Benchmark Model Suite

Report Participants

Joseph Cotchen,[1] Lloyd Huang,[1] Sean Moran,[1] Scott Spychala,[1] Aaron Tyo,[1] Jeff Wegener,[1] Christopher Young[1]

1 Naval Nuclear Laboratory

Scientific Achievement

This work provides the modeling and qualification for a suite of unclassified Physics Unified Modeling and Analysis Application Programming Interface (PUMA-API) and MC21 benchmark models to support general-purpose qualification of the Common Monte Carlo Design Tool (CMCDT).

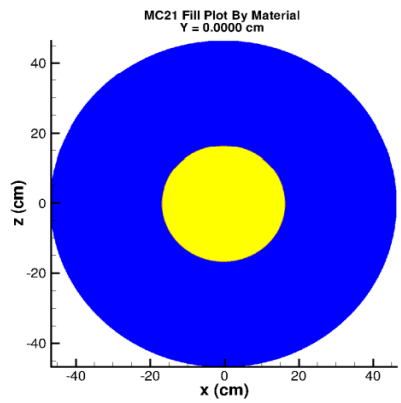


Figure 1. Example MC21 plot of model PST023.

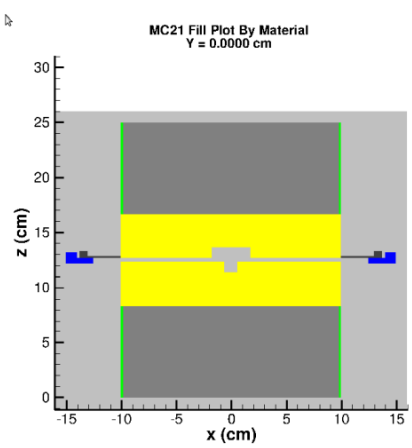


Figure 2. Example MC21 plot of model HMF092.

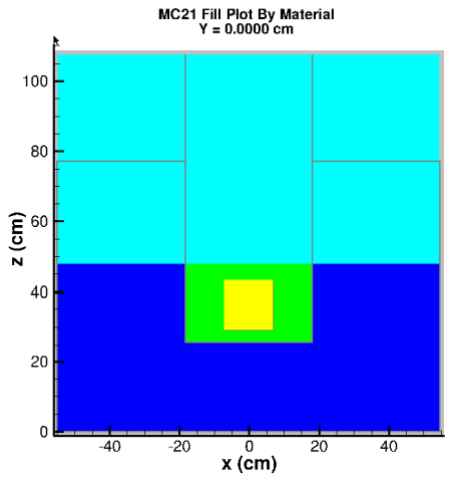


Figure 3. Example MC21 plot of model PST003.

Significance

Developing benchmark models using the PUMA-API, nuclear data cross sections, and critical eigenvalues generated by the MC21 Monte Carlo transport code will allow the development of an end-to-end qualification of CMCDT for use in general-purpose criticality analyses. It will also be more maintainable than using translated MC21 models. The development of a CMCDT-based general-purpose criticality analysis methodology will eventually allow the retirement of the legacy codes.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.19. Computational Design of Alloy Chemistry to Mitigate Fuel-Cladding Chemical Interactions in Uranium-Based Metallic Fuels

Report Participants

Samrat Choudhury,[1] Rabi Khanal,[1] Nicholas Ayers[1]

1 University of Idaho

Scientific Achievement

In U-based metallic fuels, lanthanide fission products react with the cladding materials leading to fuel-cladding-chemical interactions (FCCI). The FCCI results in reduced cladding integrity and eventual rupture of the cladding. Addition of dopant(s) to arrest lanthanides within the fuel-matrix by forming intermetallic compounds have generated considerable attention due to its effectiveness. However, there is lack of generic principle to choose appropriate dopant that can be effective in arresting a series of lanthanides. In this work, we have developed ab-initio-based thermodynamic alloy design principles which can be effective in identifying dopant(s) that can bind each lanthanide inside the fuel-matrix. We further investigated the role of alloying elements, such as Zr, on the dopant-lanthanide interactions. It was shown that easily available intrinsic characteristic of the dopant and lanthanides such as electronic configuration, covalent radius, and electronegativity can guide our choice of dopants to arrest a given lanthanide. Our approach correctly identifies both known dopants like Pd and new dopants such as As and Se which can be effective in binding lanthanides within U-matrix. Our predicted dopant-lanthanide behavior from ab initio calculations was verified experimentally. Later, the calculations and experiments were also performed in diffusion couples to further examine the ability to prevent FCCI in realistic scenarios.

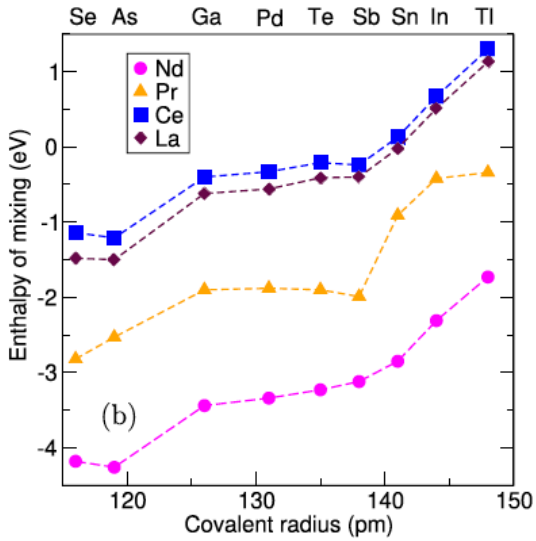


Figure 1. The correlation between enthalpy of mixing of the dopant obtained from electronic structure calculations and covalent radius of the dopant.

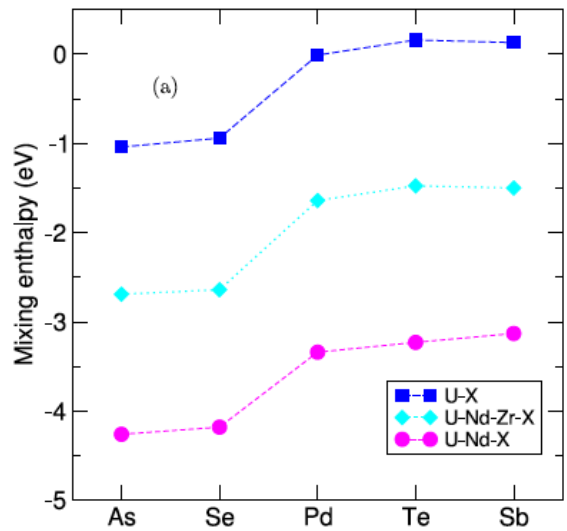


Figure 2. Calculated mixing enthalpy of dopant (X) in U, U–Nd, and U–Zr–Nd matrix.

Significance

This research provides a significant leap in alloy design beyond typically used empirical approaches such as Hume-Rothery rules or Darken-Gurry map. It was shown that solely based on readily available intrinsic features of dopants and lanthanides it is possible to predict the tendency of a given dopant to form intermetallic within the metallic matrix. We showed that the desired alloy chemistry can be predicted without creating complicated binary/ternary phase-diagrams, as currently needed. Finally, the work published in the journal *Nuclear Materials and Energy* (R. Khanal 2020) was listed among the the most downloaded articles.

Key Publications

- Khanal, R., N. Ayers, N. Jerred, M. Benson, R. Mariani, I. Charit, and S. Choudhury. 2021. "Role of zirconium in neodymium-dopants interactions within uranium-based metallic fuels," *Nuclear Materials and Energy*, 26:100912. https://doi.org/10.1016/j.nme.2021.100912.
- Jerred, N., R. Khanal, M. Benson, R. Mariani, S. Choudhury, and I. Charit. 2020. "Nd, SbNd and Sb3Nd4 and their interactions with the cladding alloy HT9," *Journal of Nuclear Materials*, 541:152387. https://doi.org/10.1016/j.jnucmat.2020.152387.
- Khanal, R., N. Jerred, M. Benson, Y. Xie, R. Mariani, I. Charit, and S. Choudhury. 2020. "Interactions and immobilization of lanthanides with dopants in uranium-based metallic fuels," *Journal of Nuclear Materials*, 540:152372. https://doi.org/10.1016/j.jnucmat.2020.152372.
- Khanal, R., N. Jerred, M. Benson, D. A. Andersson, R. Mariani, I. Charit, and S. Choudhury. 2020. "A novel approach to selection of dopant to immobilize neodymium in uranium-based metallic fuels," *Journal of Nuclear Materials*, 529:151922. https://doi.org/10.1016/j.jnucmat.2019.151922.
- Jerred, N., R. Khanal, M. Benson, E. Perez, J. King, M. Dubey, J. Burns, I. Charit, S. Choudhury, and R. Mariani. 2019. "Evaluation of tellurium as a fuel additive in neodymium-containing U-Zr metallic fuel," *Scientific Reports*, 9:16043. https://doi.org/10.1038/s41598-019-51852-z.
- Choudhury, S. 2020. "Computational design of alloy chemistry in uranium-based metallic fuels," School of Mechanical and Materials Engineering, Washington State University, Pullman, WA, October 8, 2020.

- Benson, M., Y. Xie, J. King, J. Harp, L. He, I. Charit, S. Choudhury, and J. Zhang. 2019. "Fuel additives to mitigate FCCI in metallic fuels," Materials in Nuclear Energy Systems, Baltimore, MD, October 6–10.
- Khanal, R., N. Jerred, I. Charit, M. Benson, R. Mariani, and S. Choudhury. 2019. "Guiding Principles of the Dopants Selection to Immobilize Lanthanide Fission Products in Uranium-based Metallic Fuels," TMS Annual Meeting, San Antonio, TX, Mar 10–14.

Sponsor/Program

Nuclear Energy University Program (NEUP)

A.20. Computational Modeling of Advanced Fuel Irradiation Experiments for Swelling and Fission Gas Release

Report Participants

Chris Ellis,[1] Hangbok Choi,[1] Jonas Opperman[1]

1 General Atomics

Scientific Achievement

Simulations were conducted to estimate pre-irradiation performance of uranium dioxide (UO2) and uranium carbide (UC) fuel kernels planned for irradiation in Oak Ridge National Laboratory's (ORNL's) HFIR. General Atomics (GA) fabricated fuel kernels and performed calculations of fuel swelling and fission gas release using the BISON code. This required new calculation modules for the UC thermal, mechanical and irradiation properties.

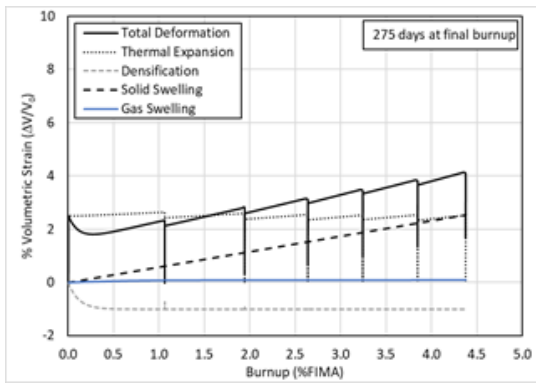


Figure 1. UO2 kernel volumetric strain during six HFIR cycles.

Significance

The new BISON modules successfully estimated the fuel deformation including the fuel densification, thermal expansion, and swelling. The fuel volumetric strain at the end of six HFIR cycles (~4.3 atom% burnup) is 4.1% and 8.3% for the UO2 and UC fuel kernels, respectively. The estimated UC swelling is 7%, which is reasonably close to the theoretically estimated value of ~5%. However, as the fuel irradiation is planned below 1173 K, BISON does not predict any fission gas release. Therefore, simulations continued to release the fission gases from the irradiated fuel kernels through an annealing test during the post-irradiation examination. It is expected that annealing above 1473 K for 10 days would release 2.6% and 2% of fission gases from the UO2 and UC fuel kernels, respectively.

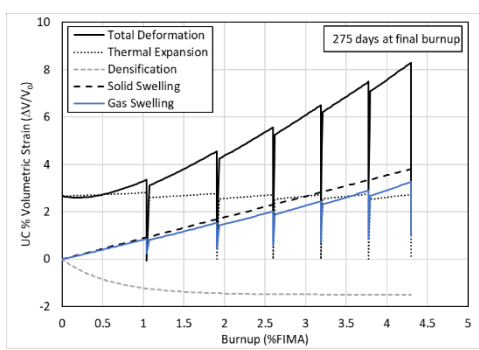


Figure 2. UC kernel volumetric strain during six HFIR cycles.

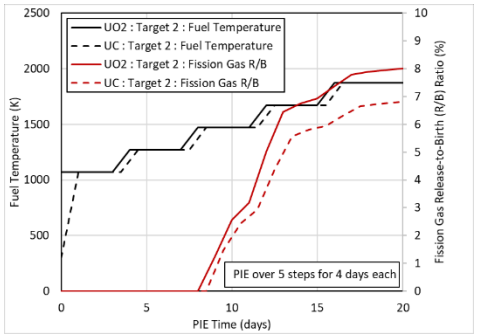


Figure 3. UO2 and UC kernel annealing tests.

Key Publications

- Ellis, C., H. Choi, and J. Opperman. 2020. "Preliminary Simulation of Advanced Fuel Irradiation Experiments for Swelling and Fission Gas Release," Proceedings of 2020 28th International Conference on Nuclear Engineering, Joint with the ASME 2020 Power Conference, ICONE28-POWER2020, Anaheim, CA, August 2–6.

Sponsor/Program

Work prepared for U.S. Department of Energy (Office of Nuclear Energy) under U.S. Government Contract Number DE-NE0008819.

Program: Combining Multi-Scale Modeling with Microcapsule Irradiation to Expedite Advanced Fuels Development.

A.21. Computer Modeling of Ag Diffusion in Crystalline and Amorphous SiC

Report Participants

Xianming Bai,[1] Chao Jiang[2]

1 Virginia Tech

2 Idaho National Laboratory

Scientific Achievement

Silver (Ag) is an important fission product in tristructural isotropic (TRISO) particle fuel. Experimentally, it has been observed that Ag can penetrate the SiC barrier layer in the TRISO fuel. However, its diffusion mechanism in the SiC is still not fully understood. In this work, we use MD simulations to study Ag diffusion in both crystalline and amorphous SiC. The former represents bulk SiC, while the latter represents regions with disordered SiC such as at grain boundaries or radiation-damaged regions. If successful, the results could elucidate the preferential diffusion path of Ag in SiC.

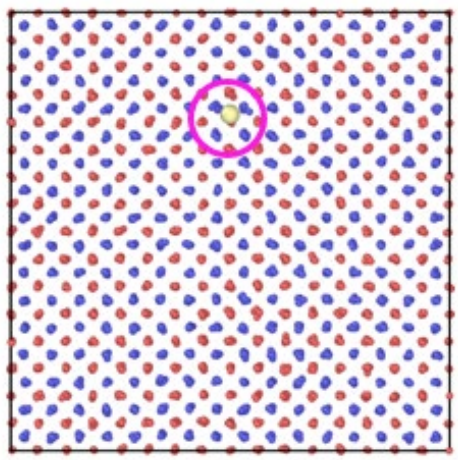


Figure 1. MD simulation of Ag (yellow sphere in the pink circle) diffusion in the crystalline SiC at 2400 K.

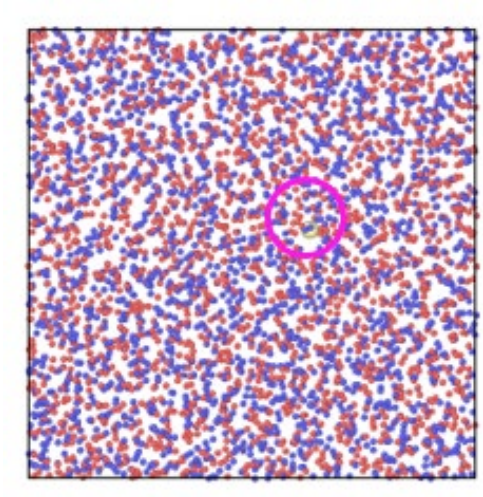


Figure 2. MD simulation of Ag (yellow sphere in the pink circle) diffusion in the amorphous SiC at 2400 K.

Significance

We have conducted MD simulations of Ag diffusion in both crystalline and amorphous SiC (first two figures below). The mean square displacement (MSD) of Ag is tracked during long-time simulation. To obtain statistical meaningful resutls, the MSD of Ag is averaged over 10 independent simulations. Our preliminary result shows that Ag can diffuse in both structures. At 2400 K, interestingly Ag diffusion in the crystalline SiC is much faster than in the amorphous SiC (third Figure below). If this is true, Ag diffusion at disordered grain boudaries could be slower than in the crystalline bulk, which is counter-intuitive. Currently, we are conducting more simulations see if this trend is still held.

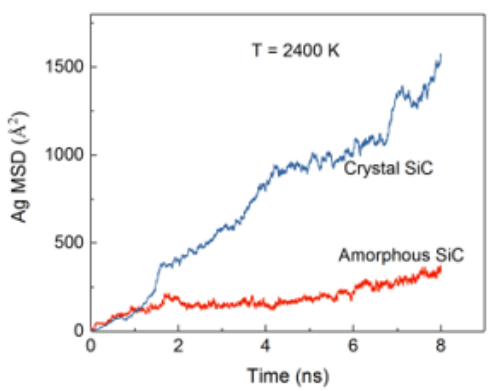


Figure 3. MSD of the Ag in the crystalline and amorphous SiC at 2400 K. Preliminary result shows that Ag diffuses faster in the crystalline SiC than in the amorphous SiC.

Key Publications

None. These are fairly new and preliminary results. If the results are significant, we will prepare a journal manuscript in the future.

Sponsor/Program

NEAMS and INL Joint Appointment Program.

A.22. Computer Modeling of Mn-Ni-Si Based G Phase in BCC and FCC Fe

Report Participants

Xianming Bai,[1] Brent Heuser[2]

1 Virginia Tech

2 University of Illinois at Urbana-Champaign

Scientific Achievement

Mn-Ni-Si-based G phase is widely found in Fe-based steels during irradiation or thermal annealing. Recently, our experimental team found that Mn-Ni-Si-based G phase can form in delta Fe, which has a body-centered-cubic (BCC) structure but not in gamma Fe, which has a face-centered-cubic (FCC) structure. To understand the underlying mechanism, we have conducted density functional theory (DFT) modeling to calculate the interface energies between G phase and Fe of different phases/structures.

Significance

G phase precipitates play an important role in affecting the mechanical properties of steels. Understanding their formation mechanism is important for predicting their precipitation kinetics in Fe-based alloys. Using DFT modeling, our results show that the interface energy between G phase and bcc Fe is lower than that between G phase and fcc Fe. The results provide a science-based explanation for our experimental observations.

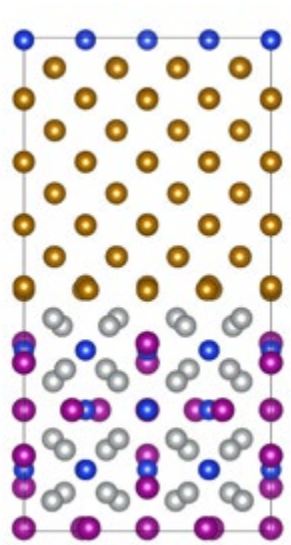


Figure 1. Interface between Mn-Ni-Si-based G phase (bottom) and bcc Fe (top).

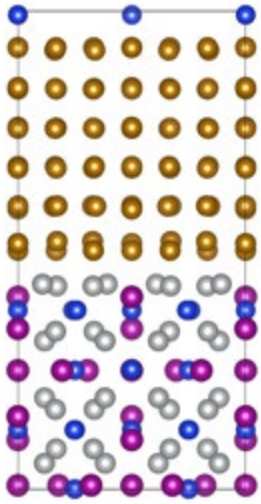


Figure 2. Interface between Mn-Ni-Si-based G phase (bottom) and fcc Fe (top).

Key Publications

- Li, Z., X. Zhan, X. M. Bai, S. C. Lee, W. Zhong, B. J. Sutton, and B. J. Heuser. 2021. "Modified Microstructures in Proton Irradiated Dual Phase 308L Weldment Filler Material," *Journal of Nuclear Materials*, 548:152825. https://doi.org/10.1016/j.jnucmat.2021.152825.

Sponsor/Program

NEUP and INL Joint Appointment Program.

A.23. Coupled Neutronic and Thermal Hydraulic Analysis of a Natural Circulation-Based Small Modular Reactor Using VERA-CS

Report Participants

Santosh Bhatt,[1] Andrew Godfrey,[1] Aaron Graham,[1] Jordan D. Rader,[1] Clayton D. Lietwiler,[2] Hunter Smith[2]

1 Oak Ridge National Laboratory

2 Holtec International

Scientific Achievement

ORNL and Holtec teams are able to utilize a common HPC framework at INL to facilitate collaboration on VERA model development for the Holtec small modular reactor (SMR)-160 design and analysis. The project uses the VERA codes MPACT, CTF, and VERAView on Sawtooth. The project has also made use of JupyterLab and interactive login sessions via hpcondemand.inl.gov.

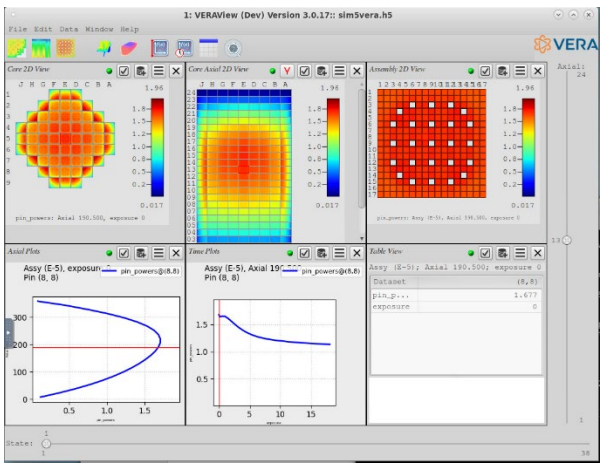


Figure 1. Example VERA results.

Significance

Note this project is still in progress. Holtec's SMR-160 is a fully passive circulation PWR. For at-power operation, the primary flow through the core is driven only by natural circulation; therefore, the nuclear and thermal-hydraulic parameters of the primary system are inherently coupled. As the SMR-160 design fully relies on natural convection for maintaining the coolant flow, eliminating the need for coolant pumps and external coolant loops inherent to conventional PWR designs, it raises operational challenges relating to neutronics of the core and on the core thermal hydraulics. This provides an exceptional opportunity for the SMR-160 to utilize the capabilities of the VERA-CS, which has the key advantage of coupling between its communicative counterparts, providing a multiphysics simulation capability that captures feedback behavior in the reactor core. The unique design of SMR-160 would greatly benefit from the tight coupling between the VERA codes and the resulting high fidelity of the solutions. Specifically, the coupling of deterministic neutronic solver MPACT with the thermal-hydraulics code CTF to calculate the subchannel level and the core wide thermal-hydraulic conditions during anticipated transients and accident scenarios for the SMR-160 design.

Key Publications

A final report will be submitted for this project at its completion in February 2022. The work is official use only (OUO) cooperative research and development agreement (CRADA) protected, and export controlled. An appropriately redacted conference paper may be prepared at the conclusion of the project.

Sponsor/Program

DOE GAIN Voucher

A.24. Davis-Besse Dosimetry Benchmark Using VERA and Shift

Report Participants

Herschel Smith,[1] Greg Hobson,[1] Justin Thomas (uncredited technical reviewer)[1]

1 Framatome

Scientific Achievement

Evaluation and benchmarking of VERA and Shift for use in commercial nuclear reactor excore fluence analysis.

Significance

VERA was found to provide accurate results for the incore power distributions, core reactivity calculations, and excore analysis neutron source terms of an operating commercial nuclear power plant in the United States. When coupled with the Shift Monte Carlo code, the simulation suite was found to provide accurate predictions of excore dosimeter fluences relative to measured data. Accurate prediction of excore fluence is of continual importance as the U.S. nuclear fleet begins to apply for further life extensions.

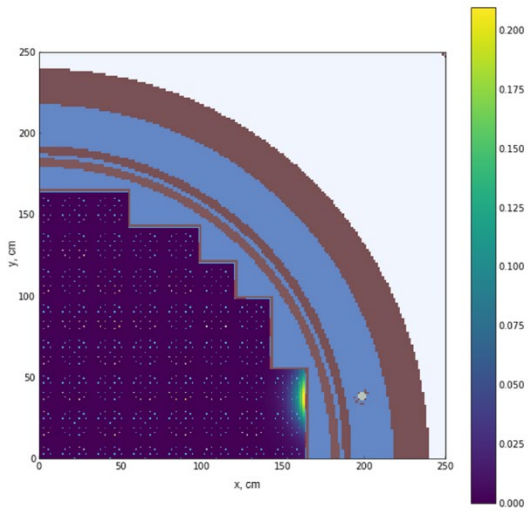


Figure 1. Shift adjoint flux calculation results.

Key Publications

- Smith, H. and G. Hobson. 2020. "Davis-Besse Dosimetry Benchmark using VERA and Shift," The Consortium for Advanced Simulation of Light Water Reactors Virtual Meeting, (282–286). https://dx.doi.org/10.13182/PCASL-32955.

Sponsor/Program

CASL, VERA User Group participation

A.25. Demonstration of Utilization of High-Fidelity NEAMS Tools to Inform the Improved Use of Conventional Tools Within the NEAMS Workbench on the NEA/OECD C5G7-TD Benchmark

Report Participants

Grigorios K. Delipei,[1] Joseph Fustero,[1] Maria Avramova[1]

1 North Carolina State University

Scientific Achievement

Multiphysics core uncertainty quantification studies at the pin-by-pin level are computationally very challenging. For this reason, simplifications are introduced to each coupled physical domain. In neutronics, direct transport calculations are replaced by the conventional two-step lattice/core calculations. In thermal-hydraulics, CFD modeling is replaced by average nodal values and simplified turbulence modeling. In fuel performance, the detailed coupling of 3D thermal, mechanical, and physico-chemical effects are replaced by a 1.5D modeling of the thermal feedback. In this project, the goal is to develop consistent high to low-fidelity (Hi2Lo) approaches for each physical domain and perform an improved low-fidelity pin-by-pin coupled calculation using the NEAMS workbench tools. Our contribution to this project focuses on the fuel performance Hi2Lo using BISON as the high-fidelity code and CTFFuel as the low-fidelity code.

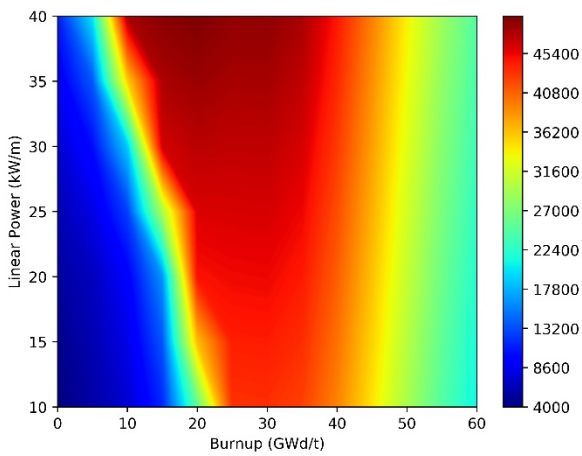


Figure 1. BISON generated 2D mean gap conductance table.

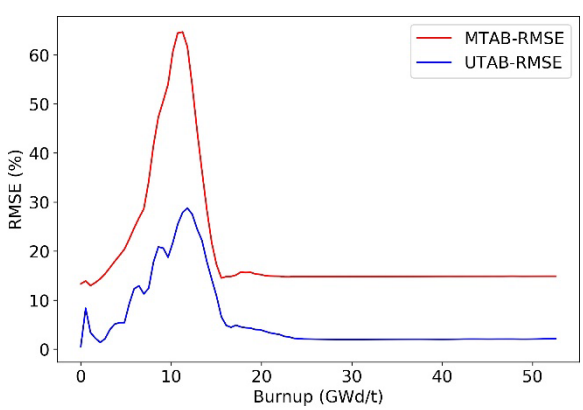


Figure 2. Proof of concept impact of the proposed UTAB approach on the gap conductance.

Significance

As the available computational power increases, multiphysics pin-by-pin calculations are becoming to be feasible. This imposes new challenges both in terms of efficient Hi2Lo approaches for each coupled physical domain and of consistent uncertainty propagation across the different domains and fidelities. With this work, we address the fuel performance Hi2Lo by focusing on the gap conductance due to the complex physical effects that are involved in its computation and due to its significant impact on fuel temperatures. A novel approach called UTAB was developed for gap conductance Hi2Lo as an extension of the 2D tabulated approaches typically employed in industrial applications. The BISON generated mean gap conductance table can be seen in Figure 1. The UTAB approach proof of concept study showed a significant improvement in the gap conductance prediction and a better understanding of its uncertainty due to high-fidelity modeling uncertainties as highlighted in Figure 2.

Currently ongoing research focuses on extending the UTAB approach to 3D gap conductance tables to incorporate the impact of historical effects and finalize the low-fidelity fully coupled pin-by-pin calculations. The impact of the UTAB approach is already significant on the gap conductance, but it should be also quantified on the low-fidelity fuel temperatures and on quantities from the other coupled physical domains.

Key Publications

- Fustero, J., G. K. Delipei, A. Abarca, A. Bennett, M. Avramova, and K. Ivanov. 2021. "High to Low Methodology for Gap Heat Transfer in an Uncertainty Quantification Framework for Depletion," American Nuclear Society, Mathematics & Computation, virtual meeting, pp. 1676-1687.

Sponsor/Program

NEUP, NEAMS

A.26. Developing the Miner Python Package for Processing Results from the MC21 Monte Carlo Reactor Physics Code

Report Participants

Daniel Gill,[1] Jeffery Wegener[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Miner is a post-processing system developed for the Monte Carlo reactor physics code MC21. Miner is developed as a Python package built on top of the Pandas and xarray packages. These packages are sophisticated tools for processing data at near-compiled speed with the convenience of being Python-based. Whereas Pandas is optimized for two-dimensional data, xarray is geared towards the type of multidimensional data encountered in the physical sciences. INL HPC resources were used for the development of new capability in Miner, the development of an automated test suite via pytest, and the creation of a fully featured user guide.

Significance

Modern reactor simulation tools like MC21 are very powerful and flexible in the types of calculations they allow. However, they have the potential to produce hundreds of gigabytes of output spread over hundreds of files in a single simulation. Miner greatly improves the accessibility of this data and gives MC21 users direct access to current data analysis capability to interrogate and manipulate this data either through a Python script or a Jupyter Notebook. The work done on the INL HPC to further the develop of Miner directly supports its first production release at NNL.

Key Publications

No publicly available reports or presentations are available.

Sponsor/Program

Nuclear Science and Technology

A.27. Development and Assessment of Advanced Modeling Capabilities for Fission Gas Behavior and Nuclear Fuel Performance

Report Participants

Giovanni Pastore[1]

1 University of Tennessee, Knoxville

Scientific Achievement

The BISON code is used to perform simulations of nuclear fuel behavior in the framework of U.S. DOE-funded projects at the University of Tennessee, Knoxville (UTK) and in collaboration with the BISON team at INL. Specific technical applications are modeling of fuel rod irradiation experiments form the International Fuel Performance Experiments database and modeling experiments from the Halden Reactor Project, including Cr2O3-doped UO2 fuel rod tests as well as loss-of-coolant accident (LOCA) experiments. Another area of application for the BISON code at UTK is modeling TRISO particle fuel, which also is in collaboration with INL.

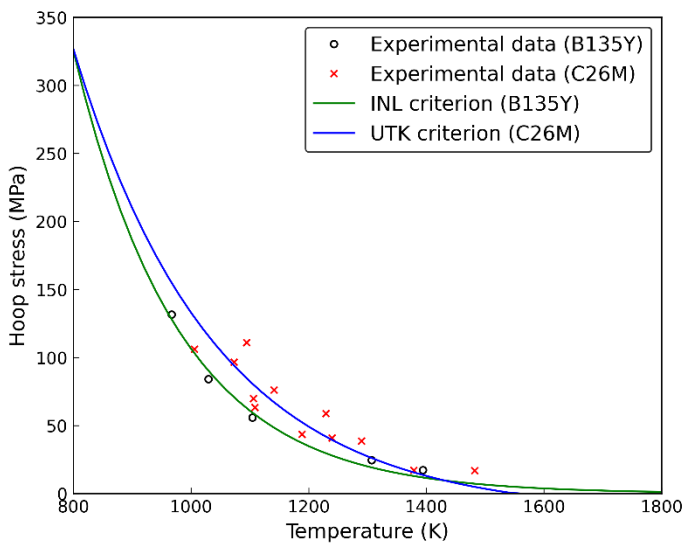


Figure 1. FeCrAl cladding failure criteria in BISON, including the recently implemented model from UTK (from BISON documentation, 2021).

Significance

The research performed with the BISON code through this request will positively impact multiple DOE research projects that rely on the use of BISON. In particular, it is foreseen that the work performed will advance the development and validation of BISON in areas such as fission gas behavior in LWR oxide fuel and accident tolerant fuel (ATF) cladding, in particular, iron-chromium-aluminum (FeCrAl) steel cladding. These are important focus areas in current U.S. DOE research projects. Specific projects that involve the usage of BISON at UTK are Contract No. 237499 between INL and UTK, the DOE SciDAC project on Fission Gas Behavior and the NEUP-IRP project on multiphysics fuel performance modeling of TRISO-bearing fuel in advanced reactor environments.

Work performed to date with BISON at UTK under this HPC account has included modeling and validation of LWR fuel rod behavior under LOCA conditions, fission gas behavior modeling under the aforementioned DOE-NE SciDAC project, as well as the implementation and testing in BISON of new models for iron-chromium-aluminum (FeCrAl) ATF cladding.

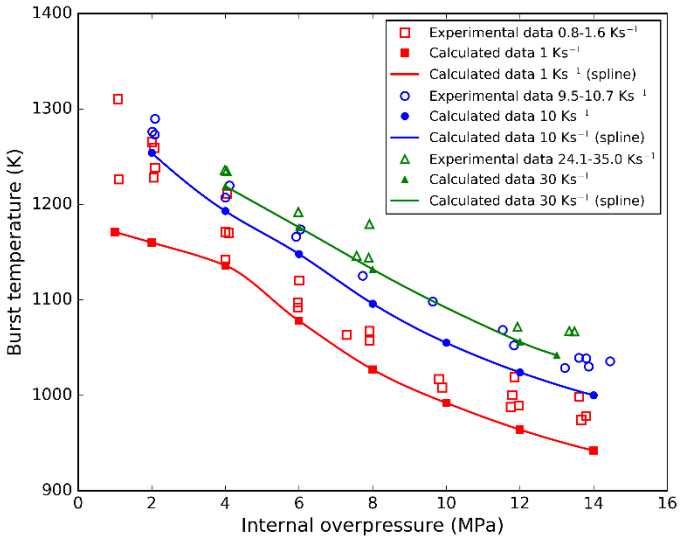


Figure 2.3 BISON calculations and experimental data of cladding burst temperature for the LOCA tests REBEKA (G. Pastore 2021).

Key Publications

- Pastore, G., K. A. Gamble, R. L. Williamson, S. R. Novascone, R. J. Gardner, and J. D. Hales. 2021. "Analysis of fuel rod behavior during loss-of-coolant accidents using the BISON code: Fuel modeling developments and simulation of integral experiments," *Journal of Nuclear Materials*, 545:152645. https://doi.org/10.1016/j.jnucmat.2020.152645.
- Pastore, G., R. L. Williamson, R. J. Gardner, S. R. Novascone, J. B. Tompkins, K. A. Gamble, and J. D. Hales. 2021. "Analysis of fuel rod behavior during loss-of-coolant accidents using the BISON code: Cladding modeling developments and simulation of separate-effects experiments," *Journal of Nuclear Materials*, 543:152537. https://doi.org/10.1016/j.jnucmat.2020.152537.
- Gamble, K. A. et al. 2021. Presentation on BISON Accident Tolerant Fuels developments, NEAMS Fuels Technical Area—Spring Meeting. In preparation.

Sponsor/Program

NEAMS, SciDAC, NEUP-IRP

A.28. Development of a Mechanistic Hydride Behavior Model for Spent Fuel Cladding Storage and Transportation

Report Participants

Edward M. Duchnowski,[1] Seokbin Seo,[1] Miles O'Neal,[1] Nicholas R. Brown[1]

1 University of Tennessee, Knoxville

Scientific Achievement

Implementation of a hydrogen migration and redistribution model in BISON is demonstrated. Two main components such as hydrogen diffusion and precipitation kinetics are assessed using separate effect test simulations. The concentration-penetration curve of hydrogen was retrieved from BISON predictions, and the diffusion coefficient was estimated.

The prediction of hydrogen distributions is validated using historical experiments and ongoing experiments conducted within the scope of project. Both existing and the improved hydrogen models are tested using the same simulations under both experimental conditions.

Sensitivity analysis of BISON model was conducted to determine the impact on accuracy of key parameters relating to hydrogen behavior.

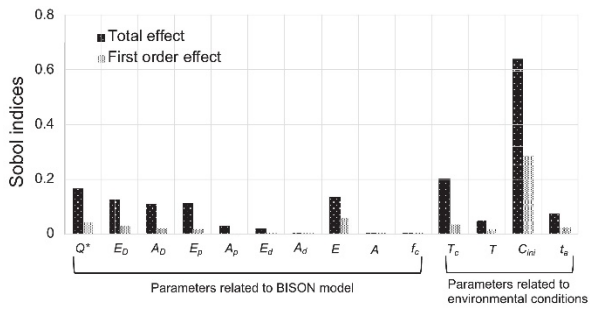


Figure 1. Sobol indices of key parameters for BISON with the target being accuracy of the model against experimental data.

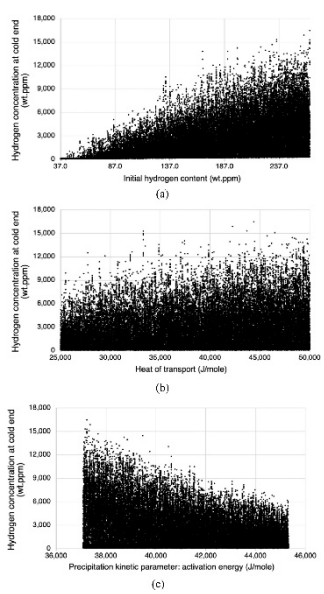


Figure 2. Scatter plots of total hydrogen content at one end verses (a) initial hydrogen content (b) heat of transport (c) activation energy for precipitation.

Significance

The study finds that BISON predictions of diffusion behavior of hydrogen in zirconium is in a reasonable agreement with the experimental data. BISON prediction of precipitation kinetic parameters in comparison with experimental data shows that BISON follows closely the historical data. In addition, BISON accurately predicts the total hydrogen distribution along the sample where the concentration increases towards the colder regions.

The improvement in precipitation and dissolution kinetics of BISON model, referred to as the HNGD model, appeared in the prediction of hydrogen distribution under historical and ongoing experiments, showing that the new model was successfully implemented into BISON.

Senstivitity analysis shows that initial conditions on the experiment have the most importance in accuratly predicting hydrogen behavior. Based on this analysis, updated parameter values may be used to better match experimental resutls for hydrogen diffusion.

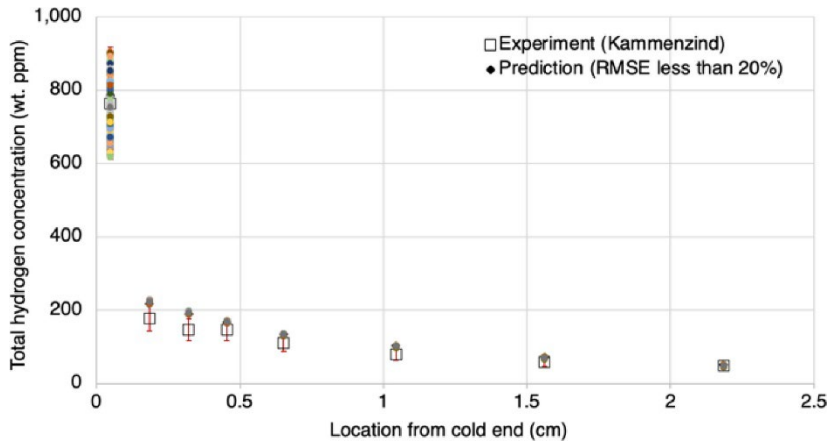


Figure 3. BISON calculation with updated parameter values from sensitivity analysis and compared against experimental results.

Key Publications

- Aly, Z., A. Casagranda, G. Pastore, and N. R. Brown. 2019. "Variance-based sensitivity analysis applied to hydrogen migration and redistribution model in Bison. Part I: Simulation of historical experiments," *Journal of Nuclear Materials*, 524:90–100. https://doi.org/10.1016/j.jnucmat.2019.06.035.
- Aly, Z., A. Casagranda, G. Pastore, and N. R. Brown. 2019. "Variance-based sensitivity analysis applied to the hydrogen migration and redistribution model in Bison. Part II: Uncertainty quantification and optimization," *Journal of Nuclear Materials*, 523:478–489. https://doi.org/10.1016/j.jnucmat.2019.06.023.
- Seo, S., E. M. Duchnowski, N. R. Brown. 2020. "The Impact of Model Parameters and Local Conditions on the Hydrogen Migration and Redistribution Model in Bison," Proceedings of ANS Annual Meeting 2020, June 8–11.
- Seo, S. B., E. M. Duchnowski, M. O'Neal, A. T. Motta, F. Passelaigue, S. Kang, and N. R. Brown. 2021. "Sensitivity analysis of BISON model for characterization of impact of experimental parameters on hydrogen migration and redistribution in zirconium-based alloys," *Journal of Nuclear Materials*, 550:152941. https://doi.org/10.1016/j.jnucmat.2021.152941.

Sponsor/Program

U.S. DOE IRP-FC-1

A.29. Development of a New Gibbs Energy Minimiser for MOOSE-Based Corrosion Modeling Application YellowJacket

Report Participants

Parikshit Bajpai,[1] Max Poschmann,[1] Markus H.A. Piro[1]

1 Ontario Tech University

Scientific Achievement

Corrosion of structural materials by the molten salt is of particular interest in molten-salt reactors (MSRs). Corrosion is an electrochemical process driven by thermodynamics that occurs at a rate controlled by reaction kinetics which in turn is significantly affected by material microstructure. Corrosion modeling at mesoscale requires coupling thermodynamic equilibrium calculations with the phase field method. A new MOOSE-based tool, YellowJacket, is currently being developed to perform such simulations and provide quantities such as the rate of material loss, corrosion product production, and precipitate production in liquid. As part of this project, a new Gibbs energy minimiser is being developed to predict the Gibbs energies, chemical potentials, and driving forces for the various phases which can be present in the system in order to inform the phase field module. This will help in improving the accuracy of corrosion prediction.

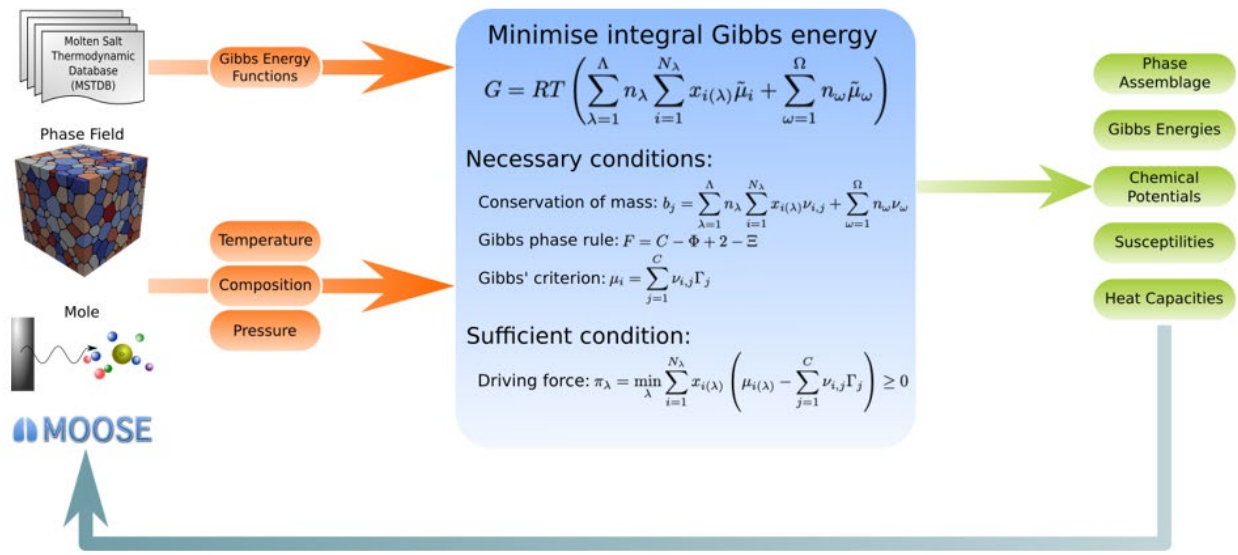


Figure 1. Principle of Gibbs energy minimization along with inputs and outputs and their exchange between the YellowJacket modules. The exchange is also possible with other MOOSE-based apps such as Mole.

Significance

Currently, the thermodynamic equilibrium solver can predict the phase assemblage for solution phases modeled using ideal solution, substitutional solution or modified quasichemical (MQM) models. The initial focus is on Ni alloys interacting with molten-LiF-KF salts, and the GEM capabilities are demonstrated using the KF-NiF2 binary system shown in Figure 2. A square with molar composition 0.7 KF + 0.3 NiF2 under a linear temperature gradient has been solved for thermodynamic equilibrium. Currently, the compound energy formalism is being implemented in the GEM solver. This would make YellowJacket GEM solver fully compatible with the Molten Salt Thermodynamic Database (MSTDB). Coupling of GEM and phase field modules will start soon.

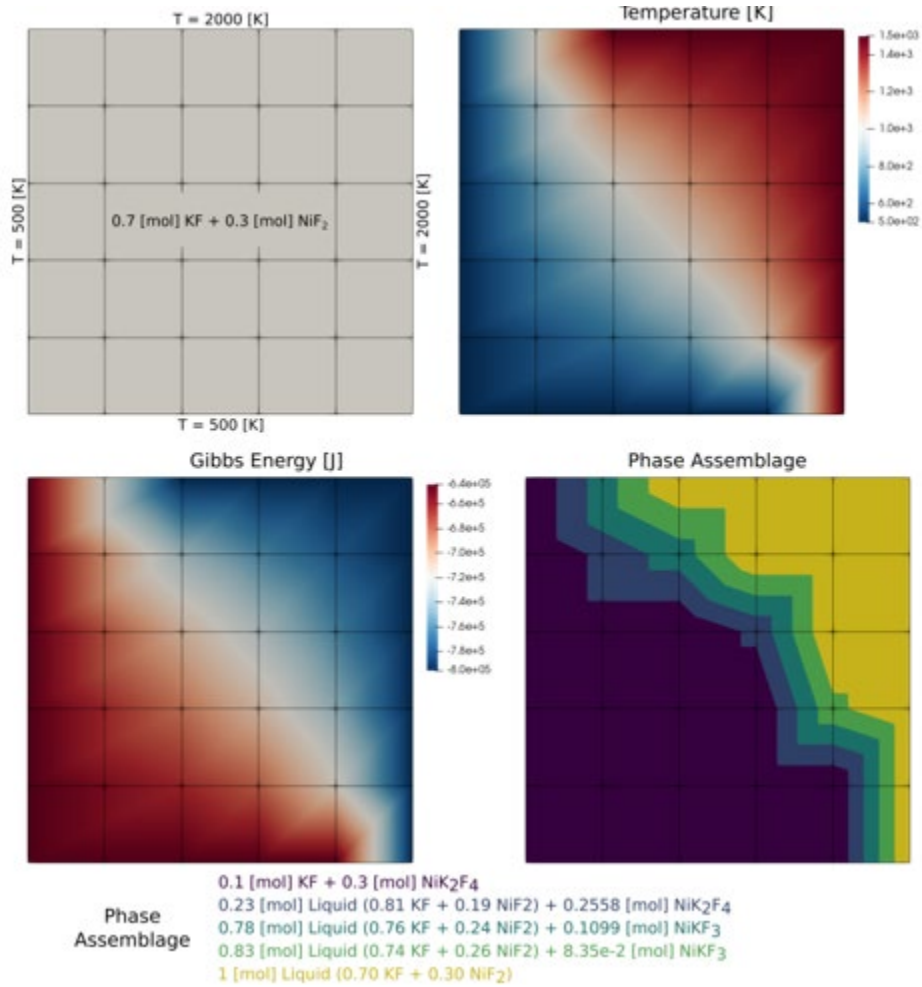


Figure 2. Demonstration problem mesh with the applied boundary conditions (top-left), temperature gradient (top-right), Gibbs energies (bottom-left), and stable phases (bottom-right).

Key Publications

- Bajpai, P., M. Poschmann, and M. H. A Piro. 2021. "Derivations of Partial Molar Excess Gibbs Energy of Mixing Expressions for Common Thermodynamic Models," *Journal of Phase Equilibria and Diffusion*, 42:333–347. https://doi.org/10.1007/s11669-021-00886-w.
- Bajpai, P., M. Poschmann, D. Andrš, C. Bhave, M. Tonks, and M. H. A Piro. 2020. "Development of a New Thermochemistry Solver for Multiphysics Simulations of Nuclear Materials," In TMS 2020 149th Annual Meeting & Exhibition Supplemental Proceedings, 1013-1025. New York City: Springer, Cham.
- Piro, M. H. A., M. Poschmann, and P. Bajpai. 2019. "On the interpretation of chemical potentials computed from equilibrium thermodynamic codes: Applications to molten salts," *Journal of Nuclear Materials*, 526:151756. https://doi.org/10.1016/j.jnucmat.2019.151756.

Sponsor/Program

DOE NEAMS

A.30. Development of a Subchannel Analysis Model for Liquid Metal Reactors

Report Participants

Aydin Karahan[1], David Andrs[2], Vasileios Kyriakopoulos[3], Sebastian Schunert[2]

1 Argonne National Laboratory

2 Idaho National Laboratory

3 Texas A&M University

Scientific Achievement

Subchannel analysis is one of the essential pieces to perform design and safety analysis of nuclear reactors. A MOOSE-based subchannel analysis model is being developed for sodium and lead fast reactors which are promising advanced reactor designs. The resulting code will directly assist vendors such as TerraPower and Westinghouse in their design, safety analysis, and licensing process.

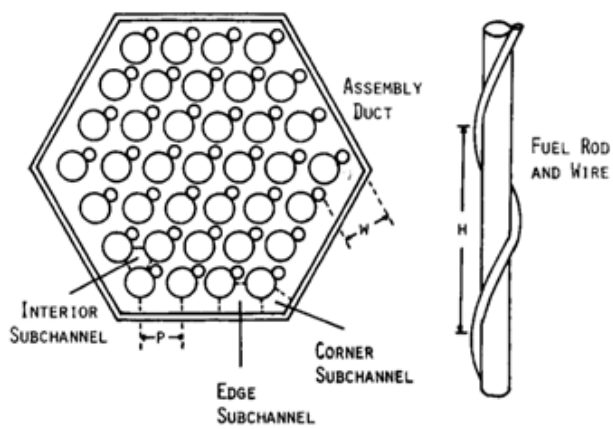


Figure 1. SFR subassembly.

Significance

The MOOSE-based subchannel analysis code developed for the water coolant has been extended to sodium-fast reactor (SFR) conditions using sodium coolant. There are distinct differences between light-water reactors (LWRs) and SFR subassemblies. Figure 1 shows that typical SFR subassembly is in hexagogonal shaped with a wrapper and each pin is wrapped with a wire. In order to model the friction and cross-flow behavior for this specific condition, detailed Cheng-Todreas model has been implemented into the code. In addition, the solver has been extended to enable uniform inlet pressure boundary condition. Figure 2 shows a typical code output for a SFR subassembly coolant temperature distribution where central parts are hotter then the edges.

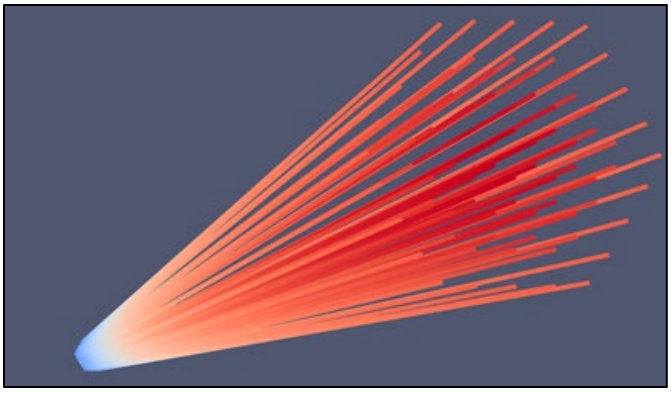


Figure 2. Subchannel analysis simulation—coolant temperature.

Key Publications

None.

Sponsor/Program

NEAMS

A.31. Development of a Tritium Transport Model for Coupled Multiphysics Analysis and Optimization of Fusion Reactor Blanket Systems

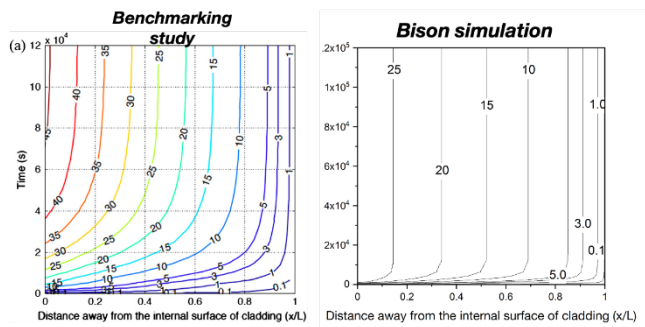
Report Participants

Niles O'Neal,[1] Seokbin Seo,[1] Nick Brown[1]

1 University of Tennessee, Knoxville

Scientific Achievement

The objective is to establish a framework for tritium transport analysis of fusion reactor blankets to be coupled with neutronics and thermal hydraulics models for multiphysics analysis. This would provide a method for analyzing and optimizing fusion blanket designs. Initial modeling focuses on steel materials due to their use as the main structural materials for blankets such as a DCLL design. Using BISON's hydrogen transport code, 1D modeling of stainless-steel structures for verification and validation purposes have been conducted. Root-mean-square error analysis of steel structures and their studies are being conducted to improve model accuracy and develop a methodology for blanket optimization.



Hu et al., "Hydrogen permeation in FeCrAl alloys for LWR cladding application." J. Nucl. Mat. 461, 2015.

Figure 1. BISON prediction of hydrogen concentration in FeCrAl cladding as a function of position.

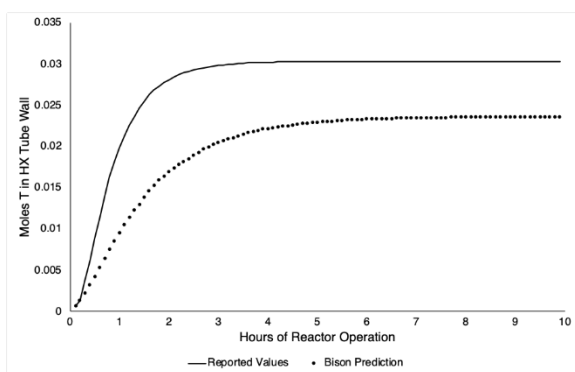


Figure 2. BISON prediction of tritium content in heat exchanger steel wall as a function of time.

Significance

Comparing with reported data, BISON has been able to reasonably predict the diffusion behavior of hydrogen isotopes in steel structures. This includes transient conditions for steels which supports BISON's ability to provide meaningful analysis of fusion blanket systems.

Key Publications

None.

Sponsor/Program

U.S. DOE, Office of Fusion Energy Sciences under Contract No. DE-AC05-00OR22725

A.32. Development of an Efficient Scoring Algorithm for Local Differential Tallies in Monte Carlo Simulations

Report Participants

D.P. Griesheimer,[1] G. Kooreman[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Recent investigations into the use of low-order approximations as surrogate physics models in multiphysics simulations has motivated a renewed interest in the use of differential operator tallies for calculating local derivatives during Monte Carlo transport calculations. However, the traditional algorithm for scoring differential operator tallies requires information to be collected for every tally at every particle event (i.e., collision and surface crossings), which can be computationally inefficient when estimating local derivatives by region for large problems, such as a reactor core. In this work, we propose an alternate scoring algorithm for differential operator tallies that exhibits improved scalability with respect to the number of simultaneous tallies collected during a simulation. Formal analysis shows that the proposed scoring algorithm is more efficient and uses less memory in cases where the number of differential operator tallies is greater than the expected number of events per particle history. A prototype version of the proposed method was implemented in a Python-based Monte Carlo transport mini-application (minimc) within the Simplified Mini-Applications for Radiation Transport (SMART) framework. Numerical results using the prototype implementation confirm the accuracy and computational efficiency of the scoring algorithm for a series of realistic test problems.

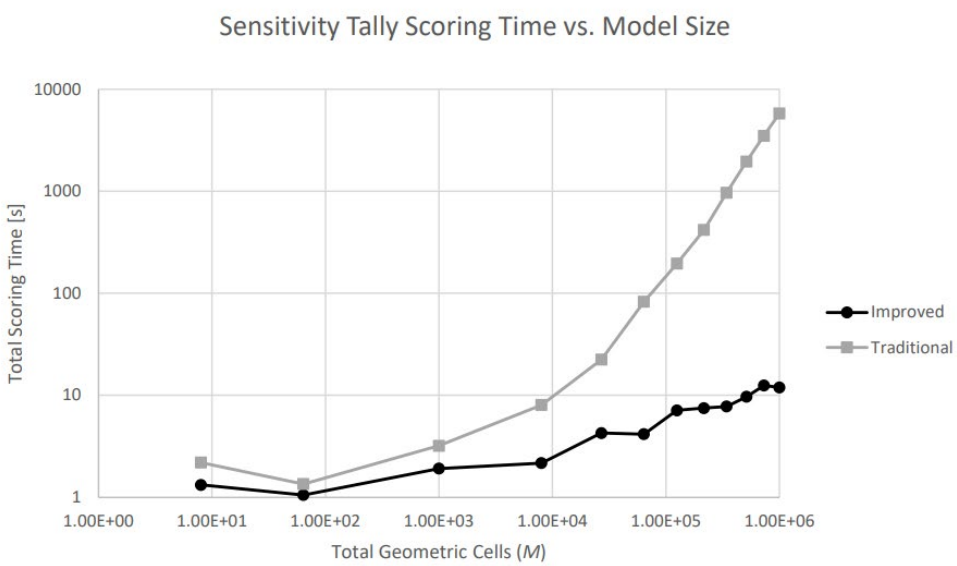


Figure 1. Comparison of total scoring time for improved and traditional differential operator tally implementations with respect to model size (i.e., number of cells in the model).

Significance

This work resulted in the development of an improved algorithm for scoring differential operator (DO) tallies in Monte Carlo radiation transport simulations. The novel scoring algorithm collects event data for each history and then processes the data in reverse sequential order to score all DO tallies with a non-zero contribution from the corresponding history. The computational cost for the alternate scoring algorithm is independent of the number of tallies present in the model, unlike the traditional algorithm, where the total cost of scoring scales linearly with the number of tallies. Numerical experiments were used to demonstrate the accuracy and improved performance of the alternate scoring algorithm. These results confirm that the improved scoring algorithm significantly outperforms the traditional scoring approach for collecting local sensitivity tallies in large models, with a 500x speedup observed for a model with 1×106 tallies. Testing with non-uniform density perturbations on a 2D PWR assembly suggests that cellwise estimates of reactivity derivatives produced with DO tallies can be used to approximate reactivity feedback effects up to ~10% change in water density. These encouraging results suggest that it may be possible to use local derivative tallies with first-order perturbation theory to implicitly account for reactivity feedback effects during Monte Carlo transient calculations using improved quasistatic or predictor-corrector quasistatic time discretization methods.

Key Publications

- Griesheimer, D. P and G. Kooreman. 2021. "Efficient Scoring Algorithm for Local Differential Operator Tallies in Large Models," Proceedings of The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021), Raleigh, North Carolina, October 3–7, 2021.

Sponsor/Program

Nuclear Science and Technology

A.33. Development of Data-Driven Constitutive Models for Structural Materials in Nuclear Energy

Report Participants

Aaron E. Tallman,[1] Stephen Novascone,[2] Laurent Capolungo[1]

1 Los Alamos National Laboratory

2 Idaho National Laboratory

Scientific Achievement

Our scientific achievements include developing microstructure sensitive, mechanistic models of high-temperature creep, irradiation creep, and visco-plasticity in Grade 91 steel, HT-9 steel (Tallman et al. 2021), and other material systems and implementing them in the MOOSE finite element method framework. In this project, mechanistic constitutive models of thermal and irradiation creep, calibrated to experiments, are employed in a Visco-Plastic Self-Consistent (VPSC) framework. This framework is used in tandem with an in-house Python package to generate and manage very large databases of VPSC simulations (>10,000s). These databases are employed in fitting regression models that operate as a data-driven constitutive model, at a small fraction (1%) of the computational cost of the VPSC simulations.

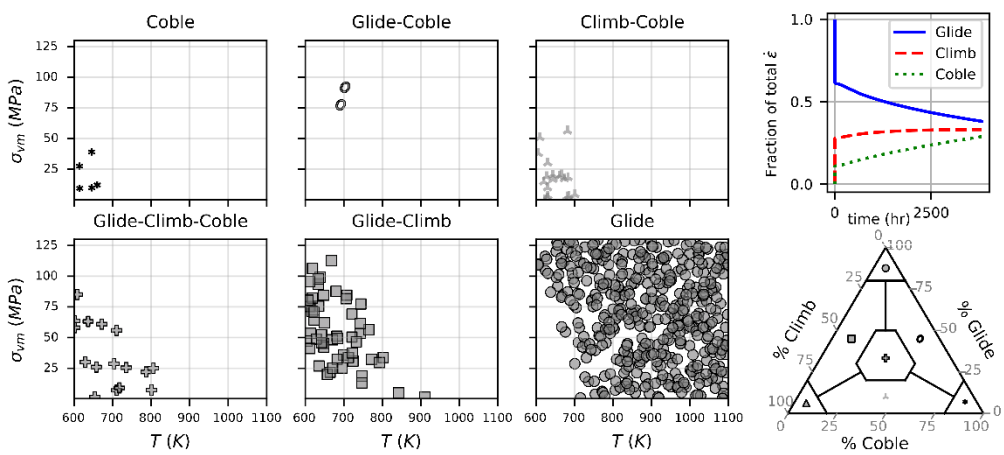


Figure 1. The mechanisms contributing to deformation vary across the range of temperatures and applied stresses in HT-9.

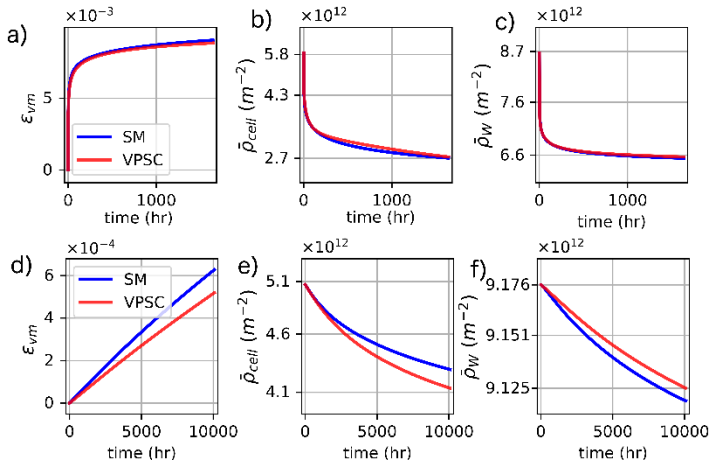


Figure 2. The predictions of the surrogate model (SM) compared to the original VPSC simulation of a creep test (HT-9).

Significance

The developed model, Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations (LARomance), can be applied in MOOSE simulations at the component scale, allowing primary and secondary creep to be considered in constant-load, cyclic-load, and cyclic-temperature conditions. These modeling capabilities are not yet found in any other computational-cost-competitive modeling approach. These new modeling capabilities will impact the development of components that will experience cyclic loading during long service lifetimes.

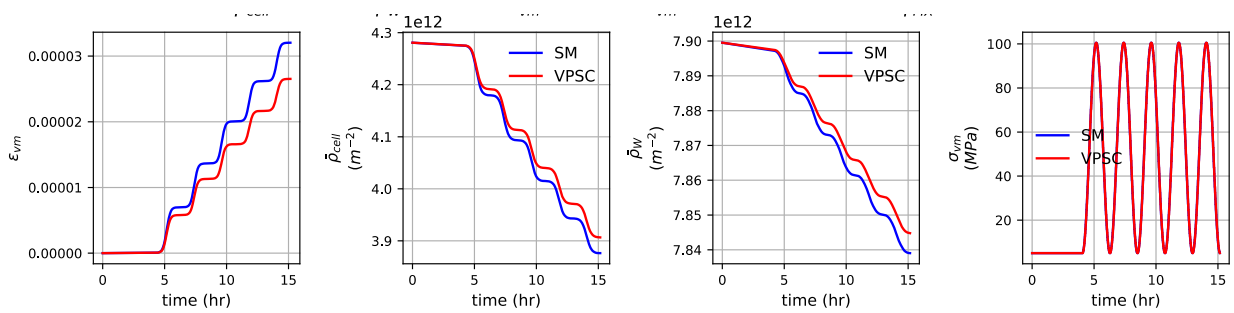


Figure 3. The predictions of the SM compared to the original VPSC simulation of transient strain under cyclic stress (P91 steel).

Key Publications

- Tallman, A. E., M. A. Kumar, C. Matthews, and L. Capolungo. 2021. "Modeling of Viscoplasticity in Steels: Application to Thermal, Irradiation Creep and Transient Loading in HT-9 Cladding," *Journal of The Minerals, Metals & Materials Society*, 73(1):126–137. https://doi.org/10.1007/s11837-020-04402-2.

Sponsor/Program

NEAMS

A.34. Development on an OpenFOAM Interface for ENRICO

Report Participants

L. Bullerwell,[1] P. Shriwise,[2] P. Romano,[2] R. Rahaman,[2] J. Hou[1]

1 North Carolina State University

2 Argonne National Laboratory

Scientific Achievement

ENRICO is an open-source multiphysics application utilizing multiple neutronics and thermal hydraulics (TH) solvers that can be selected at runtime to perform in-memory coupling. Previously, Nek5000/NekRS, Shift, and OpenMC were supported as solvers in ENRICO. This work includes an additional TH solver, the FoamDriver, which provides a TH solution based on the multi-region conjugate heat solver in OpenFOAM.

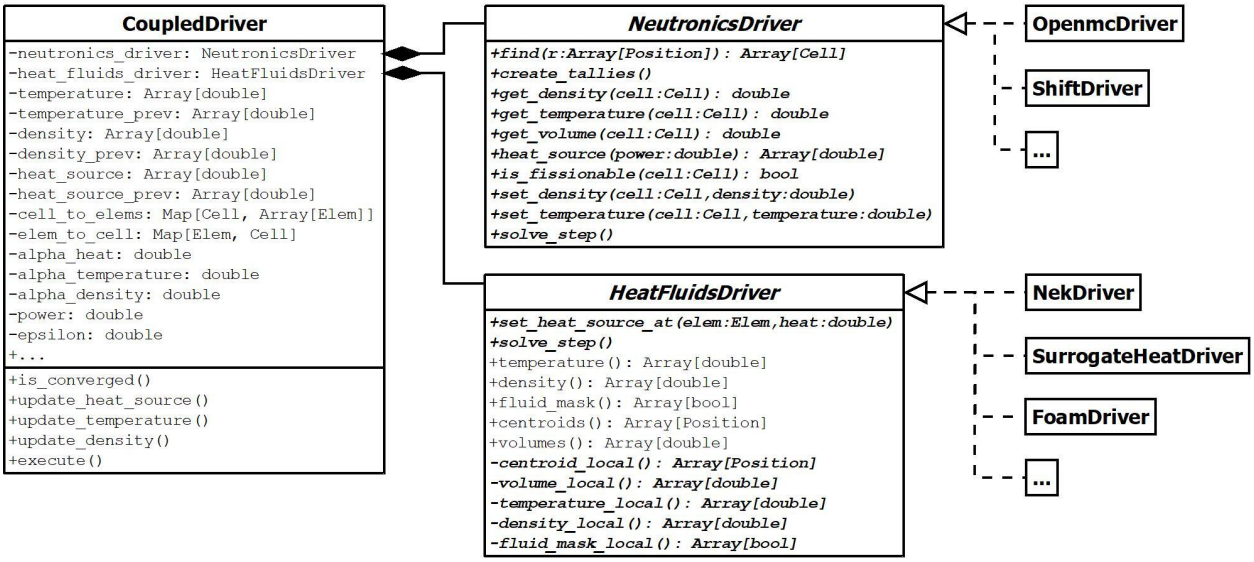


Figure 1. ENRICO class diagram.

Significance

ENRICO is intended to be a framework for in-memory coupling of neutronics and TH codes for exascale architecture that is agnostic to the underlying neutronics and TH solvers employed. The inclusion of an OpenFOAM TH solver validates the design of ENRICO's interfaces and coupling schemes. Additionally, it provides a pathway for OpenFOAM users to perform multiphysics simulations and perform cross-code comparisons against Nek5000/NekRS with a consistent coupling approach.

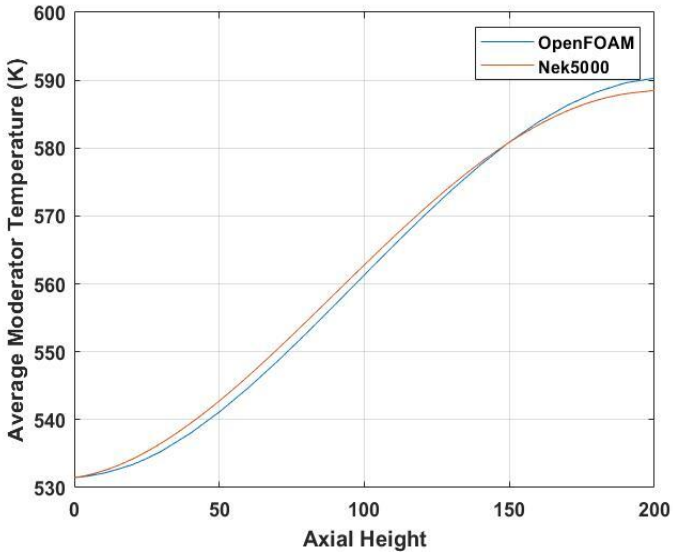


Figure 2. Axial temperature profiles of a coolant channel in a 17x17 assembly modeled after the NuScale SMR design.

Key Publications

- Romano, P., S. Hamilton, S, R. Rahaman, A. Novak, E. Merzari, and S. Harper, et. al. 2020. "A Code-Agnostic Driver Application for Coupled Neutronics and Thermal-Hydraulics Simulations," *Nuclear Science and Engineering*, 195:391–411. https://doi.org/10.1080/00295639.2020.1830620.
- Bullerwell, L., P. Shriwise, P. Romano, R. Rahaman, and J. Hou. 2021. "Development of an OpenFOAM Interface for ENRICO," American Nuclear Society Mathematics and Computation 2021 Meeting. Raleigh, NC. Oct. 3–7, 2021.

Sponsor/Program

DOE ECP - ExaSMR

A.35. DNS and LES of a 5x5 Rod Bundle with Impacts of a Central Control Rod Thimble Tube

Report Participants

Adam Kraus,[1] Elia Merzari,[1] Thomas Norddine,[2] Sofiane Benhamadouche,[2] Oana Marin[3]

1 Penn State University

2 EDF R&D

3 Argonne National Laboratory

Scientific Achievement

This project used the highly scalable Nek5000 code to simulate the fluid flow through a 5x5 square rod bundle with dimensions typical of LWR fuel. This is the smallest representative geometry for the fuel bundle class, in that there is no direct geometric linking between the edge and central subchannels. The geometry notably includes an outer wall that represents a more realistic advancement over some prior "infinite lattice" studies found in the literature. The high-fidelity approaches of large eddy simulation (LES) and direct numerical simulation (DNS) were performed for the baseline 5x5 geometry to generate very detailed representations of the turbulent flow field. LES was also performed for a 5x5 case with a larger central tube, representing a control rod guide thimble tube. These simulations are enabled by HPC and are believed to represent the first systematic analyses of this class of geometry with high-fidelity approaches.

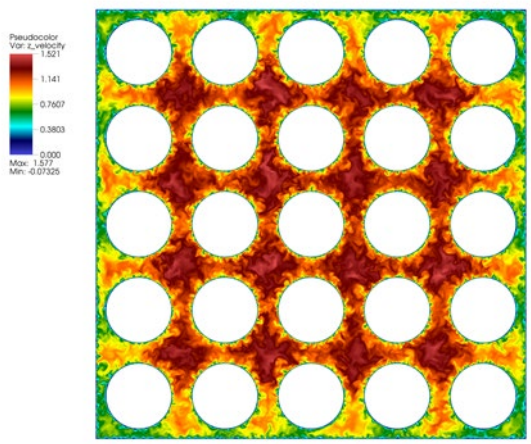


Figure 1. Instantaneous streamwise velocity in a 5x5 rod bundle.

Significance

The work is believed to be the first DNS of a 5x5 rod bundle in the open literature. The DNS provides full and unfettered access to the flow field, and can be used as a reference data set that supplements and in some areas expands upon traditional physical experiments. This work also presented the first publication of turbulent kinetic energy budgets for this class of geometry. Similarly, the project provided what is believed to be the first systematic analysis of the impacts of a central thimble tube on flow behavior with a high-fidelity approach. A number of post-processing techniques were used to describe notable aspects of the flow field. These included a novel invariant analysis technique which demonstrated a transition toward two-component turbulence that is present in the narrow gaps at the edge walls and near the central thimble tube. All of these findings can be used as highly detailed validation data to guide and improve lower-fidelity modeling approaches, ranging from coarser CFD to subchannel and applying to other codes that are included under the NEAMS umbrella. An ongoing phase of the work is to use the high-fidelity data to mechanistically improve subchannel and porous media models in Pronghorn. This work is part of a current Integrated Research Project (IRP) led by Penn State.

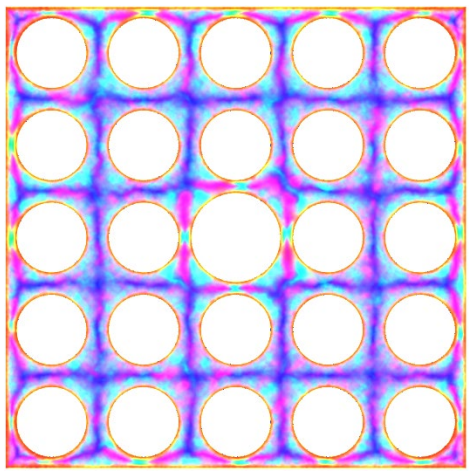


Figure 2. Anisotropy invariant analysis demonstrating the transition toward two-component turbulence in the thimble vicinity and in the narrow wall gaps.

Key Publications

- Kraus, A., E. Merzari, T. Norddine, O. Marin, and S. Benhamadouche. 2021. "Direct Numerical Simulation of Fluid Flow in a 5x5 Square Rod Bundle," *International Journal of Heat and Fluid Flow*, 90:108833. https://doi.org/10.1016/j.ijheatfluidflow.2021.108833.
- Kraus, A., E. Merzari, T. Norddine, O. Marin, and S. Benhamadouche. 2021. "Large Eddy Simulation of a 5x5 rod bundle: Impacts of a central control rod thimble tube," *Nuclear Engineering and Design*, 381:111337. https://doi.org/10.1016/j.nucengdes.2021.111337.
- Kraus, A., E. Merzari, T. Norddine, and S. Benhamadouche. 2020. "Invariant Analysis of Flow in a 5x5 Rod Bundle with a Central Thimble Tube." 2020 ANS Winter Meeting, Nov. 16–19, Virtual.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulations (NEAMS)

A.36. Duke Energy PWR Core Model Benchmarking, Reactor Vessel Fluence Predictions, and Crud Layer Predictions with VERA

Report Participants

Matthew C. Adler[1]

1 Duke Energy

Scientific Achievement

The VERA code developed for the DOE CASL project is a state-of-the-art pin-resolved reactor simulation suite, integrating core neutronics (MPACT), thermal-hydraulics (CTF), fuel performance (BISON), chemistry (MAMBA), and excore neutron transport (Shift) models. These capabilities allow for detailed integrated models of certain phenomena particular to commercial PWRs which are challenging for current industry methods. Near term projects include the benchmarking of VERA core models for Duke PWRs against measurements to validate the tool. Once basic benchmarking is complete, the chemistry and fuel crud and corrosion models may be employed to investigate VERA's ability to predict the PWR phenomena crud-induced power shift (CIPS) and crud-induced localized corrosion (CILC) fuel failures. Additionally, excore neutron transport capabilities in VERA may be used to predict vessel fluence for licensing applications and to potentially design capsule placement schemes for non-beltline fluence measurements.

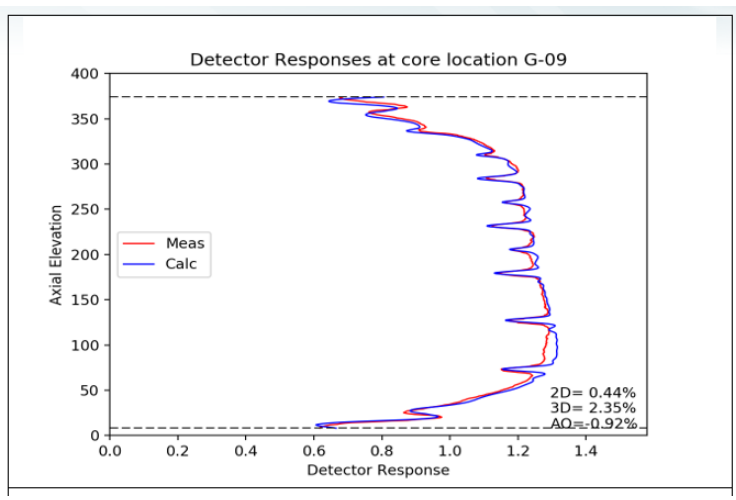


Figure 1. Measure vs. VERA predicted fission chamber reaction rate.

Significance

Validation of VERA chemistry (CIPS/CILC) capabilities and excore neutron transport capabilities would yield incredible value to the commercial nuclear power industry and would allow for a variety of practical analysis applications not currently possible with standard industry modeling tools.

Key Publications

In progress conference presentations for CASL/NEAMS VERA User's Group.

Sponsor/Program

VERA User's Group (CASL/NEAMS)

A.37. Effect of Grain Boundary Migration on Radiation-Induced Segregation in Polycrystalline Metal

Report Participants

Aashique A Rezwan,[1] Yongfeng Zhang,[1] Daniel Schwen[2]

1 University of Wisconsin-Madison

2 Idaho National Laboratory

Scientific Achievement

Irradiation produces point defects in metallic alloy. Fraction of the point defect diffuses to and get absorbed by the geometrical sink like grain boundaries (GBs). The transport of point defects induces coupled transport of alloying element resulting in either enrichment or depletion of alloying element from the GBs, which is termed as RIS. While in coarse-grained alloys, the GBs and the grain size are regarded as static under irradiation, in nanocrystalline materials RIS is accompanied by grain growth via GB migration. In this project, we investigate the effect of GB migration on RIS in ternary Fe-Cr-Ni alloy considering both the vacancy and interstitial mediated diffusion, as well as defect production, recombination, and absorption. The phase field module of the MOOSE framework has been used to perform the investigation.

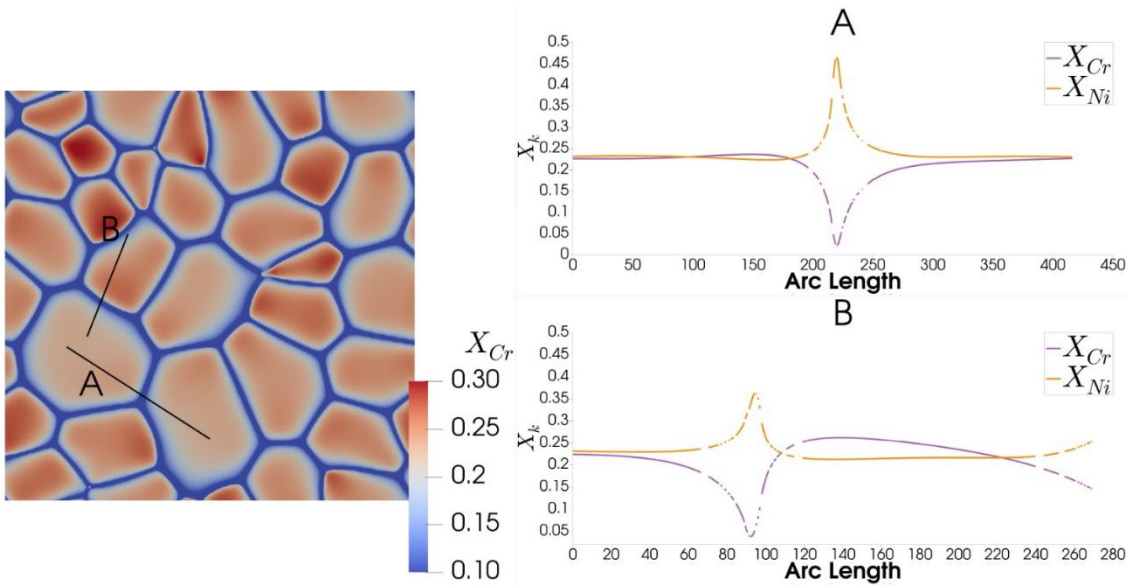


Figure 1. Segregation behavior and concentration profile under migrating grain polycrystal in Fe-Cr-Ni ternary alloy. (a) Cr concentration profile over the polycrystal. Cr concentrations increase ahead of the moving grain and thus shrinking grain gained higher concentration of Cr, while Cr concentration depleted behind the moving grain, and thus the expanding grain showed reduced Cr concentration. (b) Asymmetrical profile of the concentration observed across the moving GB (line B on polycrystal) as compared to stationary GB (line A on polycrystal).

Significance

RIS can detrimentally degrade the mechanical properties and corrosion resistance of materials used in nuclear reactors. With static GB and no grain growth, Cr tends to be depleted at GBs because of it has the fastest diffusion rate among the three elements via the vacancy mechanism, while Ni tends to be enriched. When grain growth is activated simultaneously, RIS is found to increase with increasing grain size. An inhomogeneous concentration profile observed across different grain. At a moving GBs, the segregation profile becomes asymmetrical, in contrast to the symmetrical segregation profile at static GBs. While Cr is still depleted behind a moving GB, it becomes enriched instead of depleted in front of the moving GB. The opposite profile is observed for Ni.

Key Publications

- Rezwan, A, Y. Zheng, and D. Schwen. "Effect of Grain Boundary Migration on Radiation Induced Segregation in Polycrystalline Metal." Computational Materials Science (in progress).

Sponsor/Program

LDRD

A.38. Evaluation of BISON's Fission Gas Release Model in UO2 MiniFuel Under Temperature Transient Conditions

Report Participants

Amani Cheniour,[1] Nathan Capps[1]

1 Oak Ridge National Laboratory

Scientific Achievement

The fuel performance code BISON was used to evaluate the fission gas release (FGR) model at different burnup and temperature transient conditions by applying it on UO2 MiniFuel. The results show a good qualitative agreement with experimental data. However, the model must be developed further to quantitatively model FGR with good accuracy. Several gaps in the model were identified through detailed analysis and validation. A paper will be submitted to a peer-reviewed journal documenting these results.

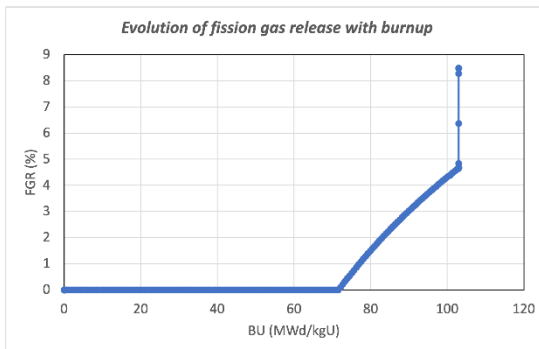


Figure 1. FGR evolution with burnup under steady state and then temperature transient conditions (at ~103 MWd/kgU).

Significance

FGR results in the degradation of the pellet-cladding gap heat transfer, which increases the fuel temperature. It is therefore necessary to account for the effects of FGR when analyzing the thermomechanical behavior of nuclear fuels in BISON through accurate models. BISON's FGR model is based on a fission gas diffusion model in addition of a purely temperature-dependent microcracking model. The latter was developed based on the results of power ramps tests. In this work, the model's accuracy is evaluated on UO2 MiniFuel using hypothetical and real temperature transient cases. The results show that the model requires further development to account for the formation of the high-burnup structure as well as the overpressurization of bubbles in the rim region of the fuel.

Key Publications

A milestone report was completed (unpublished) and an upcoming publication is in progress.

Sponsor/Program

This work was funded by the Advanced Fuels Campaign of the U.S. Department of Energy Office of Nuclear Engineering.

A.39. Evaluation of QustomWeld Software for Performing Welding Simulations

Report Participants

Alex Harrouff[1]

1 Naval Nuclear Laboratory

Scientific Achievement

This project assessed the capability of QustomApps software, QustomWeld, to perform welding simulations in Abaqus. Modeling the welding process is very complicated and time consuming due to the evolving loads and boundary conditions as elements are activated. QustomWeld automates much of the setup process and the creation of the subroutines which control the element activation, evolving heat flux, and evolving film conditions. Prior to purchasing the software, NNL performed high-level evaluations at INL to ensure the basic capabilities were functional, including 2D and 3D analyses, autogenous welding, and a variety of heat sources including those that support both arc and laser welding.

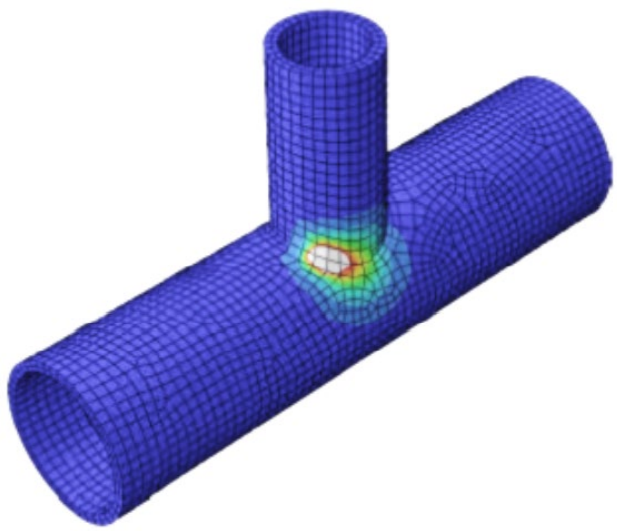


Figure 1. Temperature distribution of a pipe weld with gray region representing melt pool.

Significance

This work allowed NNL to work closely with the vendor during the initial evaluation phase and identify any major issues prior to purchasing QustomWeld. During the evaluation process, NNL was able to address major bugs with the vendor and obtain new releases for testing. The evaluations completed gave NNL confidence in the cababilities of the new software and were a key part of the risk mitigation plan. At the conclusion of this evaluation, NNL purchased QustomWeld which offers welding analysis capabilities not provided by other welding codes.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.40. Evaluation of Thermophysical Properties of the LiCl-KCl System via Ab Initio and Experimental Methods

Report Participants

Kai Duemmler,[1] Benjamin Beeler,[1,2] Yuxiao Lin,[2] Michael Woods,[2] Toni Karlsson,[2] Ruchi Gakhar,[2]

1 North Carolina State University

2 Idaho National Laboratory

Scientific Achievement

The self-diffusion coefficient can be calculated through both the Einstein relationship and the Green-Kubo relationship. Historically, it has not been calculated in ab initio molecular dynamics (AIMD) due to computational constraints but with the advancement of computers and the increased efficiencies with simulation software, it is now possible to calculate the self-diffusion coefficient from AIMD.

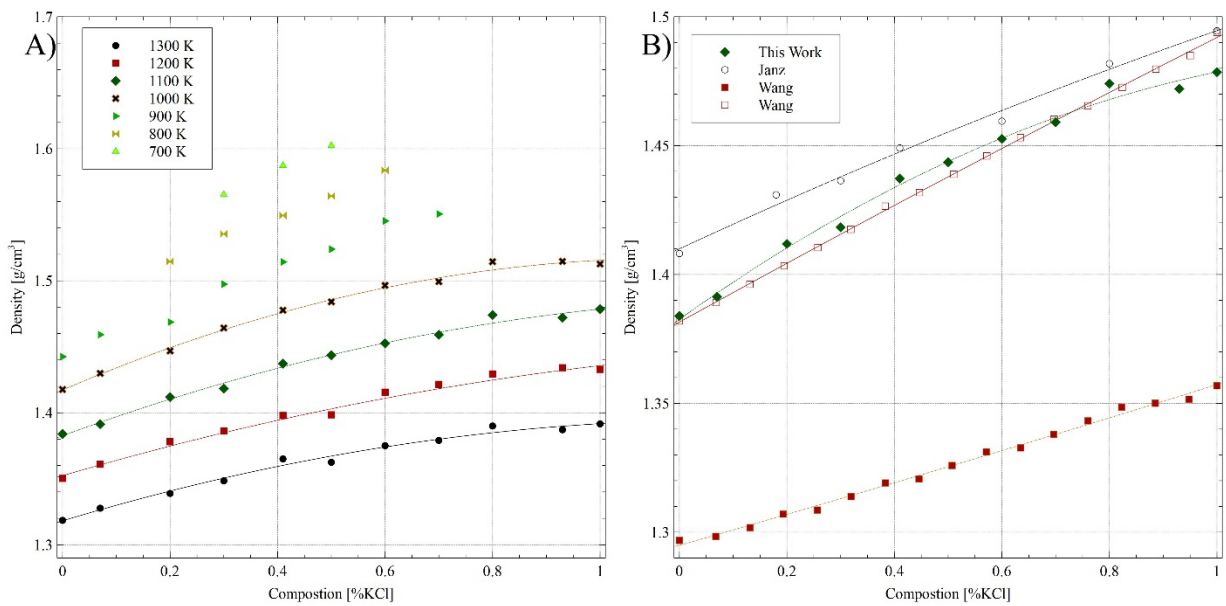


Figure 1. LiCl-KCl density calculations for temperature range of 700 to 1300.

The diffusion coefficient is also calculated and below in Figure 2. Which shows the diffusion coefficient for the system with various sizes and run steps to see what the minimum requirements are for diffusion coefficient for AIMD. Below in Figure 2, the diffusion coefficient is plotted for each component of the salt system (K, Li, and Cl), and each is run for a total time length of 100 ps, so the 25 ps case is an average of four runs. The influence of time is shown for the first two rows for both 100 and 200 atoms respectively, and the last row shows the influence of system size for the 100 ps runs.

Significance

Molten salts are of interest for their use in various generation four (Gen-IV) reactor designs. There is a lack of literature for some high-temperature properties including the self-diffusion coefficient and other thermophysical properties. Below is an illustration of the calculation of density for the molten-salt LiCl-KCl for a temperature range of 700 K to 1300 K compared to experimental work. There is good agreement between the AIMD simulations, and the experimental measurements are for diffusion coefficient for AIMD. Below in Figure 2, the diffusion coefficient is plotted for each component of the salt system (K, Li, and Cl), and each is run for a total time length of 100 ps, so the 25 ps case is an average of four runs. The influence of time is shown for the first two rows for both 100 and 200 atoms respectively, and the last row shows the influence of system size for the 100 ps runs.

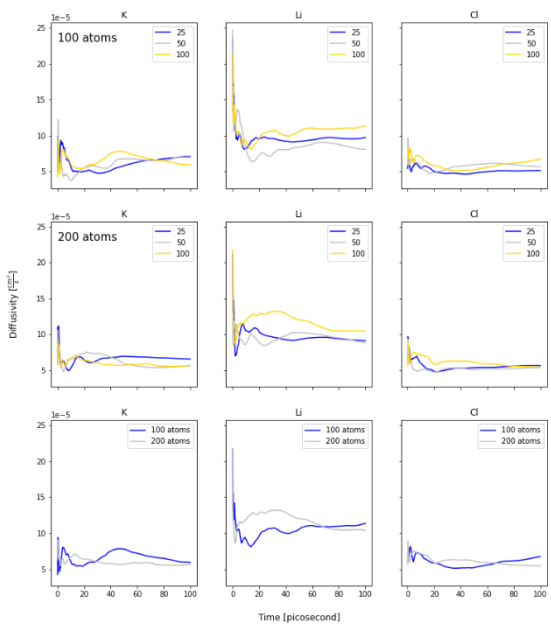


Figure 2. The self-diffusion coefficient for eutectic LiCl-KCl at 1200 K for various simulation segment lengths with a total run time of 100 ps.

Key Publications

To be submitted.

Sponsor/Program

LDRD

A.41. Evaluation of VERA Transient Capability for Analyzing PWR Control Rod Ejection Accident

Report Participants

Vefa Kucukboyaci,[1] Brendan Kochunas,[2] Thomas Downar,[2] Aaron Wysocki,[3] Robert Salko[3]

1 Westinghouse Electric Company

2 University of Michigan

3 Oak Ridge National Laboratory

Scientific Achievement

Control rod ejection events were simulated for the AP1000® reactor core at the end of cycle hot zero power (HZP), part-power, and hot full power conditions and for the Farley Unit 1 core at HZP conditions using the VERA code system developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL). Calculations were performed first to deplete the core to end of cycle, and then restart calculations were performed to simulate the rod ejection events in full-core geometry. These simulations were performed using the MPACT neutronics code-coupled to the CTF subchannel analysis thermal-hydraulics code within VERA. It was found that the VERA code system can simulate full-core geometry rod ejection events in a stable manner with the expected power pulse resulting from a super-prompt critical reactivity insertion and the resulting negative doppler reactivity feedback. A select set of results from VERA were compared to those from current Westinghouse methods. Both peak power and reactivity insertion values agree well between VERA and the Westinghouse codes, confirming VERA calculations.

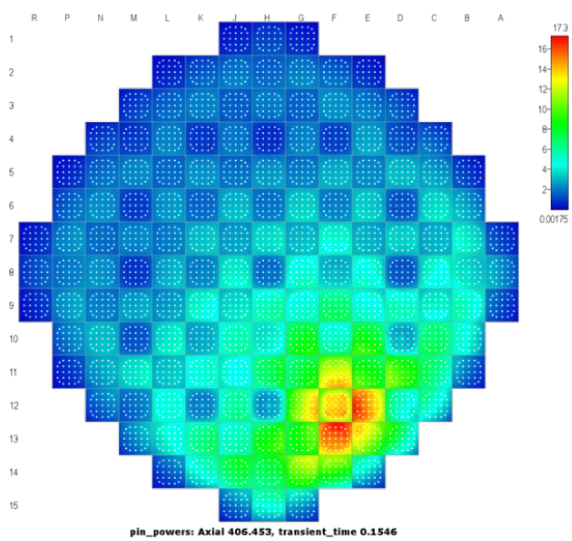


Figure 1. AP1000 reactor core radial pin power distribution at the peak of the power pulse due to rod ejection at HZP.

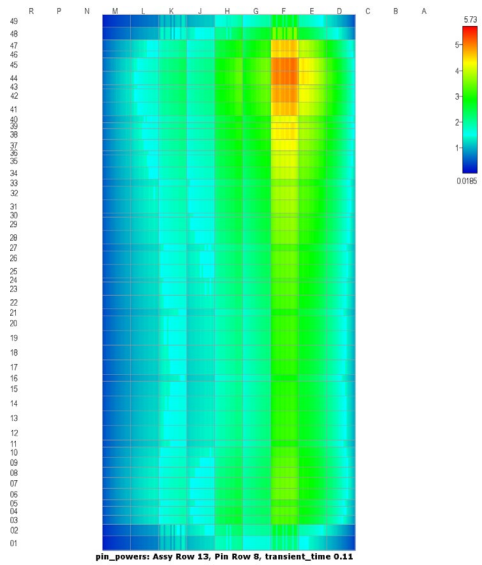


Figure 2. AP1000 reactor core axial pin power distribution at the peak of the power pulse due to rod ejection at hot full power.

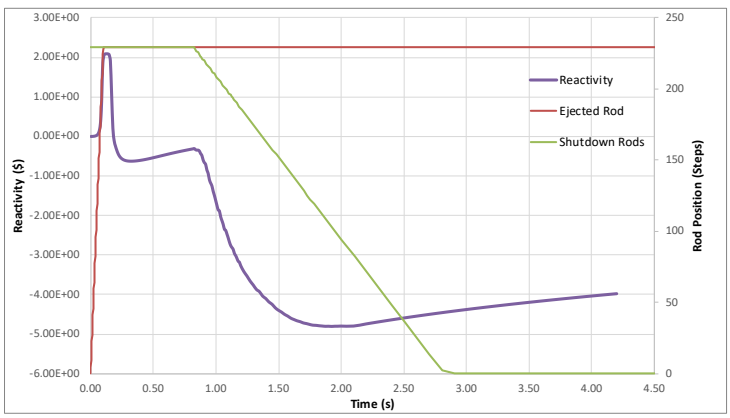


Figure 3. Farley Unit 1 core total reactivity and ejected rod position for HZP rod ejection.

Significance

The control rod ejection accident is a design basis reactivity insertion accident (RIA) event for PWRs. The consequences of RIA are a rapid reactivity insertion and core power increase together with an asymmetric core power distribution, possibly leading to localized fuel rod damage. The reactivity insertion is initially mitigated by the doppler feedback and delayed neutron effects followed by a reactor trip, initiated by a high neutron flux signal in ex-core detectors. Depending on the amount and rate of reactivity insertion, fuel rods may experience several degradation mechanisms and failure modes, including fuel melting, pellet clad mechanical interaction, and departure from nucleate boiling (DNB). With high-fidelity simulation capabilities, the VERA core simulator can support the nuclear industry on RIA analyses to gain margin against expanding regulatory requirements and to address data gaps through simulation for new fuel designs such as accident tolerant fuel (ATF) and high-burnup applications. VERA-coupled code system, developed by CASL, includes coupled neutronics, thermal-hydraulics (T/H), and fuel temperature components with an isotopic depletion capability. The neutronics capability is based on the three-dimensional whole-core transport code MPACT, and the T/H and fuel temperature models are provided by the CTF subchannel code. By modeling and simulating two Westinghouse reactor designs, the AP1000® reactor Cycle 1 and Joseph M. Farley Unit 1, Cycle 27, on the INL HPC system, VERA's transient capability to simulate RIA events has successfully been demonstrated and evaluated, paving the way for non-traditional applications such as those with high-enrichment/high-burnup fuel, for which data gaps exist, and reference solutions are necessary to verify current methods.

Key Publications

- Kucukboyaci, V. 2020. "Evaluation of VERA Transient Capability for Analyzing PWR Control Rod Ejection Accident," CASL Symposium at the 2020 ANS Virtual Winter Meeting, November 2020.
- Kucukboyaci, V., F. Franceschini, Z. McDaniel, Z. Karoutas, Y. Sung, and R. Brewster. 2020. "VERA Applications and Commercial Deployment at Westinghouse," CASL Symposium at the 2020 ANS Virtual Winter Meeting, November 2020.
- Ray, S., V. Kucukboyaci, Y. Sung, P. Kersting, R. Brewster, K. Clarno, and A. Godfrey. 2018. "Industry Use of CASL Tools," Global/ Top Fuel 2018, Prague, Czech Republic, September 30–October 4, 2018.
- Kucukboyaci, V., B. Kochunas, T. Downar, A. Wysocki, and R. K. Salko. 2018. "Evaluation of VERA-CS Transient Capability for Analyzing the AP1000® Reactor Core Control Rod Ejection," PHYSOR 2018, Cancun, Mexico, April 22–26, 2018.

Sponsor/Program

CASL, Industry

A.42. Explore Collaboration Opportunities with RELAP5-3D

Report Participants

Francis X. Buschman,[1] Cajon Gonzales,[1] Tammy Petranka,[1] Michael Meholic,[1] Zachary Bacon[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Our work on the INL HPC thus far has been focused primarily in two areas. The first is related to evaluating our capability to establish a more collaborative development relationship with the RELAP5-3D team at INL. The second is related to developing and running models of open literature experimental facilities or canonical problems using RELAP5-3D. We have been working with INL to identify software limitations and availability on the INL HPC system that can be targeted to make this a more effective collaboration environment. Through our efforts and a parallel "remote relap" effort at INL, some of these limitations are being addressed that could make this a more viable workspace for RELAP5-3D development and use in the near future.

Significance

Understanding the capabilities and limitations of performing collaborative development and assessment of RELAP5-3D, between NNL and INL, on the INL HPC enviroment is important in shaping the strategic direction of RELAP5-3D use and development at NNL.

Key Publications

No publications.

Sponsor/Program

Nuclear Science and Technology

A.43. Fidelity Enhancement of Nuclear Power Plant Simulators Utilizing High-Fidelity Simulation Predictions

Report Participants

Hisham Sarsour[1], Igor Arshavsky[1], Benjamin Collins[2], Aaron Graham[2], Robert Salko Jr. [2], Aaron Wysocki[2], Paul Turinsky[3]

1 WSC, INC.

2 ORNL

3 Statehouse, LLC

Scientific Achievement

A fully integrated code (RELAP-NESTLE-CTF) that is designed to be used as a nuclear engineering simulator by nuclear industry, national laboratories, and university researchers was developed. In addition, a real-time nuclear reactor simulator was developed based on the above methodology. Please see Figure 1.

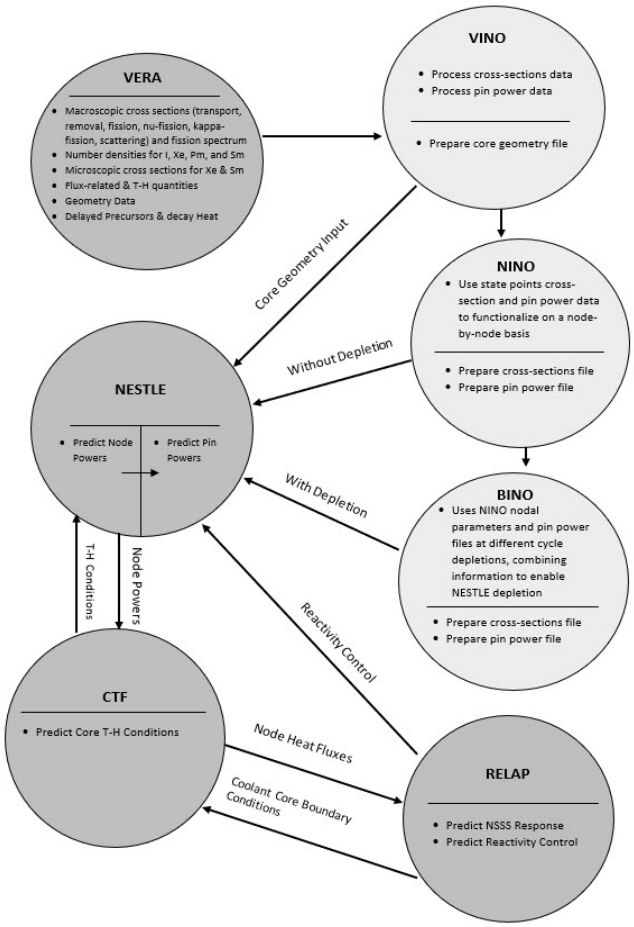


Figure 1. Combined Figure that shows the target code package for this DOE project (an integrated NESTLE\CTF\RELAP5-3D model).

Significance

The DOE-funded ORNL and other institutions spent 10 years to build the ultimate core simulator, VERA, which is based on the transport equation with more than 50 energy groups. Running VERA is very expensive in terms of run time and memory, where 1000s of cores are needed for modeling a nuclear plant. Our approach is based on running limited number of cases using VERA and then applying our methodology to improve the accuracy and fidelity of a nodal code based on the two-energy diffusion equation. This technology is the basis for WSC, INC, new engineering, and real-time training simulators.

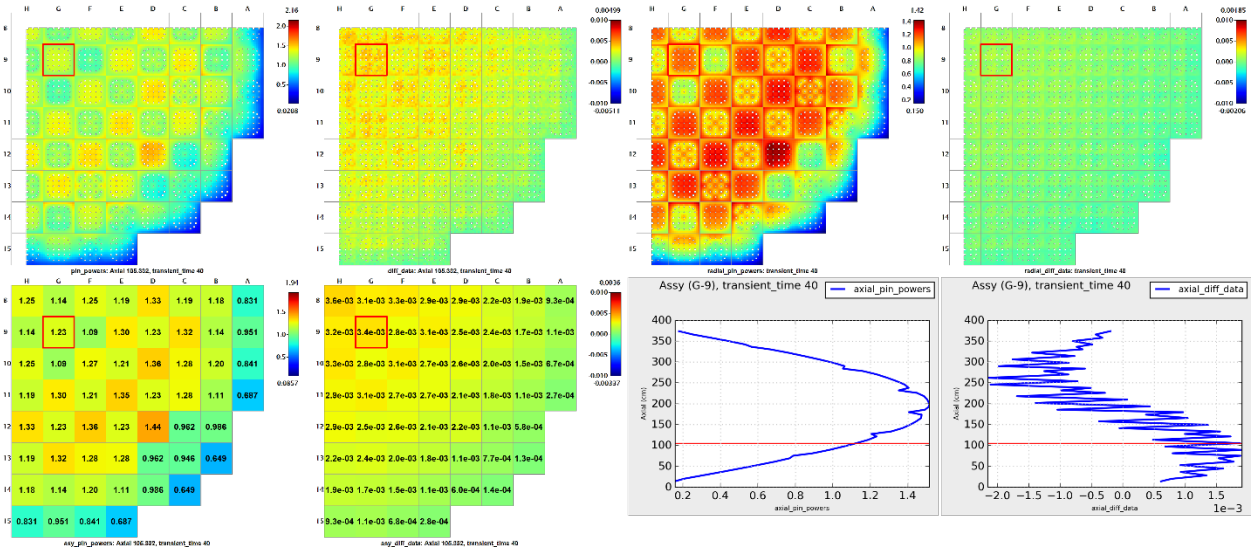


Figure 2. Relative power distributions and differences for the boron dilution transient at t=40 seconds.

Key Publications

- Turinsky, P., A. Graham, H. N. Sarsour, and B. Collins. 2020. "Generation of Nodal Core Simulator Utilizing VERA," PHYSOR 2020: Transition to a Scalable Nuclear Future, Cambridge, United Kingdom, March 29th–April 2nd, 2020.
- Wysocki, R. S. and I. Arshavsky. 2022. "Coupling of CTF And Relap5-3d within an Enhanced Fidelity Nuclear Power Plant Simulator," The 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6–11, 2022.

Sponsor/Program

DOE, SBIR/STTR, CASL, NEAMS

A.44. First-Principles Investigation of Nuclear Fuel Properties

Report Participants

Vancho Kocevski,[1] Michael Cooper,[1] David Andersson[1]

1 Los Alamos National Laboratory,

Scientific Achievement

Utilizing DFT to calculate various properties of uranium mononitride (UN) nuclear fuel, namely defect formation energies, and finite temperature phonon dispersions and crystallographic properties. The formation energies of the U and N defect in UN were calculated under U-rich and N-rich conditions using PBE and AM05, with added on-site Coulomb repulson term (+U), with and without spin-orbit coupling (SOC). Also, stoichiometric formation energies in UN were calculated using the different methodologies. The defect formation energies provide an insight into the observed tendency for forming hypostoichiometric UN. The finite temperature properties of UN were calculated using PBE and PBE+U. The calculations were performed using VASP.

Significance

The lowest energy (dominant) defects in the U-rich region are N vacancies and U in N antisites (see Figure 1a), which would increase the U concentration in UN, while N interstitial, U vacancy, and N vacancy are dominant defects in the N-rich region (see Figure 1b), slightly decreasing the U concentration in UN. Furthermore, the formation energies of the dominant defects in the U-rich region are slightly lower compared to the formation energies of the dominant defects in the N-rich region, which indicates that this might be the driving force for the small hypostoichiometry when UN is synthesized. We observed that magnetic ordering has influence on the defect formation energies, especially for U in N antisites, and we are suggesting to further analyze the influence of magnetism on the stability of UN and its defects. In the case of the stoichiometric reaction energies, we show that the N Frenkel pairs and Schottky defect energies are very similar, which indicates that both would have almost equal concentration in UN. We also show the U-dumbbell interstitial (UU-D) has lower energy than the U-tetrahedral interstitial (Ui-t) and demonstrate that it comes from steric effects and lowering of the density of states (DOS) at the Fermi level in the UU-D. We also showed that when SOC is used, the energy difference between Ui-t and UU-D is significantly increased compared to when SOC is not used, which we argue comes from further decreases of the strain and lowering the DOS at the Fermi level in UU-D.

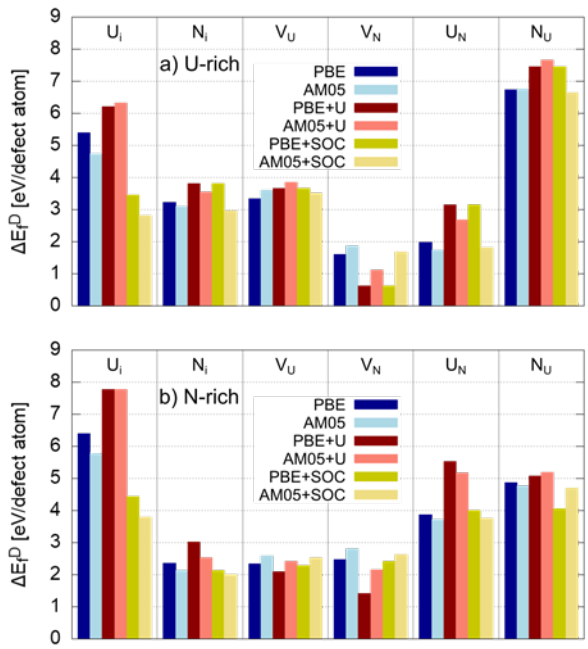


Figure 1. UN point defect formation energies (ΔEDf) in: a) U-rich and b) N-rich regions. The ΔEDf calculated using GGA, GGA+SOC, and GGA+U are shown in blue, red, and yellow, respectively. ΔEDf calculated using PBE and AM05 are shown in dark and light shade, respectively.

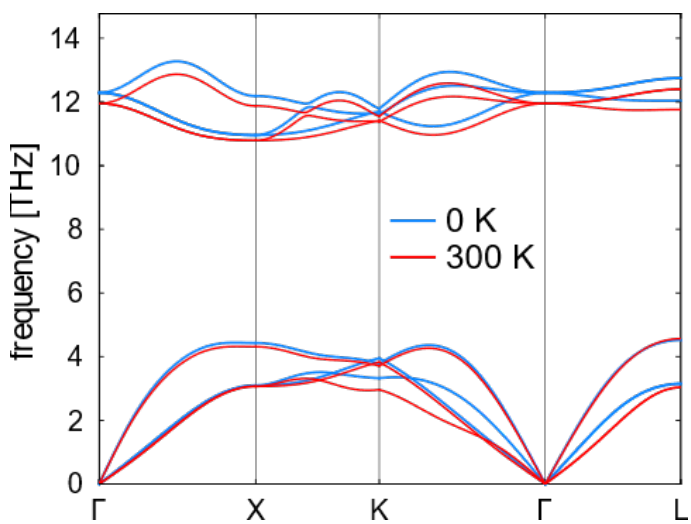


Figure 2. UN phonon dispersion calculated using PBE, at 0 K and 300 K, shown in blue and red, respectively.

To study the finite temperature behavior of UN, we performed ab initio MD (AIMD) simulations at five different temperatures: 300, 600, 900, 1300, and 1800 K. The simulations were done using two thermostats: constant volume Nose-Hoover thermostat (NVT) and constant pressure Langevin thermostat (NPT). The NVT simulations were used to calculate the finite temperature phonon dispersions, while the NPT simulations were used to calculate the temperature dependence of the crystallographic parameters. The NVT simulations show softening of both the acoustic and optical phonon modes with increasing temperature (see Figure 2). A further investigation of the influence of this softening of the phonon modes on the elastic properties of UN will be performed. The NPT simulations give a lattice thermal expansion that is similar to the experiment, with the lattice parameters being slightly lower compared to the experiment. Moreover, the average UN unit cell resembles a cube even when PBE+U is used for the antiferromagnetic ordering, implying that finite temperature needs to be used to get better UN model when using PBE+U.

Key Publications

Works in progress:

- "First-principles investigation of uranium mononitride (UN): Effect of magnetic ordering, spin-orbit interactions and exchange correlation potential," led by Vancho Kocevski.
- "Ab-initio Molecular Dynamic study of the temperature dependent crystallographic, phonon and elastic properties of uranium mononitride (UN)," led by Vancho Kocevski.

Sponsor/Program

NEAMS

A.45. Gadolinium Depletion Studies in MC21 and VERA/MPACT

Report Participants

Jane Derboven[1]

1 Naval Nuclear Laboratory

Scientific Achievement

This study recommended energy group structure changes to improve accuracy of Gd depletion predictions in Consortium for Advanced Simulation of Light Water Reactors (CASL) VERA/MPACT. VERA/MPACT (method of characteristics [MOC]) models containing Gd yield eigenvalue differences from Shift (Monte Carlo [MC]) at high depletions, with differences exacerbated at high void conditions. One hypothesized cause of these discrepancies is VERA's use of a poor energy group structure relative to the 155Gd total cross-section (e.g., Figure 1 shows that the 2.47eV–3.73eV group (orange), straddles a ~100× drop in 155Gd cross-section magnitude, suggesting that collapsing across this range is undesirable). High void conditions reduce thermalization, leading to a higher population of neutrons in the offending epithermal energy group(s), consistent with the observed eigenvalue effect.

This hypothesis was tested by analyzing depletion of the Gd-bearing CASL VERA progression problem 2o (Figure 2) using both VERA/MPACT and the NNL MC tool MC21 on the INL HPCs. A coarse depletion history accelerated acquisition of highly depleted edits, a strategy enabled by consistency across both tools, as depletion errors introduced by this coarseness are irrelevant to code-tocode comparisons. Figure 3 shows absorption edit ratios collected at each time step in the inner and outer Gd-bearing pins, with energy grouping colors matching the colored bars in Figure 1. These ratios confirm the under depletion of 155Gd at early steps due to too few absorptions in groups 2 and 3 from Figure 1, leaving more residual Gd mass at later steps when the Gd has become less black, and eigenvalues are more sensitive to small mass differences. The recommended solution is an additional energy group breakpoint at 3 eV and, if necessary, also at 2.15 eV. Follow-up calculations to test this recommendation are pending, and will be performed upon availability of updated cross-section files which follow the recommended group structure.

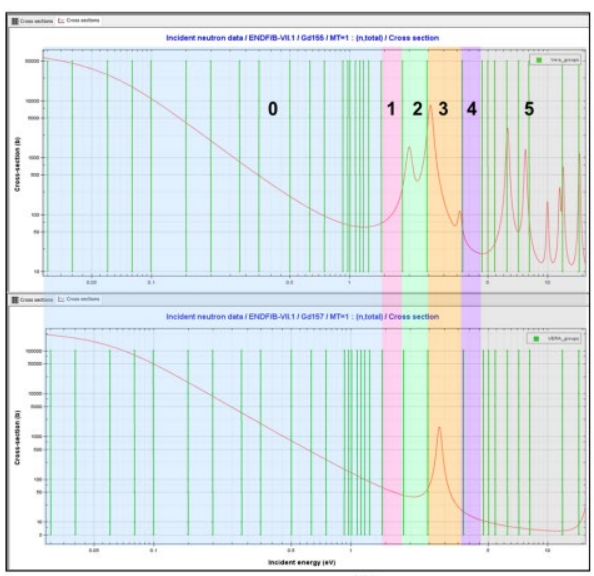


Figure 1. Total cross-section of 155Gd (top) and 157Gd (bottom) from ENDF/B VII.1 via JANIS. Green lines indicate VERA/MPACT energy group breakpoints. Colored overlays indicate groupings used for this study and correspond to the scatter plot colors in Figure 3.

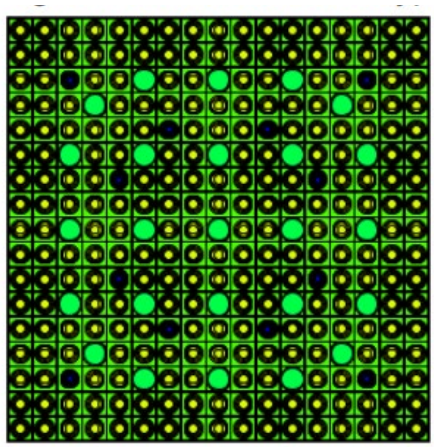


Figure 2. CASL VERA progression model 2o, with Gd-bearing fuel pins shown in dark blue.

Significance

Recommended energy group stucture could improve nuclide inventory and eigenvalue predictions in Gd-bearing VERA/MPACT models.

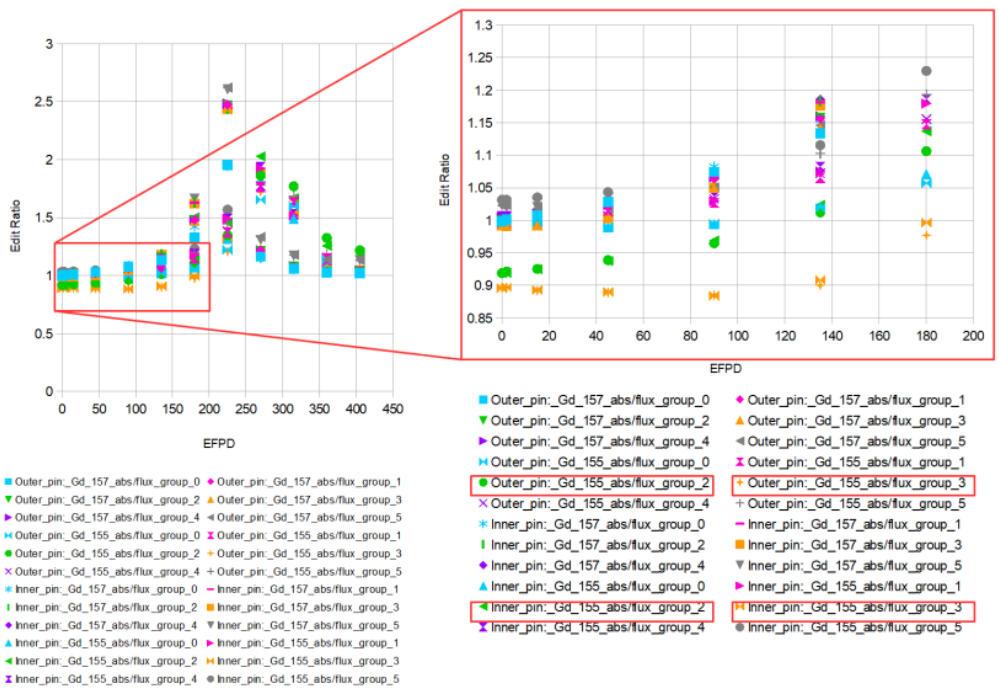


Figure 3. VERA/MC21 absorptions/n-cm edit ratios for inner and outer Gd-bearing pins in model 2o, showing under depletion of 155Gd at early time steps, leading to higher 155Gd inventories, more absorptions, and more noticeable eigenvalue differences at later depletion steps, as Gd becomes less black.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology, Consortium for Advanced Simulation of Light Water Reactors (CASL)

A.46. Great White

Report Participants

Benjamin Ramirez Flores[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Great White (GW) was implemented using the material of defect library (MoDELib) and the MOOSE platform. GW is a 3D Discrete Dislocation Dynamic (DDD) application which is capable of performing simulations of dislocation that include not only glide motion and cross slip but also climb motion. These features make GW a unique tool to study the dislocation behavior under creep conditions.

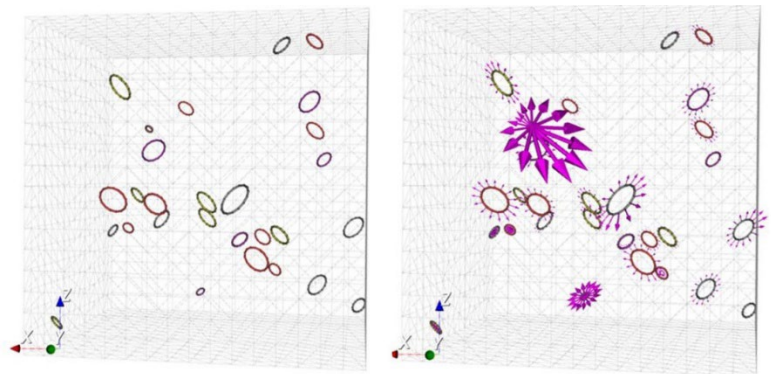


Figure 1. The implementation of the climb algorithm was tested by simulating 28 circular loops of 14nm average radius (deviation 4nm).

Significance

DDD simulations are limited in almost all implementations to simulate inelastic deformation due to dislocations glide. But for higher temperatures, it is necessary to add creep. GW objective is to work as a virtual creep test. We can build many different microstructure for a range of dislocation density population under different conditions of temperature, stress, and flux to complement experimental tests and increase the design space. The results from the simulations could be used to develop constitutive relationships. GW will allow us to target testing such that the time required to develop constitutive material laws could be reduced.

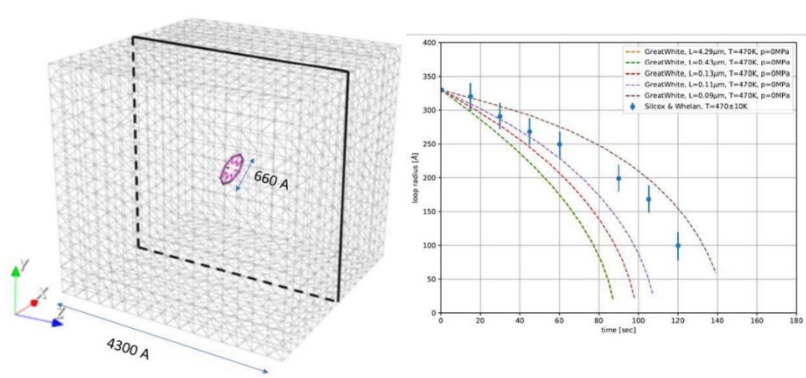


Figure 2. The implementation of the climb velocity was benchmark with observations by Silcox, J. in 1959.

Key Publications

- Po, G., Y. Huang, N. Ghoniem, B. Ramirez, C. Baker, T. Black, and J. Hollenbeck. 2021. "A Model of 3D Dislocation Climb and Annealing in Irradiated Materials," ICFRM conference, Granada, Spain Oct 24–29, 2021.
- Po, G., Y. Huang, N. Ghoniem, B. Ramirez, C. Baker, T. Black, and J. Hollenbeck. 2021. "A Model of 3D Dislocation Climb and Annealing in Irradiated Materials," MMM conference Baltimore, MD Oct 2–7, 2022.
- Po, G., Y. Huang, N. Ghoniem, B. Ramirez, C. Baker, T. Black, and J. Hollenbeck. ND. "A Computational Method for Dislocation Climb with Application to Vacancy Loop Annealing in Polycrystals," In progress.

Sponsor/Program

Nuclear Science and Technology

A.47. High-Energy High-Burnup 24 Month Cycle VERA Models for Farley NPP

Report Participants

Mykola Boychenko,[1] David Salazar,[1] Fausto Franceschini[1]

1 Westinghouse Electric Company

Scientific Achievement

This work's purpose is to assess feasibility of transition from the fuel enrichment below 5.0 w/o to higher than 5.0 w/o for the three-loop plant. The increase in-core average enrichment promise to upend the nuclear industry and improve reactor economics and resource utilization. HPC was utilized to conduct 3D VERA modeling of transition and estimated equilibrium cycles. The results of peaking factors and burnup distribution were compared with current production models and showed good agreement. This provided the basis for the estimation of the current design safety system capabilities.

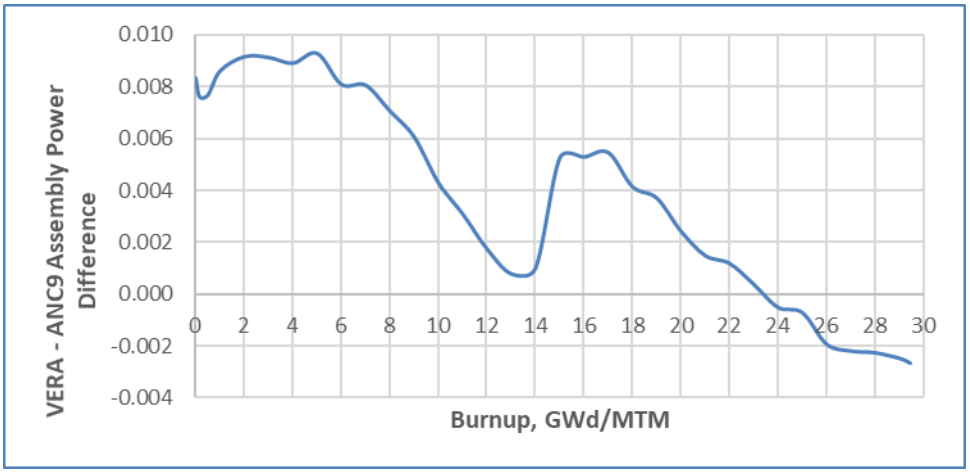


Figure 1. Equilibrium cycle VERA - ANC9 assembly power difference.

Significance

Toward the goal of introducing high-burnup (HB) and high-enriched (HE) fuel in the operating fleet and developing optimal transition from currently operating cycles to equilibrium fuel cycles with HE/HB fuel based on 2-year, 3-year, and 4-year refueling cycles and utilizing HE up to 10 w/o 235U and HB up to 75,000 MWD/MTU rod average burnups. An optimal multi-cycle refueling strategy is assessed based on relevant industry expertise, including advanced burnable absorber usage for optimal power shaping and reactivity control over the extended cycle length. The use of VERA advanced simulation capabilities for analysis of the HB/HE cores enables accurate assessment of fuel and core design constraints which are driven by the normal operation and accident simulation scenarios that are the design basis for NRC licensing under the standard review plan for LWR Transient and Accident Analysis (NUREG-0800). This work assesses HB/HE constraints that include thermal and reactivity margin licensing limits as well as operational constraints, both anticipated and unanticipated, for irradiated fuel under long cycle operating scenarios. These constraints relate to risk mitigation and may involve a need to design with additional local operating margin relative to current licensing limits. One such example is a constraint on CIPS which is a function of the core excess reactivity (i.e., maximum soluble boron) as well as localized fuel rod subcooled boiling integrated over time. Another example might be fuel assembly bow produced under sustained power gradients during long cycles. Such power gradients are characteristic of current low-leakage core designs that may require mitigation through use of additional margin on local power peaking.

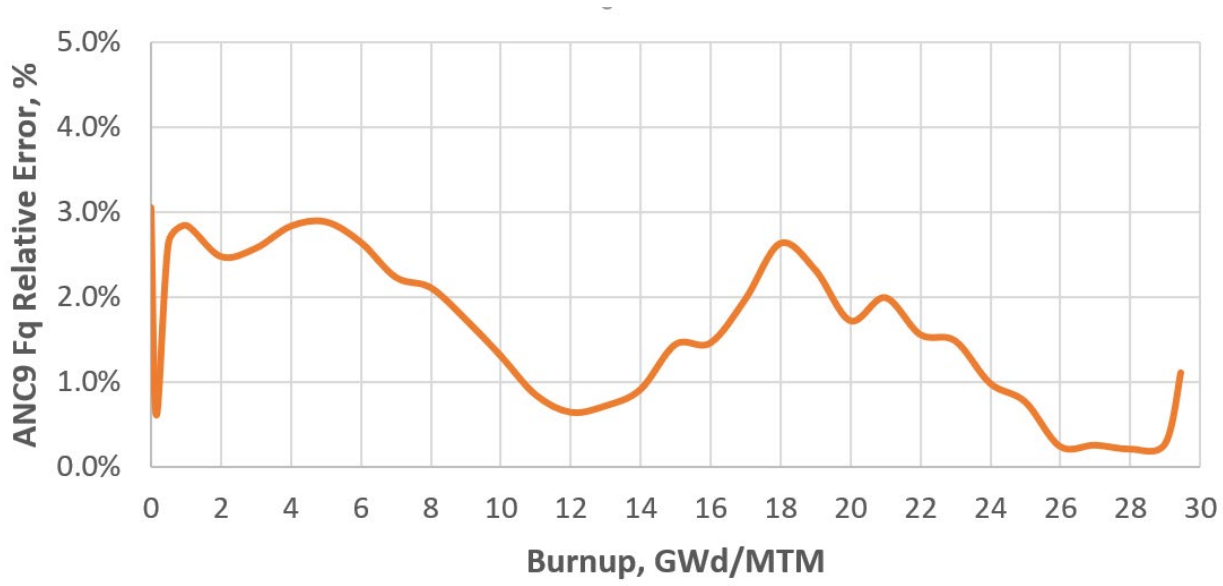


Figure 2. Equilibrium cycle WEC ANC9 Fq relative error.

Key Publications

- M. Boychenko. 2021. "24 Month Transition Cycles Farley VERA Models," CN-GEN-MISC-315, Westinghouse Electric Company LLC.

Sponsor/Program

Westinghouse Electric Company

A.48. ICSBEP Modeling MCF003 and MCF004

Report Participants

Emily Ziolkowski[1]
1 Naval Nuclear Laboratory

Scientific Achievement

I am in process of recreating MIX-COMP-FAST-003 (MCF003) and MIX COMP FAST-004 (MCF004) model in MC21 for NNL.

Significance

MC21 is a Monte Carlo solver, which is part of NNL's CMCDT analysis package. Representation of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) models MCF003 and MCF004 in MC21 will facilitate benchmark calculations to expand MC21's qualification basis and provide insight to target further code improvements. This work is currently in progress; the models in question are still under development, and no significant results are available yet.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.49. Innovative Enhanced Automation Control Strategies for Multi-Unit Small Modular Reactors

Report Participants

Brendan Kochunas,[1] Sooyoung Choi[1]

1 University of Michigan

Scientific Achievement

The scientific achievements of this project address the challenges of optimizing load follow through enhanced automation control strategies for multi-unit SMRs. The specific objectives of this project are to develop a hierarchy of automation control strategies for flexible power operation using the NuScale plant as the reference SMR design. This entails innovative work in the area of automation for control of systems necessary for providing (1) supervisory control for load following, (2) tactical control for prognostic health management, and (3) strategic control for the operation of multiple units at a single site. As the initial step, we have used VERA to develop and run high-fidelity calculations of the NuScale reactor to get its approach to equilibrium and analyzed the variation in important reactor dynamics parameters. Additionally, we have used these models to develop lower order expressions for degradation of reactor components such as the fuel, control rod drives, and vessel due to load follow maneuvers.

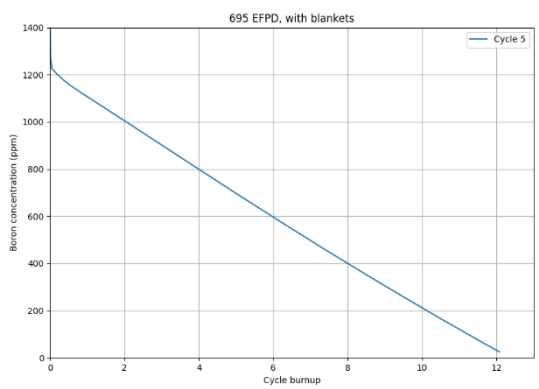


Figure 1. VERA calculated critical boron letdown curve for NuScale cycle 5.

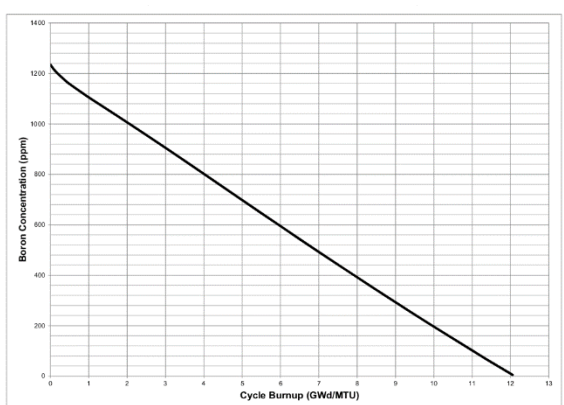


Figure 2. NuScale calculated critical boron letdown curve for equilibrium cycle from design certification application.

Significance

The significance of this work, so far, is additional, high-fidelity models within the public domain that include not just the NuScale equilibrium cycle but all cycles leading up in the approach to equilibrium. This will enable the many other significant contributions of this work to be achieved in the 2nd and 3rd year of this NEUP.

Key Publications

- Baker, U., M. Garrouste, S. Choi, G. S. Gonzalez, B. Lindley, and B. Kochunas. 2021. "Development of a high-fidelity multi-cycle model of the NuScale Small Modular Reactor using VERA," International Conference on Physics of Reactors 2022 (PHYSOR 2022), Pittsburgh, PA. Manuscript submitted for publication.
- Choi, S., M. Garrouste, U. Baker, B. Lindley, and B. Kochunas. 2021. "Development of Learning-based Model Predictive Control Framework for SMRs," NE/8975-2021-011-00, University of Michigan.

Sponsor/Program

NEUP, Project 20-19737, DOE Award Number DE-NE008975

A.50. Investigating the Effects of Sodium Coolant Infiltration of the Metallic Uranium Fuel on Its Thermal Conductivity from First Principles

Report Participants

Ahmed Aly,[1] Benjamin Beeler,[1,2] Maria Avramova[1]

1 North Carolina State University

2 Idaho National Laboratory

Scientific Achievement

Metallic uranium alloyed with Zr or Mo is a potential fuel candidate for Gen-IV SFRs. The high density of the fissile materials leads to the possibility of operating the fuel pins on a higher power levels than conventional oxide fuels used in LWRs. The heat transfer process from the fuel to the coolant must be as efficient as possible in order to protect the integrity of the fuel. Therefore, the heat conduction between the fuel and cladding through the gap is enhanced by filling the gap with a bonding sodium. With time, some of the bonding sodium might infiltrate the fuel leading to degradation in its thermal properties.

The goal of this project is to investigate the effect of the sodium infiltrate on the fuel thermal conductivity using ab initio methods for the U-Zr-Na systems. The ab initio calculations were performed using VASP code. The work performed so far consists of ab intio investigation of the fuel thermal and structural properties. This included the evaluation of the capability of VASP to capture the heat capacity, equilibrium lattice parameter, bulk modulus, heat of formation, and surface energy. The results were compared to previous computational work and/or experimental values and demonstrated the capability of ab initio methods to perform this task. The work progressed to the evaluation of the speed of sound in U-Zr alloys of interest in the metallic fuel. This is an initial step required to evaluate the kapitza resistance between the fuel and the bonding sodium. The work will later progress to evaluate the interactions between the bonding sodium and the fuel.

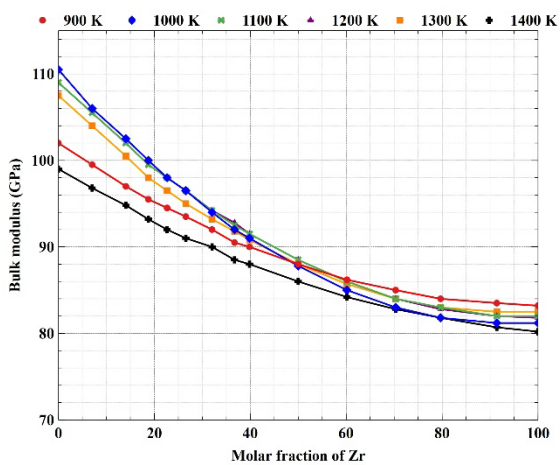


Figure 1. The Bulk modulus as a function of Molar fraction of Zr.

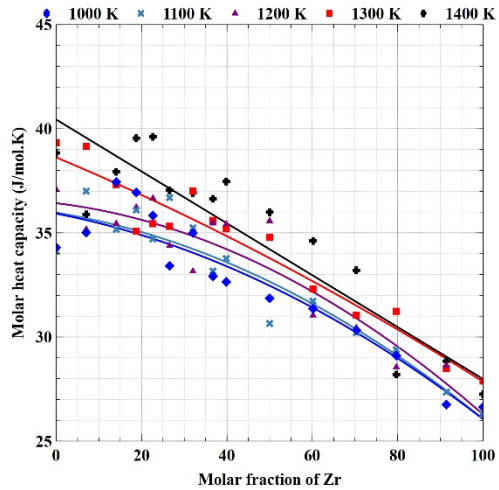


Figure 2. The molar heat capacity as a function of the zirconium content in UZr. Discrete points are the average values obtained from the results of three simulated configurations. The solid lines are the fittings of the simulation data.

Significance

Currently, the work is still in progress. So far AIMD was used to investigate UZr system properties for the full spectrum of concetrations and temperatures between 1000 K and 1400 K for γ(U-Zr). The bulk modulus was calculated for the studied UZr system as well as the thermal expansion coefficients. The obtained values were compared to experimental data available for U and Zr, and a good matching was the data was achieved. The heat capacity was computed for the UZr, and the results matched well with the available experimental points for UZr. The surface energy was computed for two surface orientations (100) and (110) and showed reasonable results. AIMD was used before to compute the surface energy for αU, This work is the first to use AIMD to calculate the surface energy for γU and its Zr alloys.

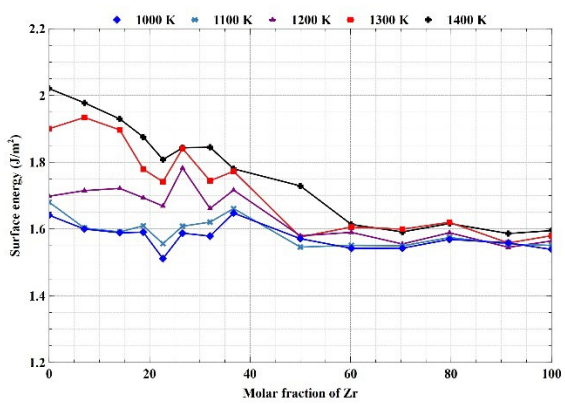


Figure 3. Surface energy as a function of zirconium content between 1000 K and 1400 K for a surface with orientation (100).

Key Publications

- Aly, A., B. Beeler, and M. Avramova. "Ab initio molecular dynamics investigation of γUZr structural and Thermal properties as a function of temperature and composition," In progress.

Sponsor/Program

NEAMS

A.51. Kairos Power – INL BISON Usage and Collaboration

Report Participants

Russell Gardner,[1] Stephen Novascone,[2] Cody Permann,[2] MOOSE Team[2]

1 Kairos Power

2 Idaho National Laboratory

Scientific Achievement

Kairos Power (KP) is an industry user/collaborator/developer of BISON, GRIZZLY, and SAM MOOSE-based code. That being said, assess to the INL HPC is required to update codes and contribute to the codes through GitLab. INL resources may be used for collaborative research and publications.

Significance

KP is the first industry user to use MOOSE-based tools in a regulatory manner, meaning results from simulations using these tools will be sent to the Nuclear Regulatory Commission (NRC) for safety and building approval.

Key Publications

While there will most likely be journal publications that spin out from this work, the most important documents will be the ones that KP submits to the NRC.

Sponsor/Program

KP – INL work is funded by multiple mechanisms including: NEAMS, KP FOA, and IRP

A.52. Learning MC21 – Basic Model Generation and Benchmarking

Report Participants

Kyle Martin[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The scientific achievements included understanding basic input and model structure for MC21. Using the HEU-MET-MIXED020 report, I created a simple geometry model which is similar to the MCNP model used in the report, and I am currently in process of comparing results to HEU-MET-MIXED-020 MCNP results.

Significance

I had very little previous experience with modeling via MC21 prior to teleworking—specifically this project. I have used MC21 extensively in my work at NNL, but I have not yet learned how the inputs affect the calculations. This project allows me to learn the basics of MC21 which include learning the various parameters used throughout the input cards and learning how to generate a model (both through the various input cards and through a program such as PUMA). My next goal is to attempt benchmarking type studies and compare MC21 results to those published in to HEU-MET-MIXED-020.

My goal is to write a benchmarking document for the NNL CMCDT group based on the HEU-MET-MIXED-020 report.

Key Publications

No publications at this time.

Project is based on:

- Nuclear Energy Agency. 2013. "HEU-MET-MIXED-020, Two Heterogeneous Cylinders of Highly Enriched Uranium, Polyethylene, and Molybdenum with Polyethylene Reflector," NEA/NSC/DOC(95)03/II Volume II.

Sponsor/Program

Nuclear Science and Technology

A.53. MC21 / CTF Simulation of OECD-NEA TVA Watts Bar Unit 1 Multi-Physics Multi-Cycle Depletion Benchmark

Report Participants

Brian N. Aviles,[1] Edwin J. Grant,[1] Daniel J. Kelly[1]

1 Naval Nuclear Laboratory

Scientific Achievement

We have been performing partial core and full-core simulations of the TVA Watts Bar Unit 1 benchmark model for submission to the OECD/NEA benchmark website. We are using the NNL Monte Carlo code, MC21, and the coupled code suite, MC21, coupled with CTF from the Consortium for Advanced Simulation of Light Water Reactors (CASL) code suite, VERA. Benchmark solutions for Exercise 1 (low power physics test) have been completed. Work continues for the high-power physics test and the depletion of Cycle 1.

Significance

This work will provide high-fidelity benchmark solutions for the OECD/NEA. MC21/CTF solutions have previously been cited as reference solutions for Exercise 2 of the benchmark suite.

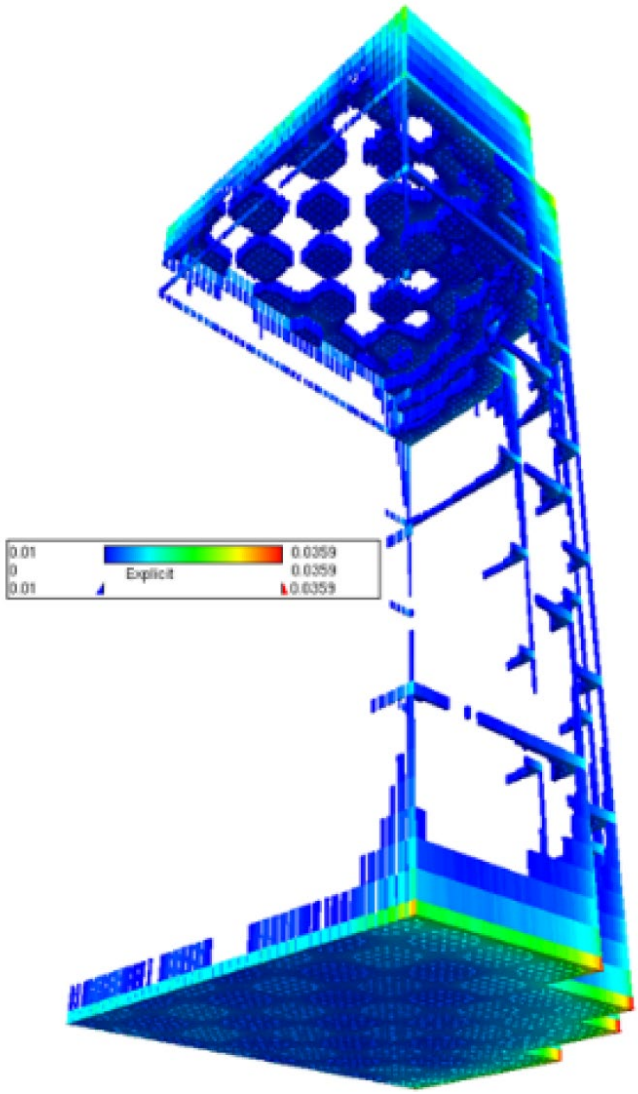


Figure 1. MC21 uncertainty >1%, TVA watts bar unit 1, exercise 2.

Key Publications

None to date. In preparation.

Sponsor/Program

Nuclear Science and Technology

A.54. MCNP®-Generated Multigroup Macroscopic Cross-Section Capability for Griffin and Validation with Hypatia Experiment

Report Participants

Alexis Maldonado,[1] Holly Trellue,[1] Mikaela Blood,[1] Michael Rising,[1] Joshua Richard[1]

1 Los Alamos National Laboratory

Scientific Achievement

We tested and developed MCNP® capability to generate multigroup macroscopic cross sections and convert this data into YAKXS format for Griffin input. This capability will allow for streamlined cross-section generation from a MCNP® model to a Griffin model. This capability has been verified with the OpenMC cross-section generation tool for Griffin. The capability has also been verified via bare sphere unit test; cross sections from MCNP® were input into Griffin, and the results were verified with existing results. Furthermore, capability is currently undergoing steady-state eigenvalue validation with the Hypatia experiment, an yttrium-hydride experiment that looked at reactivity changes of YH with respect to temperature. Hypatia was conducted at the National Criticality Experiment Research Center (NCERC). Future work includes coupling Griffin and BISON with Hypatia to create a multiphysics coupled transient simulation for the experiment and validate with existing data.

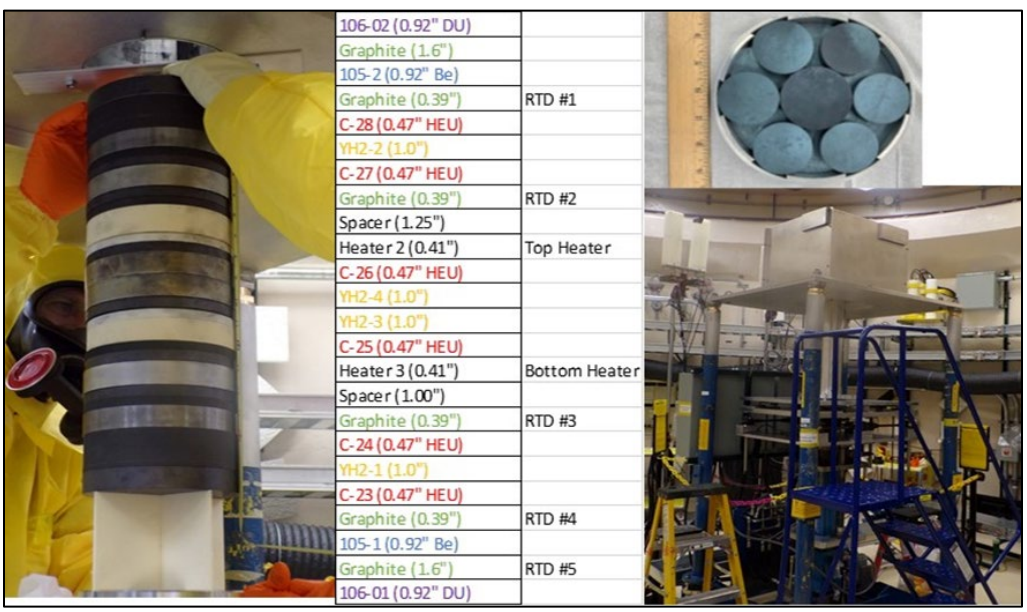


Figure 1. Hypatia experiment with HEU, YH, and graphite plates at NCERC. The Hypatia experiment took place on the planet vertical assembly machine at NCERC. This experiment has been modeled several times in MCNP®, Abaqus, and now Griffin.

Significance

This capability allows another robust physics code, MCNP®, to link to Griffin, streamlining the cross-section generation process since MCNP® is widely used. Existing work also further verifies and validates the Griffin code, increasing the robustness and confidence in the Griffin code.

Key Publications

- Trellue, H. R., M. Blood, R. Kimpland, J. Richard, and A. Maldonado. 2021. "Prediction Improvements of Transient Behavior in Advanced Reactors," LDRD-20210801ER, Los Alamos National Laboratory.

Sponsor/Program

NEAMS, LDRD, LA-UR-21-29177

A.55. MCVIZ Development – MC21 Visualization Tool

Report Participants

Brian R. Nease,[1] Victor W. Chan,[1] Ryan J. Marcellino,[1] Matthew S. Everson[1]

1 Naval Nuclear Laboratory

Scientific Achievement

MCVIZ is an interactive 3D ray tracing visualization tool used to render MC21 models. MC21 is a Monte Carlo solver used to perform reactor analyses at both NNL and INL. Historically, users could only visualize their final MC21 model by having MC21 produce non-interactive 2D slices. However, with the introduction of MCVIZ, users will now be able to interactively produce both 2D and 3D renderings of their models. In addition, the MCVIZ team expects to add capability for mesh and results visualization in future releases.

Significance

Being able to quickly and interactively visualize a model before running calculations is clearly important for model QA. However, MCVIZ development stopped when the developers began teleworking in Spring 2020, and there was no clear timeframe for when they could return to work and restart development. The developers decided to move development from NNL to INL, enabling MCVIZ to quickly restart development so that the team could finish implementing several additional important features, such as:

- Improved interactivity by performing ray tracing on a separate Qt thread
- Implemented a complete GUI test suite that covered all Qt widgets, dramatically reducing the necessary amount of manual testing
- Modularized the code so that ray tracing kernels are contained in their own plugin, making it possible for MCVIZ to visualize models from other solvers. Without access to the INL machines, completing these features would have significantly delayed the first release of MCVIZ.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.56. Modeling and Analysis of Exelon BWRs (VERA-BWR)

Report Participants

Brendan Kochunas,[1] Sooyoung Choi[1]

1 University of Michigan

Scientific Achievement

The VERA-BWR project has many members. This short report only covers those activities performed by Prof. Kochunas and Dr. Sooyoung Choi at University of Michigan, as several other activities were performed by other members at other institutions. Prof. Kochunas is a co-PI on this project. His tasks included the verification and validation of MPACT for whole-core BWR modeling. To accomplish this, several critical experiments were simulated using Sawtooth, lots of debugging was performed, and the accuracy and robustness of MPACT for simulating Peach Bottom Unit 2 cycle 1 and 2 was also carried out.

Significance

For the first time, we have validated a high-fidelity core simulator like VERA for BWR analysis. Comparisons to critical experiments show agreement in criticality which is exceptional. The Peach Bottom Cycles 1 and 2 results show quantifiable improvements over existing state-of-the-art simulation tools used by industry and regulators and agreement within approximately 95% of the estimated uncertainty of measurements.

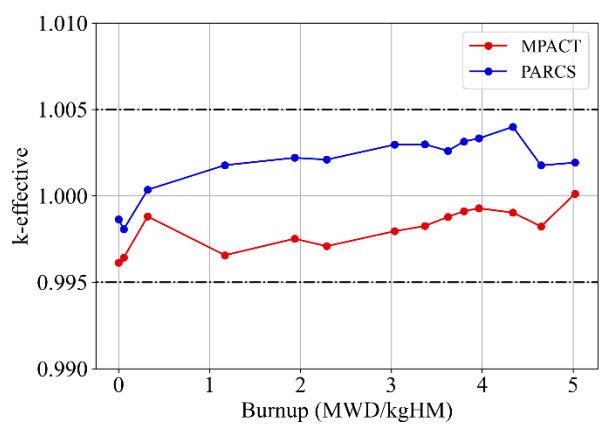


Figure 1. Peach Bottom Unit 2 cycle 2 criticality predictions.

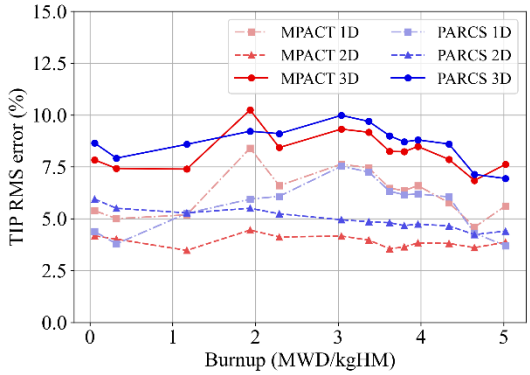


Figure 2. Peach Bottom Unit 2 cycle 2 flux measurement comparisons.

Key Publications

- Choi, S., D. Jabaay, M. Kabelitz, Y. Liu, B. Kochunas, and T. Downar. 2021. "MPACT Geometry Developments for Full-Core BWR Modeling," NURAM-2021-003, University of Michigan.
- Choi, S. and B. Kochunas. 2021. "The Limited Linear Source Approximation of the Method of Characteristics for Mitigating Negative Sources," Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021). American Nuclear Society. https://dx.doi.org/10.13182/M&C21-33635.
- Choi, S. and B. Kochunas. 2021. "PN Source Expansion Nodal Method in MPACT for Boiling Water Reactors," International Conference on Physics of Reactors 2022 (PHYSOR 2022), Pittsburgh, PA. Manuscript submitted for publication.
- Choi, S., Q. Shen, D. Jabaay, Y. Liu, B. Kochunas, and T. Downar. 2021. "MPACT Efficiency and Robustness Enhancements for Full-Core BWR Modeling," NURAM-2021-002-00, University of Michigan.
- Liu, Y., S. Choi, A. Ward, D. Jabaay, B. Kochunas, and T. Downar. 2021. "Initial Verification and Validatino of MPACT for Boiling Water Reactors," NURAM-2021-006-00, University of Michigan, Ann Arbor.
- Liu, Y., D. Jabaay, and B. Kochunas. 2021. "Validation of MPACT BWR Capabilities Against Critical Experiments," International Conference on Physics of Reactors 2022 (PHYSOR 2022), Pittsburgh, PA. Manuscript submitted for publication.

Sponsor/Program

Department of Energy

A.57. Modeling Brittle Fracture due to Anisotropic Thermal Expansion

Report Participants

Aashique A Rezwan,[1] Andrea M Jokisaari,[2] Michael R Tonks[3]

1 University of Wisconsin-Madison

2 Idaho National Laboratory

3 University of Florida

Scientific Achievement

Anisotropic thermal expansion in metal results in stress concentration at grain boundaries and triple junctions. In some materials, these stresses can lead to fracture. In this project, we investigate the impact of thermal expansion anisotropy on brittle fracture in three-dimensional polycrystal using the phase field fracture method. Investigation was performed for both increasing and decreasing temperature and the impact of crystallographic texture. A material class for anisotropic thermal expansion eigen strain was developed in the process and will merge to the Marmot framework.

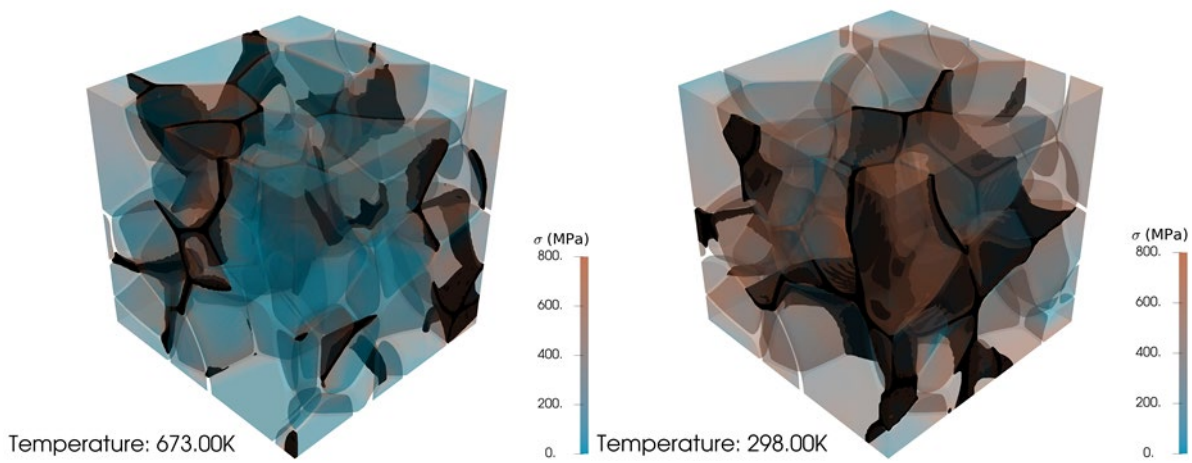


Figure 1. Fracture simulation results during heating and cooling, where (a) shows the polycrystals at the simulation end during heating, and (b) shows the same during cooling. The cracked regions are shown in black, and the domain is shaded by MPS σ.

Significance

Polycrystal material with anisotropic thermal expansion can experience fracture due to changes in temperature. This model showed significant thermal stress induced along the grain boundaries, resulting in intergrannular fracture in the three-dimensional polycrystal sample. Fracture initiated much earlier, and the final crack lengths were much more extensive during cooling than during heating since the anisotropy in α-U is more pronounced at high temperature. Increased grain misorientation affecting the crack as increasing the total fracture area. These studies provide both basic scientific insight and engineering support by predicting and explaining the complex behavior of anisotropic materials. They can offer a path forward for designing and fabricating novel materials.

Key Publications

- Rezwan, A, A. Jokisaari, and M. Tonks. “Modeling Brittle Fracture due to Anisotropic Thermal Expansion in Polycrystalline Material,” Computational Materials Science. (Under review.)

Sponsor/Program

NEAMS

A.58. Modernizing the CSAP for Use with LEU Fuel Using MC21

Report Participants

John Tortorello,[1] Ryanne Kennedy,[1] Curt Brown,[1] Michael Saitta[1]

1 MPR Associates, Inc.

Scientific Achievement

Throughout the last year, I have been working on various projects that have the big picture goal of calculating, verifying, and documenting safety pertinent quantities for the ATR. These quantities are required for the completion of the CSAP and the SAR. New calculation methods are necessary due to the planned transition from HEU to LEU.

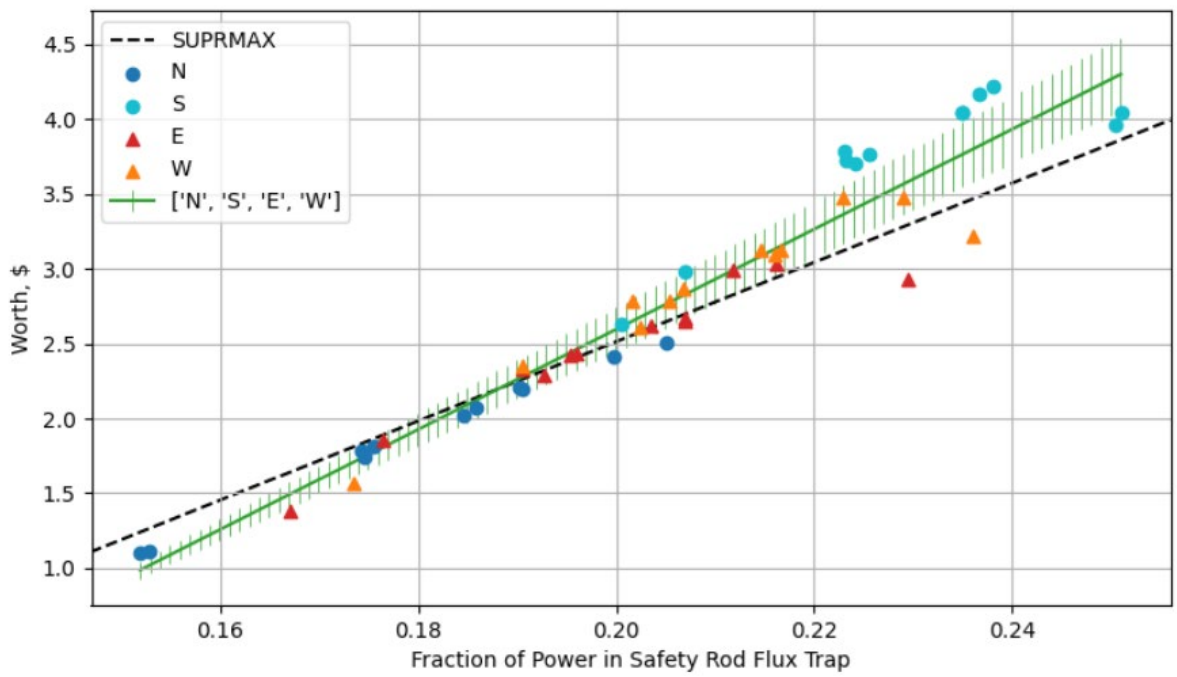


Figure 1. The Figure above shows the results of a regression that uses outputs from MC21 to predict safety rod reactivity worth in different power scenarios.

Significance

This project is calculating reactivity worths and power uncertainty in the ATR. The documentation being produced in this project is vital for a smooth transition from HEU fuel to LEU fuel in the ATR.

Key Publications

I prepared the MPR calculation document titled "Calculating ATR Safety Rod Reactivity Worth Using MC21." In addition, I was a collaborator and checker for the calculation document titled "ET-1 Local Power Uncertainty." C21 requires all information to go through NNL's public utterance process. No publications made it through the public utterance process.

Sponsor/Program

Advanced Test Reactor (ATR)

A.59. Monte Carlo Fission Source Convergence Acceleration Methods

Report Participants

C. Murphy,[1] D.P. Griesheimer[2]

1 Answers Software Service, Jacobs

2 Naval Nuclear Laboratory

Scientific Achievement

Monte Carlo codes that solve the fission eigenvalue problem have so far mainly used the power iteration technique to obtain the fundamental eigenvalue due to its simplicity and robustness to stochastic noise. However, the power iteration method is slow to converge when the ratio between the fundamental eigenvalue and the next eigenvalue is high—known as the dominance ratio. As a result, problems with a high dominance ratio often require that a large number of iterations of the Monte Carlo calculation be discarded to ensure that the result is not biased while the fission source is still converging. Alternative methods of calculating the fission eigenvalue with faster convergence rates are being prototyped and investigated using the Monte Carlo code in the Simplified Mini-Applications for Radiation Transport (SMART) suite written in Python. So far, methods that involve the Arnoldi iteration and dynamic mode decomposition techniques have been implemented.

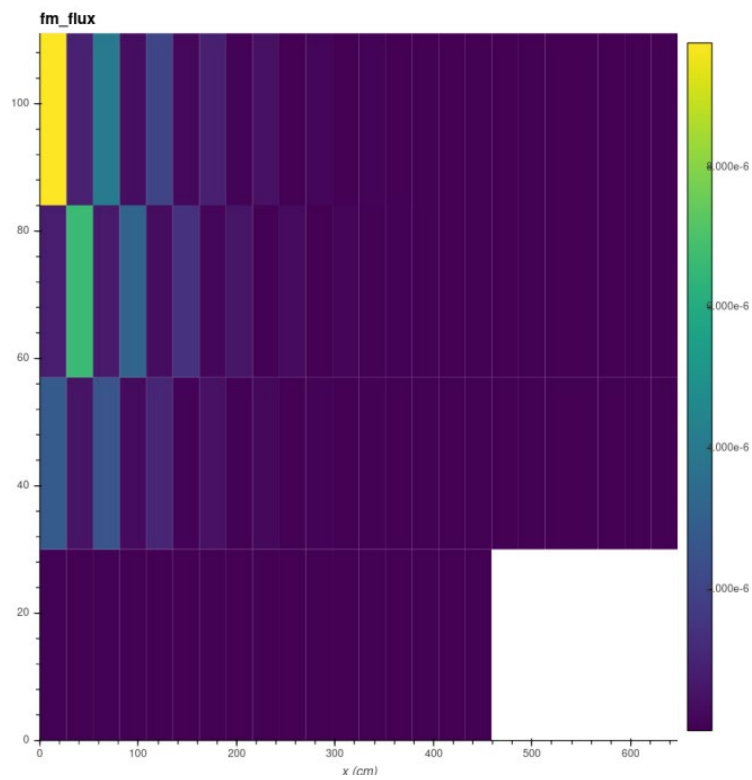


Figure 1. Neutron flux distribution of a SMART model based on the NEA checkerboard storage of fuel assemblies source convergence benchmark. This is a particularly difficult problem for Monte Carlo power iteration codes to solve.

Significance

The lessons learned from prototyping new techniques to improve the convergence rate of Monte Carlo fission eigenvalue calculations will be applied to future developments of the MC21 Monte Carlo reactor physics code.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.60. Multi-Physics Modeling and Simulations of Heat-Pipe Microreactors

Report Participants

Rui Hu,[1] Guojun Hu,[1] Joseph Kelly,[2] Javier Ortensi[3]

1 Argonne National Laboratory

2 U.S. Nuclear Regulatory Commission

3 Idaho National Laboratory

Scientific Achievement

The primary goal of this work was to develop the multi-physics modeling capability for analysis of the advanced nuclear reactors. The heat-pipe microreactor system has been demonstrated in the steady and transient simulation of a reference heat-pipe reactor design. Simulation of the heat-pipe-cooled microreactors requires capturing the phenomena of several fields of physics (e.g., reactor kinetics, system TH, and thermomechanics). The model was simulated using three submodules of Comprehensive Reactor Analysis Bundle (BlueCRAB). The MAMMOTH module is used to simulate the reactor kinetics behavior of the microreactor; the SAM module is used to simulate the heat conduction in the reactor core and heat removal through the heat-pipe heat exchangers and Reactor Cavity Cooling System (RCCS); and the MOOSE Tensor Mechanics module is used to simulate the thermal expansion of the reactor cores. The different sub-models are coupled together using the MultiApp system in MOOSE. The BlueCRAB multi-physics modeling was demonstrated by performing a steady-state analysis and transient simulation of an unprotected loss of heat sink event.

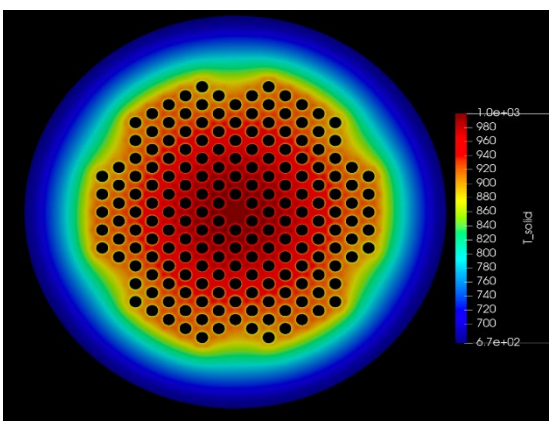


Figure 1. Steady-state solid temperature profile.

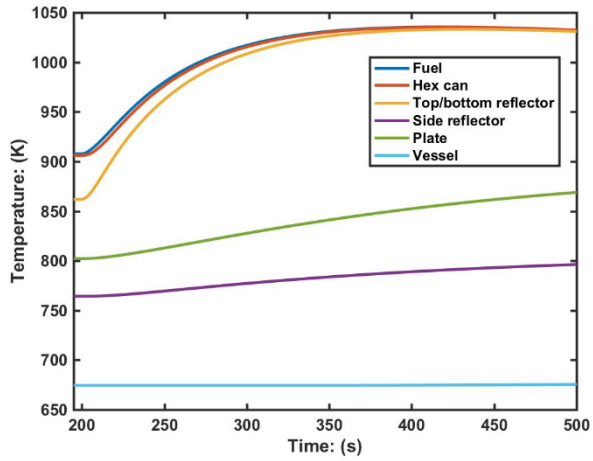


Figure 2. Transient solid temperature in different regions during an unprotected loss of heat sink event.

Significance

For plant systems analysis and assessing the adequacy of the emergency core cooling features of a design, the NRC is developing a suite of codes called the BlueCRAB. BlueCRAB is the coupled combination of NRC codes and codes developed by the Department of Energy under the under the NEAMS program. BlueCRAB is capable of simulating a broad range of conventional and advanced reactor designs. To prepare for independent analysis as part of the review and to demonstrate the capabilities of BlueCRAB, this work supported the NRC to develop a reference plant model of a heat-pipe-cooled microreactor. The purpose of a reference plant is to provides both a test bench for the BlueCRAB system and a means to identify potential modeling and simulation challenges before a design review is underway.

Key Publications

- Hu, G., R. Hu, J. M. Kelly, and J. Ortensi. 2019. "Multi-Physics Simulations of Heat Pipe Micro Reactor," ANL/NSE-19/25, Argonne National Laboratory.

Sponsor/Program

NRC, NEAMS

A.61. Multiphysics Modeling of Fracture in Sintered Uranium Dioxide Fuel Pellets

Report Participants

Levi D. McClenny,[1] M. Gomaa Abdoelatef,[2,3] Moiz I. Butt,[2] Michal J. Pate,[2] R. Harikrishnan,[4] W. Jiange,[5] Sean M. McDeavitt,[2] Karim Ahmed[2,3,*]

1 Electrical Engineering Department, Texas A&M University

2 Nuclear Engineering Department, Texas A&M University

3 Materials Science and Engineering Department, Texas A&M University

4 Aerospace Engineering Department, Texas A&M University

5 Idaho National Laboratory

* Corresponding Author: Karim.Ahmed@tamu.edu

Scientific Achievement

Commercial nuclear power plants extensively rely on fission energy from uranium dioxide (UO2) fuel pellets to provide thermal energy to the coolant in current generation reactors. UO2 fuel incurs damage and fractures during operation due to large thermal gradients between the fuel and the coolant in the reactor core. In this work, we describe an experimental study performed to understand the fuel fracturing behaviors of sintered powder UO2 pellets when exposed to thermal shock conditions, as well as a computational fracture model which accurately predicts the experimental results. Experimental data was collected from multiple experiments by exposing UO2 pellets to high-temperature conditions (900–1200°C) which are subsequently quenched in sub-zero water. The pellets were placed in contact with one side of a helium insulated copper pipe inner wall to improve heat conduction efficiency. We exhibit that the fracture results gathered in the experimental setting can be consistently recreated in a computational setting, demonstrating a reliable ability to computationally simulate thermal shock gradients and subsequent fracture mechanics in the primary fuel source of LWRs.

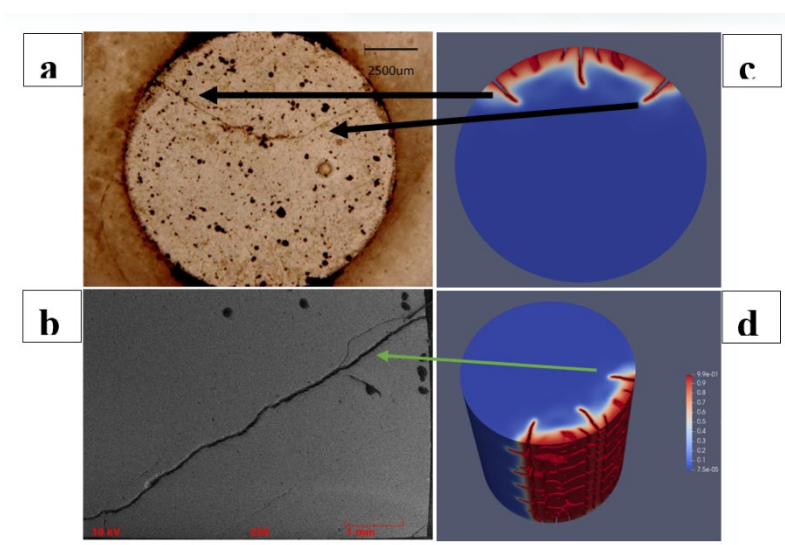


Figure 1. Comparison of final crack patterns induced by thermal shock between ([a] and [b]) this work's experiment observations after the thermal shock testing and ([c] and [d]) the elected model simulation (colored by the fractured order parameter field distribution). The model could capture the formation and evolution of primary radial cracks. As seen, there are two major (longer) radial cracks that formed immediately on the pellet circumferential boundary after the instantaneous drop in the outer temperature (thermal shock). Moreover, the simulated crack thickness was too close to the experimental observation,

as seen in (b) and (d). We noticed minor inconsistencies between the model and the experiment results (such as the middle crack shown in the model simulations). The reason for that is our model, at its current status, did not fully account for the porosity microstructure effects; overcoming such limitation is one of our future directions.

Significance

These work model parameters were calculated based on the UO2 thermomechanical properties, while the other effective parameters were determined based on a parametric study as described below. Due to the instantaneous temperature drop on the pellet surface, a large jump in the stresses throughout the pellet took place, mainly on the cooling side face. This rapid temperature change and the increased localized stresses are considered the main driving forces for the UO2 fuel cracking. To obtain initial insights with computational cost concerns, we only considered a fresh fuel (zero burnups) in this model, then compared the model results with the previously described experiment outcomes. The model did not account for the creep effect; we ignored the fission gas release and the grain growth influences. However, the qualitative effects might consider in parametric study calculations of the energy release rate (g_c), as illustrated throughout this section. The studied domain consists of a 3D fuel pellet with a 10 mm radius, and the axial direction height was set to 10 mm as well. The whole pellet's initial temperature condition was set to 50°C, while the right side only introduced to the low-temperature value, −10°C (thermal shock).

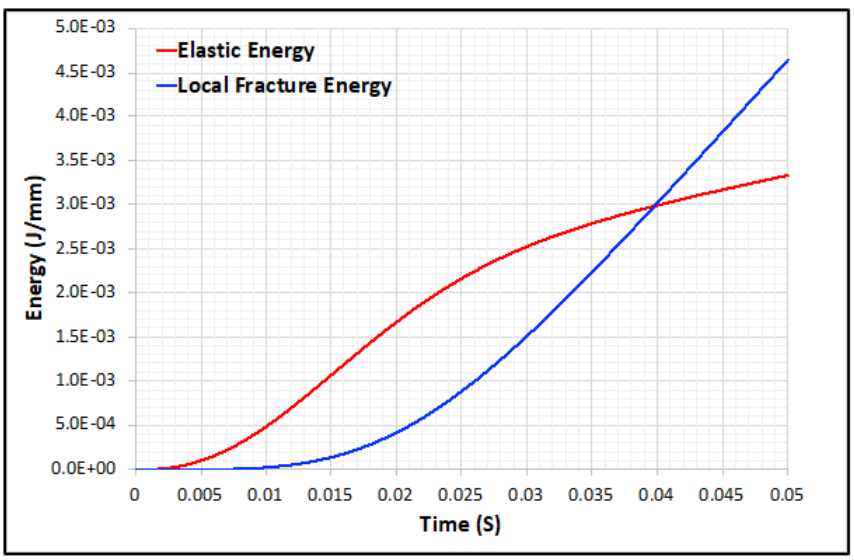


Figure 2. Evolutions of elastic strain energy and the formation and growth of the local fracture energy based on fine mesh and length-scale parameter of 10-3 mm for the elected simulation case; see the last row in Figure 4. The elastic strain energy increases with increasing the temperature difference between the inner center and the outer surface (see Figure 1). The cracks immediately initiated on the pellet outer surface at about 10-2 seconds, right after the instantaneous drop in temperature. The elastic strain energy drops quickly to generate new fracture faces.

Key Publications

The proposed manuscript is under preparation for submission/publication.

Sponsor/Program

NEAMS

A.62. Multiscale Modeling of Environmental Degradation in Structural Materials

Report Participants

Benjamin Anglin,[1] Jonathan Wormald,[1] Thomas Webb[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The NNL is developing environment sensitive, physically based plasticity models at various length scales across many orders of magnitudes. Results obtained from one length scale are readily passed to another length scale owing to the unified set of physics and understanding of underlying mechanisms built into each of these models. INL HPC supports both electronic structure calculations and novel fast Fourier transform (FFT) driven crystal plasticity simulations. These results are integrated with a multiscale physically based model for oxidation to simulate stress corrosion cracking on an explicit 3D microstructure.

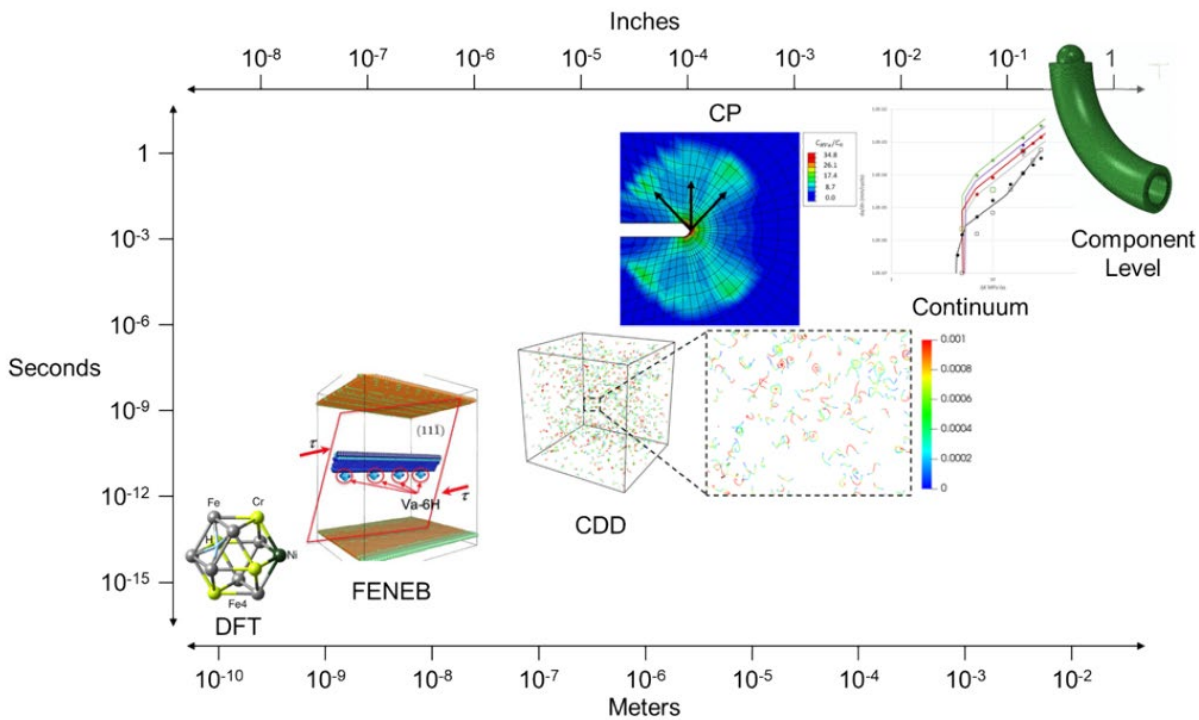


Figure 1. A schematic of the range of length scales, in both meters and inches, and time scales, in seconds, spanned in the multiscale modeling approach employed in the EICEM program. Legend: DFT = density functional theory; FENEB = free end nudged elastic band; CDD = continuum dislocation dynamics; CP = crystal plasticity.

Significance

Environmental cracking is a localized pheomenon in structural materials where only the conditions near the crack tip are of importance. In the case of stress corrosion cracking in aqueous environments, these conditions include local chemisry, stress, and material microstructure. Conventional empirical models used to predict stress corrosion cracking rely on large datasets to offer model accuracy. Whereas, physically based models developed in this project use the understanding of underlying operative physical mechanisms to build accuracy, thereby promoting confidence in model accuracy outside the available dataset. Simulations over a wide range of time and length scales, such as electronic structure theory to capture the atomic level environment and chemistry, are used to construct and inform a crystal plasticity model that explicitly accounts for mechanical deformation in the material microstructure. Stress corrosion cracking simulations of explicit microstructures quickly become intractable in finite element methods owing to the large domains required to emulate significant explicit microstructures. An alternative approach, employed here, is to use fast Fourier transforms to solve the micromechanical equations throughout a large (~104 grains) microstructure. Thus, realistic simulations of stress corrosion cracking can be achieved.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.63. Multiscale Modeling of the Evolution of Metal-Oxide Interface

Report Participants

Natalia Tymiak Carlson[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The scientific achievements included ab initio and MD calculations toward developing mechanistic corrosion rate models.

Significance

Interactive effects of oxide growth and stress evolution during aqueous corrosion of zirconium alloys are linked to degradation of the protective capability of zirconium (Zr) oxide. Understanding the interactive effects is instrumental to improving predictions of the in-service component performance. Modeling across the length scales has been undertaken for the evaluation of the factors influencing metal/oxide interface during Zr alloy corrosion.

MD evaluates the interface evolution on the nanoscale. Interfacial non-planarity develops in the simulated nano-grains assuming energy-governed metal-to oxide transformation and enhanced GB diffusion.

Ab initio evaluates the effects of factors potentially influencing corrosion rate transitions. Fracture resistance of Zr oxide. Out of all the evaluated Zr oxide phases/stoichiometries, ZrO is expected to be the most brittle. Slightly lower ductility is predicted for the monoclinic as compared to the T ZrO2. This implies a potentially negative impact of the T-M transition on fracture resistance of ZrO2.

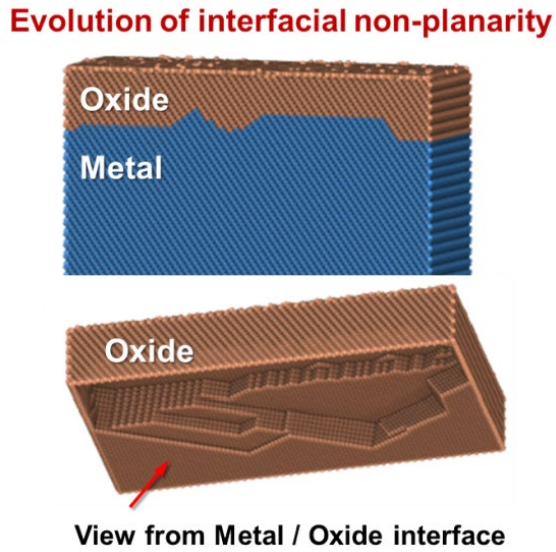


Figure 1. Evolution of the nanoscale non-planarity of metal-oxide interface (MD calculations).

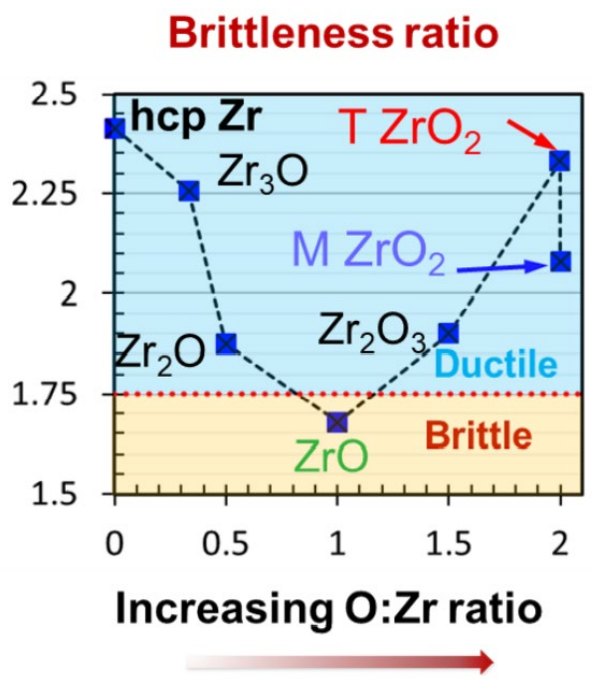


Figure 2. Effect of Zr oxide stoichiometry on its brittleness (DFT calculations).

Key Publications

In progress.

Sponsor/Program

Nuclear Science and Technology

A.64. Nanodispersion-Strengthened Metallic Composites with Enhanced Neutron Irradiation Tolerance

Report Participants

Penghui Cao,[1,2] Kangpyo So,[1] Ju Li,[1] Michael P. Short[1]

1 Massachusetts Institute of Technology

2 University of California

Scientific Achievement

We develop and study irradiation-tolerant, nanodispersion-strengthened composite structural materials by innovative manufacturing methods. These nano-composites have prolific internal interfaces between 1D/2D nanodispersoids and the metal matrix; therefore, they provide abundant radiation defect recombination venues to rapidly heal radiation damage.

Significance

We demonstrate in our recent study (Cao et al. 2021) that a metal composite made by adding 1D carbon nanotubes (CNTs) to aluminum (Al) exhibits superior radiation resistance. In situ ion irradiation with transmission electron microscopy and atomistic simulations together reveal the mechanisms of rapid defect migration to CNTs, facilitating defect recombination and enhancing radiation tolerance. The origin of this effect is an evolving stress gradient in the Al matrix resulting from CNT transformation under irradiation and the stability of resulting carbides. Extreme value statistics of large defect behavior in our simulations highlight the role of CNTs in reducing accumulated damage. This approach to controlling defect migration represents a promising opportunity to enhance the radiation resistance of nuclear materials without detrimental effects.

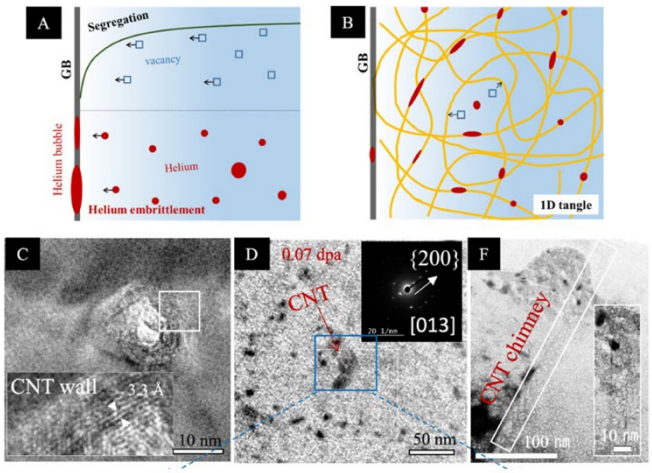


Figure 1. (A) Schematic illustration of GB-related radiation degradation such as RIS and helium gas embrittlement. The green line indicates the concentration of vacancies away from the GB. (B) 1D tangles of CNTs or NWs accommodate radiation defects and protect GB integrity. In (C–D), we demonstrate the role of CNTs in attracting radiation defects. (C) Intact wall structure of a CNT in an Al grain before irradiation and (D) defect distribution near a CNT at 0.07 DPA.

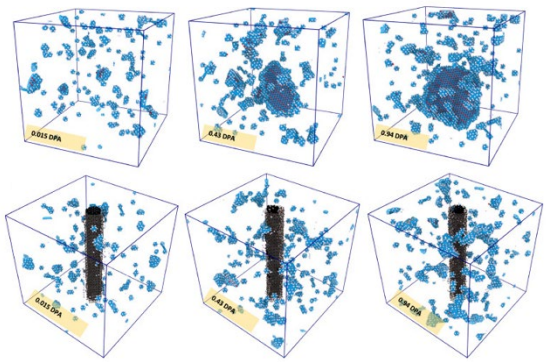


Figure 2. Evolution of defect structures in pure Al and Al-CNT, respectively. Only non-FCC atoms are shown, selected by coordination number analysis.

Key Publications

- Cao, P., K. P. So, Y. Yang, J. G. Park, M. Li, L. Yan, J. Hu, M. Kirk, M. Li, Y. H. Lee, M. P. Short, and J. Li. 2021. "Carbon nanotube (CNT) metal composites exhibit greatly reduced radiation damage," *Acta Materialia*, 203:116483. https://doi.org/10.1016/j.actamat.2020.116483.

Sponsor/Program

NEUP/NSUF

A.65. NDEX Development for NNL

Report Participants

Jason Thompson,[1] Andrew Pavlou[1]

1 Naval Nuclear Laboratory

Scientific Achievement

NDEX is NNL's primary nuclear data processor for the CMCDT project (which includes MC21). It is a Python program which is primarily focused on converting nuclear data evaluations into nuclear data suitable for use in Monte Carlo calculations. NDEX's capabilities are currently being expanded to provide a single nuclear data processing system for CMCDT.

Significance

Simplified input and more robust nuclear data processing is required to support NR program designs. Simplified input results in less engineering time developing the input and less intesive quality assurance checks. A robust code is needed to ensure all requirements are met, and all use cases are covered.

Key Publications

No publicly available reports or presentations are available for the work performed at INL.

Sponsor/Program

Nuclear Science and Technology

A.66. NEAMS – Analysis of Cladding Burst Geometry and Development of Burst Model Using the BISON Fuel Performance Code

Report Participants

Ryan T. Sweet,[1] Nathan A. Capps[1]

1 Oak Ridge National Laboratory

Scientific Achievement

This work uses the BISON fuel performance code to elucidate additional information from cladding burst tests. This is accomplished through detailed characterization of testing conditions and specimen in situ behavior. Testing conditions and cladding-specific material models are selected, and the experiment is simulated. Results from the simulations are compared against cladding strain surface maps from the experiment to determine how well current models can predict the coated-cladding behavior under transient conditions.

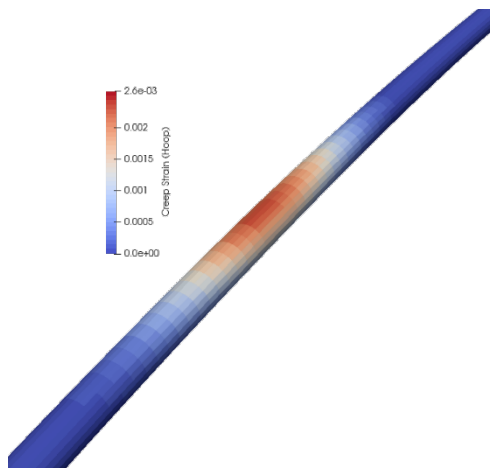


Figure 1. 3D cladding strain profile arising from variations in the azimuthal and axial temperature gradients.

Significance

This work is still in progress; however, early prototype simulations have been performed using the HPC system.

Key Publications

Final milestone report and upcoming publications are still in progress.

Sponsor/Program

This work is sponsored by the NEAMS program.

A.67. NEAMS – Shift and Griffin Development for LWR and Advanced Reactors

Report Participants

Tara Pandya[1]

1 Oak Ridge National Laboratory

Scientific Achievement

I have produced Shift Monte Carlo generated multigroup cross sections for the EMPIRE fast reactor and run these with Griffin. This capability is general and is applicable to LWR and advanced reactor multiphysics analysis.

Significance

This work will benefit NEAMS by expanding the capabilities of the NEAMS software suite, Shift and Griffin, as applied to LWR and advanced reactor multiphysics analysis. Comparisons of results from Griffin using Shift-generated cross sections and Serpent-generated cross sections serve as verification and validation.

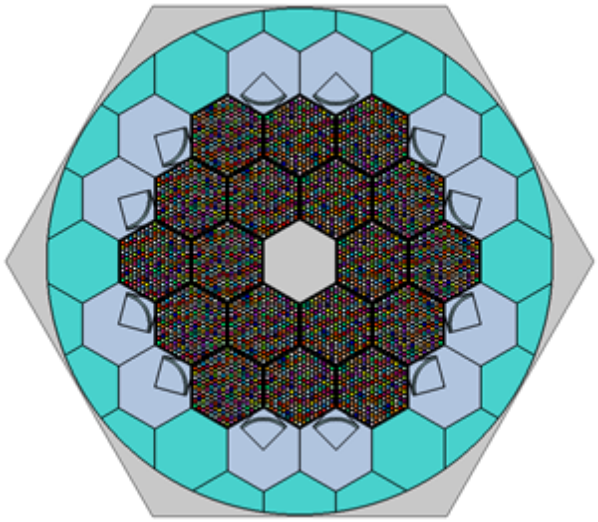


Figure 1. EMPIRE 2D core shift model (from Fulcrum).

Key Publications

In progress.

Sponsor/Program

NEAMS

A.68. NEAMS Molten-Salt Breeder Reactor Modeling and Simulation

Report Participants

Eva Davidson,[1] Benjamin Betzler[1]

1 Oak Ridge National Laboratory

Scientific Achievement

The NEAMS modeling and simulation work for this fiscal year involves running the Shift Monte Carlo code to perform dose rate calculations for the molten- salt breeder reactor (MSBR). These calculations have never been done for the MSBR and are first-of-a-kind for the MSBR.

Significance

The private sector's recent interest in the active development of MSRs has led to the need to develop and test advanced modeling and simulation tools to analyze various advanced reactor types under numerous conditions. The MSBR model integrates a Monte Carlo N-Particle (MCNP) MSBR core model with an MCNP model that was generated from a CAD model of the external components and the reactor building, which was subsequently run in Shift. This model is intended to aid in understanding radiological dose conditions during operation, as well as the iron dpa rates in the reactor vessel. The neutron biological dose rates and flux calculated in the reactor cell are much higher in the MSBR than in typical LWRs.

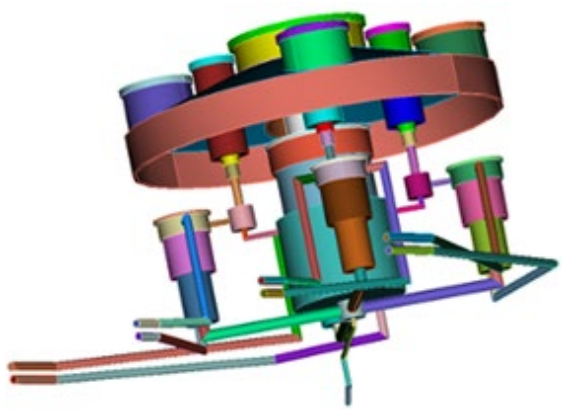


Figure 1. External MSBR components.

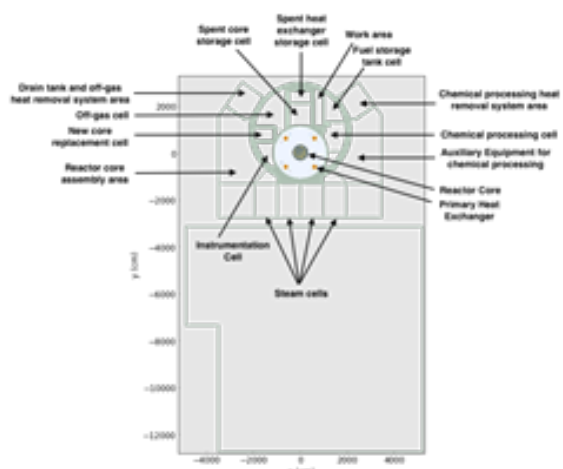


Figure 2. MSBR integrated model for radiation transport.

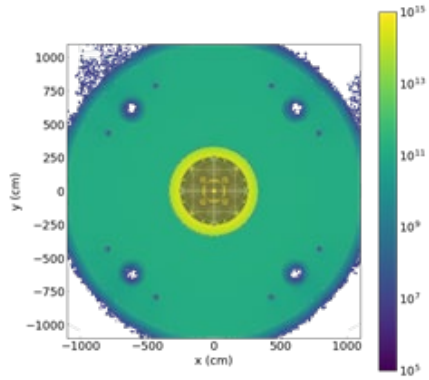


Figure 3. Neutron flux at z=0 (reactor midplane).

Key Publications

- Davidson, E. E., G. Radulescu, K. Smith, J. Yang, S. Wilson, and B. R. Betzler. 2021. "Reactor Cell Neutron Dose For the Molten Salt Breeder Reactor Conceptual Design," *Nuclear Engineering and Design*, 383:111381. https://doi.org/10.1016/j.nucengdes.2021.111381.

Sponsor/Program

NEAMS

A.69. NEK5000 Benchmark and Demonstration for NRC Use

Report Participants

Christopher Boyd[1]

1 U.S. Nuclear Regulatory Commission

Scientific Achievement

This project is not complete and is still in the preliminary stages. The achievements to date have been related to exercising the code and becoming familiar with the INL computing systems.

Significance

The work is part of a benchmark exercise being conducted by the NRC with the support of ANL staff through NEAMS. This benchmark exercise is focused on computing turbulence statistics from a jet/plume with obstacles and the jet/plumes interaction with a stratified helium layer. This work supports the NRC's efforts to build capabilities for nuclear containment type models where rising steam plumes from the primary system can interact with hydrogen layers and containment structures during postulated severe accident scenarios. Tracking and understanding the distribution of hydrogen in containtment is of interest to the NRC.

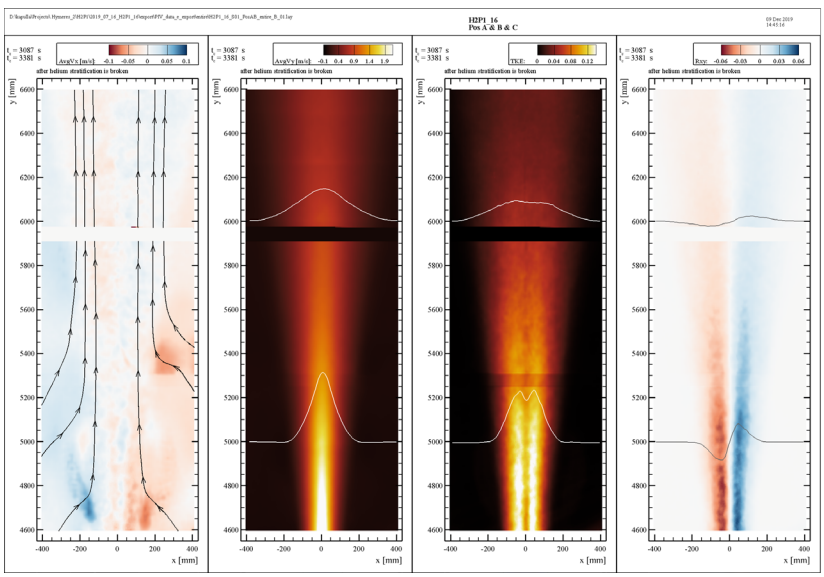


Figure 1. PIV benchmark test data from one of the tests.

Key Publications

None.

Sponsor/Program

This work is sponsored by the NRC with DOE support coming from NEAMS.

A.70. New Technology Early Access (Software and Hardware)

Report Participants

Ann Kelly,[1] Brian J. McDermott,[1] Kevin Sischo[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The NNL Future Technology organization evaluates HPC hardware and software for potential use in future HPC procurements and internal software development. Members of this organization have utilized the INL Sawtooth system to investigate multiple hardware and software options in an expedited fashion relative to what would have otherwise been required by NNL's traditional (on-premises) evaluation methods. This has included: use of GPUs (software stack and programming), Open OnDemand features and use, and general HPC user experience for an outside organization other than NNL.

Significance

Access to INL HPC has provided NNL Future Technology with a rapid method of evaluating hardware and software that would otherwise have to be purchased and installed on site at NNL, which would have required longer lead times and greater resource expenditures. The net effect is an ability for NNL to deploy new scientific computing technologies and infrastructure faster to its engineers and scientists, which ultimately enables more capable products and services to be delivered to the Navy with increased velocity. This organization will continue to access INL systems in the future to enhance their evaluation process.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.71. Non-Intrusive Neural-Network-Based Reduced-Order Modeling

Report Participants

Brandon LaFleur[1]

1 University of Michigan and Naval Nuclear Laboratory

Scientific Achievement

High-fidelity simulations of neutron transport play an important role in the design and analysis of nuclear reactor cores. Specific challenges present in numerical simulations required for nuclear reactor design, specifically the high computational cost and dimensionality often encountered, are not unique to the nuclear industry. A full order model (FOM) is often very expensive to evaluate in many engineering disciplines, particularly when considering transient simulations. The dimensionality encountered during discretization of partial differential equations often leads to hugely coupled systems of equations. In the context of making design decisions requiring quick model turnaround times, performing uncertainty quantification (UQ), or optimizing some engineering system, these FOMs can be prohibitively expensive.

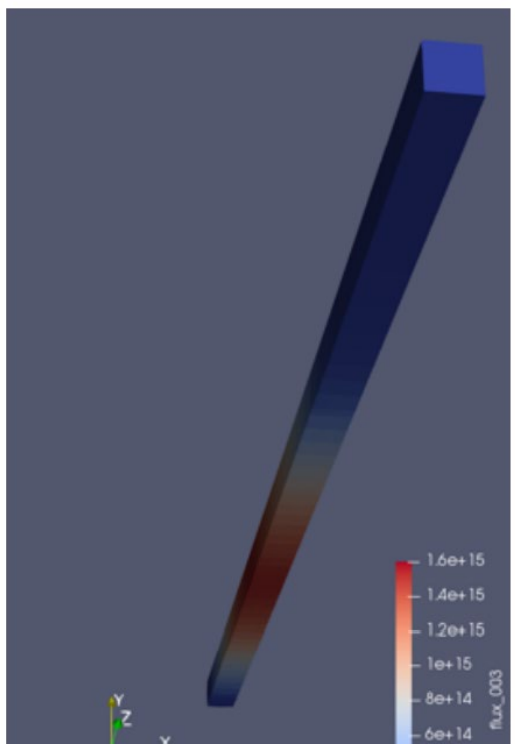


Figure 1. An MPACT single assembly model, showing relative powers axially.

This natural limitation is present in many fields and has led to the development and deployment of reduced-order modeling techniques. A reduced-order model (ROM) allows for the approximation of an FOM on a lower dimensional manifold. The goal of the ROM is to produce results that enable the engineer to make design decisions without having to incur the cost of a FOM to do so.

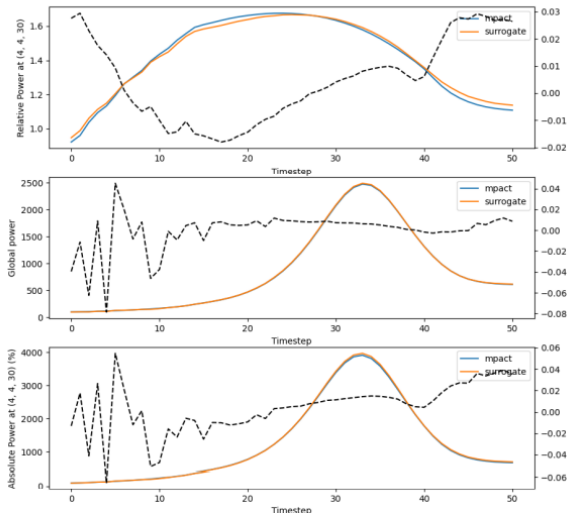


Figure 2. Transient local relative powers. It includes ROM, FOM, and associated error as a function of timestep.

Significance

This project explores the ability to perform expensive transient multiphysics calculations for some sets of model inputs much more quickly using ROM methodologies. Specifically, the work involves a non-intrusive Bayesian neural-network-based methodologies, only requiring access to code output. This work would allow nuclear designers of various sub-disciplines to explore their design space without needing to repeatedly run FOMs. To this end, Bayesian neural-network-based reduced-order models are explored as an option to fascilitate the quick exploration of a design space.

The methods are to be applied to two application problems. The first is a small scale transient model, to demonstrate the ability of the ROM to capture the time dynamics of a multiphysics calculation. The second application problem deals with a larger reactor core model but is constrainted to a steady-state scenario. This stage is intended to test the scalability of the methodology in a more realistic modeling environment.

Key Publications

No current publications. Currently performing research supporting a PhD prospectus. The work may lead to publications in the future.

Sponsor/Program

Nuclear Science and Technology

A.72. OpenFOAM Professional and Technique Development

Report Participants

Philip Sapienza[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The scientific achievements included familiarizing the participant with the use of the open source CFD code OpenFOAM and developing modeling techniques applicable to NNL problems.

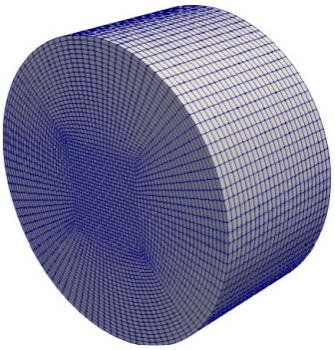


Figure 1. Disc with o-grid structure mesh.

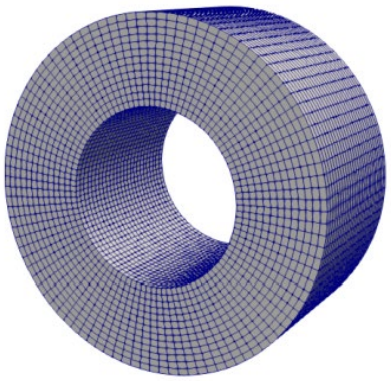


Figure 2. Ring with structured mesh.

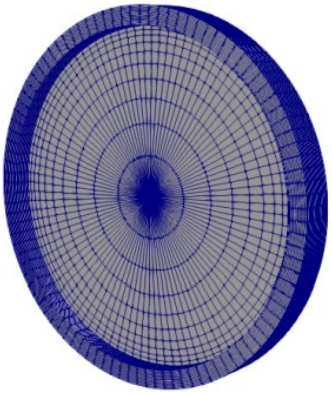


Figure 3. Combined ring and disc with structured mesh.

Significance

The participant has increased his familiarity with OpenFOAM which is being heavily used in work performed by his NNL internal organization. The particpant has also developed meshing techniques that could be of use to NNL CFD problems. Specifically, the creation of multi-block structured meshes of rings, discs, and other cylindrical or annular shapes. Finally, the participant has learned how to create these meshes parametrically.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.73. OpenMC Monte Carlo Particle Transport Code to Optimize Parallel Efficiency on Large-scale Computing Systems Using Ensemble-Averaging With Coarse Mesh Finite Differences Source Acceleration.

Report Participants

Shikhar Kumar,[1] Benoit Forget,[1] Kord Smith[1]

1 Massachusetts Institute of Technology

Scientific Achievement

This Ph.D. project focused on using the OpenMC Monte Carlo particle transport code to optimize parallel efficiency on large-scale computing systems using ensemble-averaging with Coarse Mesh Finite Differences (CMFD) source acceleration.

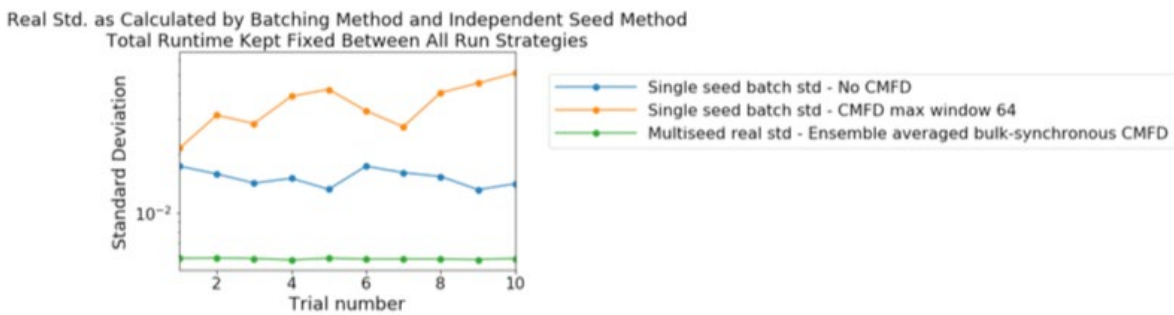


Figure 1. Real standard deviation as predicted by independent trials of bulk synchronous ensemble-averaged CMFD and by the batching method using a single seed with a large number of active generations. Runtime is kept fixed across all run strategies, and results are shown for the 2-D BEAVRS problem.

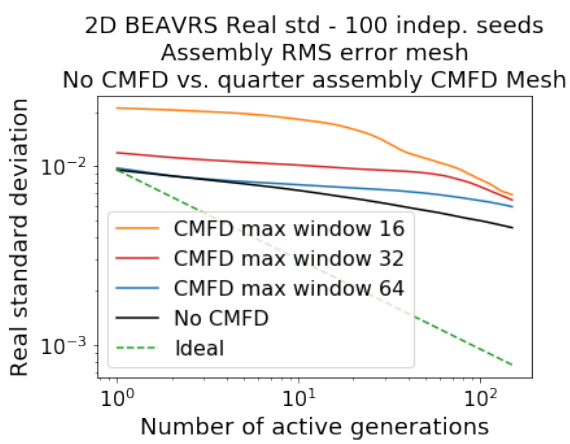


Figure 2. Real standard deviation as a function of number of active generations - No CMFD vs. Quarter assembly CMFD mesh with varying window size for 2-D problem. Real standard deviation is computed over 100 independent trials with a generation size per trial of 10 million and assembly sized RMS error mesh.

Significance

It is found that an ensemble-averaged CMFD approach improves load balancing by 5–10%, improves fault tolerance, and provides a method for true variance calculations without explicitly determining Monte Carlo correlation effects. This work will be used to report on how full-core Monte Carlo calculations can be optimized on large-scale computing systems, and this work has applications on TH multiphysics coupling, as well as on GPU-based computing platforms.

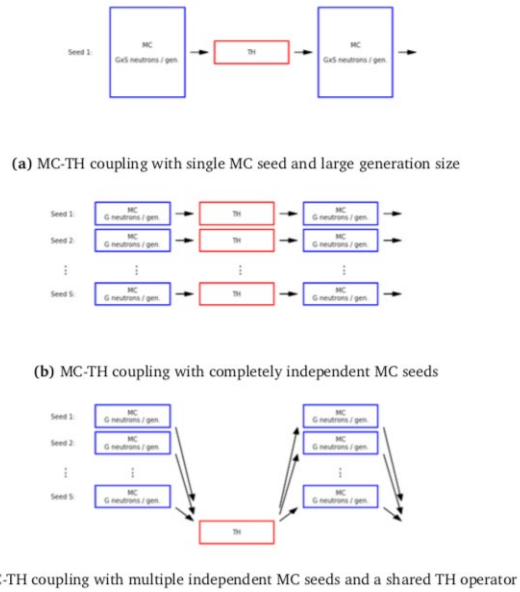


Figure 3. Schematics for running MC-TH coupling.

Key Publications

- Kumar, S., B. Forget, and K. Smith. 2020. "Stationarity Diagnostics using Functional Expansion Tallies," *Annals of Nuclear Energy*, 143:107388. https://doi.org/10.1016/j.anucene.2020.107388.
- Kumar, S., B. Forget, and K. Smith. 2019. "Analysis of Fission Source Stationarity for a 3-D SMR Core Using Functional Expansion Tallies," Proceedings of International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2019).
- Kumar, S. ND. "An Asynchronous Ensemble-Averaged Approach to CMFD Acceleration: Rearchitecting Reactor Simulation Paradigms for the Exascale Computing Age," Doctoral dissertation, Massachusetts Institute of Technology, in progress.
- Kumar, S., B. Forget, and K. Smith. ND. "An Asynchronous Ensemble-Averaging Approach to CMFD Source Acceleration for Monte Carlo Reactor Simulations," submitted to *Annals of Nuclear Energy*, in progress.
- Kumar, S., B. Forget, and K. Smith. ND. "Fission Source Variance Analysis for CMFD Source Acceleration with Monte Carlo Transport," submitted to *Nuclear Science and Technology*, in progress.

Sponsor/Program

Nuclear Energy University Program (NEUP)

A.74. OVERLORD – Bayesian Optimization for Engineering Design

Report Participants

Lloyd M. Huang,[1] Kevin Parrish,[1] Brian McDermott,[1] Michael Schneier,[1] Steven Mattis[1]

1 Naval Nuclear Laboratory

Scientific Achievement

The objective of this project is to develop a ML platform that adaptively learns from physics simulations in order to efficiently find an optimal solution to engineering design problems. New algorithms have been developed in order to improve the scalability and reliability of Bayesian optimization for production level engineering challenges. The scalability of Bayesian optimization has been improved by implementing a newly develop Bayesian neural network with a Gaussian prior. Additionally, novel or improved global heuristic optimization algorithms are combined.

Significance

This project is resulting in the reduction of necessary high-fidelity physics calculations needed to optimize engineer designs by up to orders of magnitude. Additionally, it results in automation that makes engineer design work less tedious. This results in less needed computational resources as well as engineering time to solve problems and make new designs. Currently, production software development is underway to provide this capability to a wide range of engineering applications.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.75. Parallel Low-Temperature Plasma Multiphysics Simulation Using MOOSE and MOOSE-Based Application Zapdos

Report Participants

Corey DeChant,[1] Casey T. Icenhour,[1,2] Steven Shannon[1]

1 North Carolina State University

2 Idaho National Laboratory

Scientific Achievement

The objective of this work is developing capability in the MOOSE framework ecosystem to model complex fluids and fluid/material interactions. These complex fluids are not only affected by the traditional fluid equations but also include the transport of species that can be affected by and can form coupled fields in other physics domains, such as electric and magnetic fields due to volume charge separation and current flow in the fluid. Both verification and validation studies were recently completed for the MOOSE-based application Zapdos. These studies involved using the method of manufactured solutions to verify mathematical calculations, spatial and temporal convergence studies to verify performance, and comparisons to previous validated software for both 1D and 2D vacuum plasma simulations performed by D.P. Lymberopoulos and D.J. Economou. For these studies, a temporal accelerator technique based on a shooting Newton's method were added to reduce the time needed to reach a periodic steady state. From example, non-accelerated simulations would take approximately 105 RF cycles, while accelerated simulations would take about several thousand. Both sets of studies showed reasonable result and agreement to theory and previous validated models.

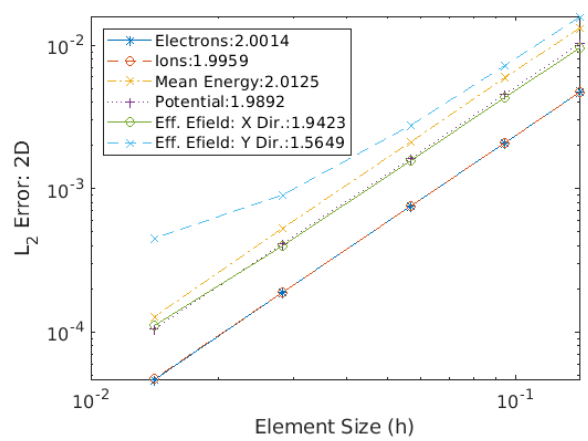


Figure 1. 2D spatial convergence study. Ideal slope = 2.

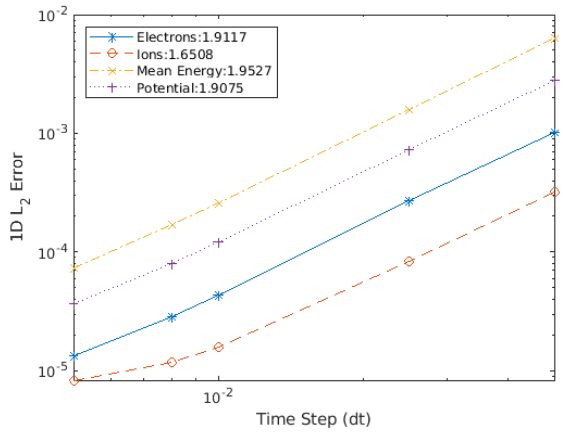


Figure 2. 2D temporal convergence study. Ideal slope = 2.

Significance

With the completion of these first sets of plasma verification and validation studies, current efforts are focused on fully coupling the MOOSE's Navier-Stokes module with Zapdos to model complex fluid species within dynamic water and on performing experimental comparisons of modeled complex fluid behavior near and on surfaces. The coupling between the two MOOSE codes, Navier-Stokes and Zapdos, would lead to simulating complex fluid species within dynamic water, such as solvated electrons. The modeling and understanding of solvated electrons are an area of interest to the DOE-NE, since it has been known that solvated electrons can be formed by radiation-induced detachment in LWR coolant channels. Most of the physics required are already within the respective codes. The main coupling effects that still need to be implemented are the heating effects unique to charged species between the two fluids. Simulations would consist of forming charged species above the water and tracking the deformation of the water surface, along with tracking the species within the water.

Key Publications

- DeChant, C. et al. 2021. "Verification and Validation of the Open-Source Plasma Fluid Code: Zapdos," submitted to *Advances in Engineering Software*, in progress.

Sponsor/Program

Nuclear Energy University Program (NEUP)

A.76. Physics-Informed Generative Adversarial Network

Report Participants

Tyrell Arment,[1] Michael Schneier,[1] John Buchanan,[1] Justin Rice[1]

1 Naval Nuclear Laboratory

Scientific Achievement

This project has achieved a novel application of physics-informed generative modeling for several use cases (i.e., heat diffusion, Taylor-Green Vortex, and Boussinesq [buoyancy driven] flow). Development is ongoing to extend the Boussinesq problem to other parametrizations (e.g., aspect ratio).

Significance

The results of this work demonstrate the capability of generative modeling to accelerate high-fidelity, parametric modeling by 3–5 orders of magnitude in terms of wall clock time. The work also forms the building blocks required for more complex model building for multiphase flows.

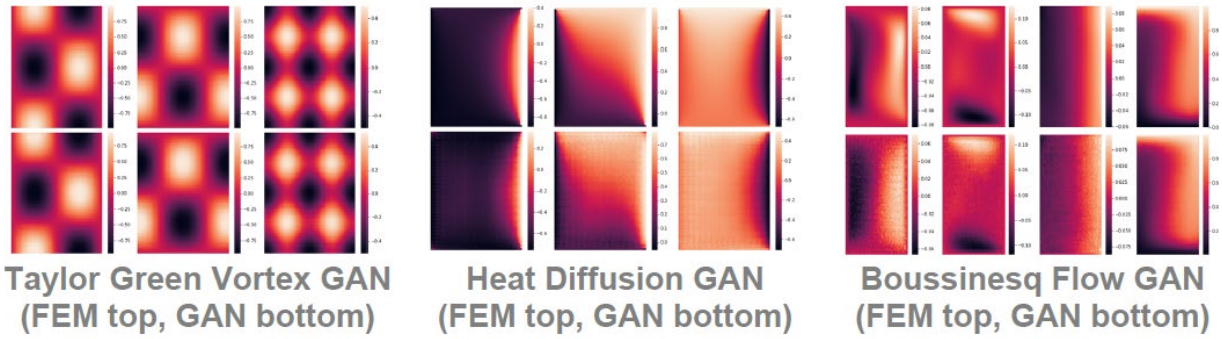


Figure 1. Several example results are shown below for the Taylor-Green Vortex, heat diffusion model, and Boussinesq flow generative models.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.77. RELAP5-3D Training: Power Plant Control

Report Participants

Mike Berkenpas,[1] Kevin Rahner,[1] Tyler Yurcisin,[1] Matt Lazor[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Training materials were developed from a RELAP5-3D model of a PWR power plant. This model simulates a four-loop nuclear power plant primary system, combining 3 of the 4 primary loops into one; it is the same model historically used for INL training classes for RELAP5-3D. NNL abruptly shifted its workforce offsite in 2020 due to the COVID-19 pandemic, limiting access to software and plant models available on NNL's classified network. INL HPC Center accounts were used to perform unclassified work, providing the means to continue training in power plant controls from a teleworking environment.

Significance

RELAP5-3D cannot be licensed to individuals, so access to the code was only available through other national laboratories. INL hosted individuals on their HPCs to provide access to the code. This provided the opportunity to do training during telework situations that would not typically be done working on the NNL site. This also provided an opportunity to maintain skills interpreting results from RELAP5-3D during the telework periods. The quick shift to performing unclassified tasks was challenging, and gaining access to RELAP5-3D was extremely helpful. Although we logged very few hours on the HPCs, the access was important.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology

A.78. Sensitivity and Uncertainty Analysis of VERA with BWR Progression Problems

Report Participants

Tomasz Kozlowski,[1] Travis Mui,[1] Katarzyna Borowiec[1]

1 University of Illinois Urbana-Champaign

Scientific Achievement

The main objective of the project is to assess the uncertainty of the VERA core simulator for boiling-water reactor (BWR) simulations. An initial analysis of the selected BWR VERA progression problems was performed to showcase the capabilities of the chosen methods and computational tools. This work is in progress.

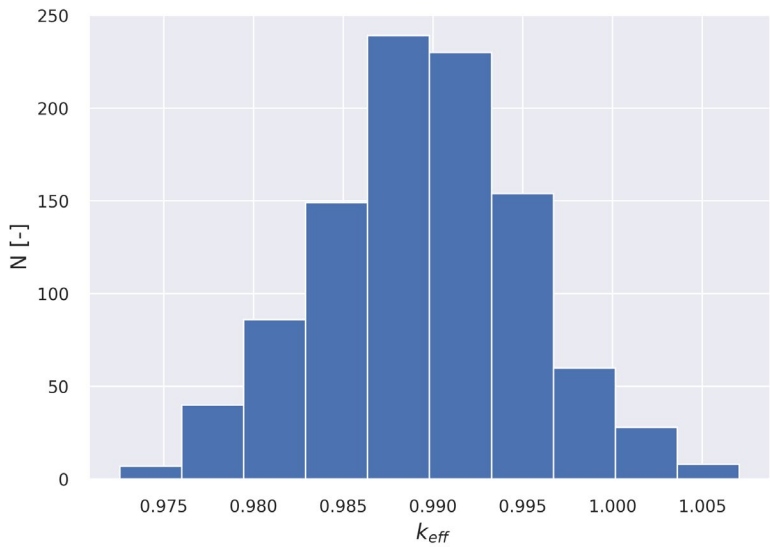


Figure 1. Histogram of keff distribution for BWR mini-core case.

Significance

A statistical uncertainty method was applied to selected BWR VERA progression problems with determined input parameters of interest and their uncertainty distributions. The results of the perturbation produced uncertainty distributions in the predicted keff and relative pin power FOMs for each progression problem. Statistical analysis of the results was presented to verify the performance including summary statistics and Pearson correlation coefficients. The predicted FOM distributions indicated a mean keff within 100 pcm of nominal with a standard deviation between 500–1000 pcm, as well as a mean relative pin power within 0.1% of nominal with a standard deviation below 1%. Additionally, the Pearson correlation coefficients indicate that generally the uncertainty in fuel enrichment has the largest impact on the predicted keff and relative pin power. These results show that TAPE can be used to propagate the uncertainties in boundary conditions and model parameters for the BWR VERA progression problems. The project is in progress.

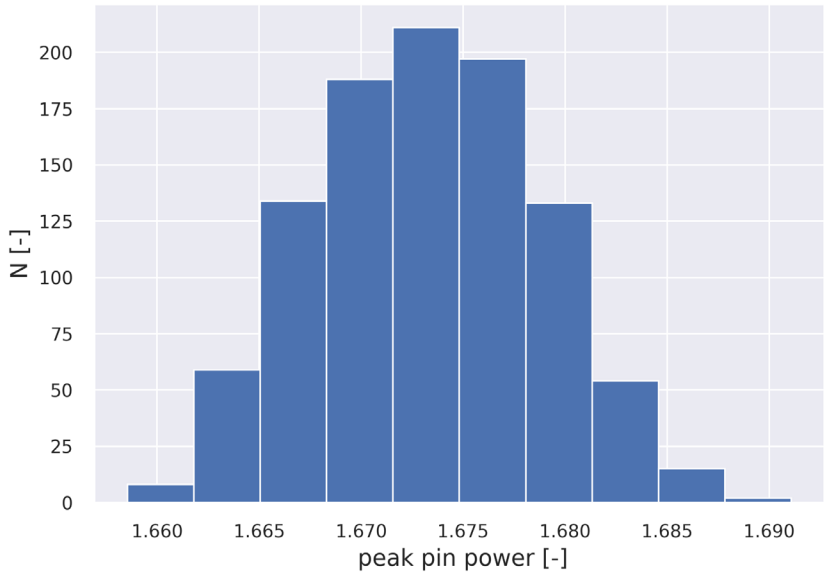


Figure 2. Histogram of relative peak pin power distribution for BWR mini-core case.

Key Publications

- Mui, T., K. Borowiec, and T. Kozlowski. 2021. "Sensitivity and Uncertainty Analysis of VERA with BWR Progression Problems," Technical report, to be submitted to ORNL, in progress.

Sponsor/Program

The project is funded by ORNL, previously part of the CASL program.

A.79. Sustaining Thermal Irradiation Capabilities Through 2085

Report Participants

Mark DeHart,[1] Joseph Nielsen,[1] Carlo Parisi,[1] Matthew Johnson,[1] Micah Gale,[1] Cole Mueller,[1] Michael Beran,[2] Michael Worrall[2]

1 Idaho National Laboratory

2 Naval Nuclear Laboratory

Scientific Achievement

The purpose of this project is to sustain the capability to irradiate materials using thermal neutrons through at least 2085. That capability is currently being filled by the Advanced Test Reactor (ATR). However, the ATR is aging and, in its current state, will not be able to operate until 2085. Studies are underway to determine the best course of action to maintain thermal irradiations capability. Major software uses on the INL HPCs include CMCDT (PUMA and MC21) and RELAP5.

Significance

The ATR is a national asset that is used by multiple organizations including the Department of Energy, naval reactors, and NASA. Studies to date have focused on pre-conceptual scoping work to support a potential replacement for ATR.

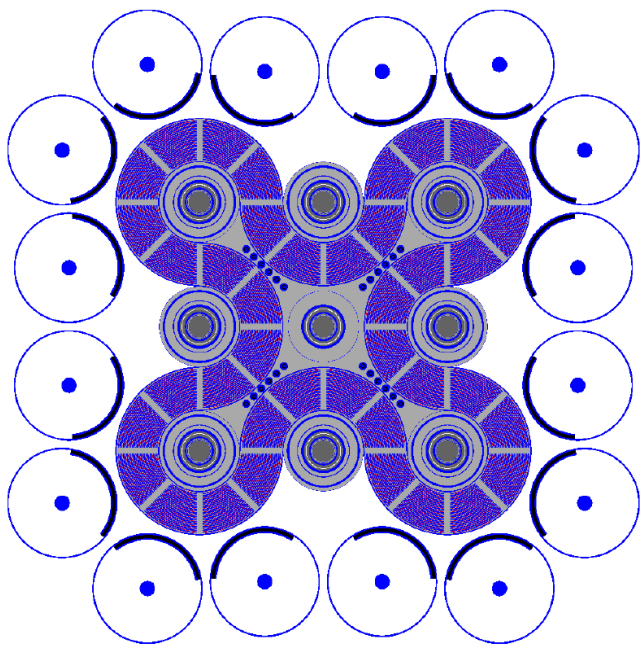


Figure 1. MC21 model of the ATR core.

Key Publications

- O'Kelly, S. and C. F. Dempsey. 2020. "Contract No. DE-AC07-05ID14517 – Recommendation for Sustaining Strategic Thermal Irradiation Capabilities," CCN 247363.

Sponsor/Program

Nuclear Science and Technology

A.80. Thermal Neutron Scattering Law Development

Report Participants

Jonathan L. Wormald,[1] Michael L. Zerkle,[1] Jesse C. Holmes[1]

1 Naval Nuclear Laboratory

Scientific Achievement

Thermal neutron scattering laws (TSLs) are nuclear data that capture the effects of chemical binding on neutron thermalization. This project includes the use of ab initio methods to calculate the vibrational spectra of materials using the MedeA simulation environment (TMMaterials Design Inc.) and subsequently use this data as input to the generation TSLs with the FLASSH code. Current projects include several materials, including metal hydrides using ab initio lattice dynamics and/or AIMD, as well as a MD study of vibrational anharmonicity in ZrHx using a MLP, which has been trained to a relevant set of ab initio calculations.

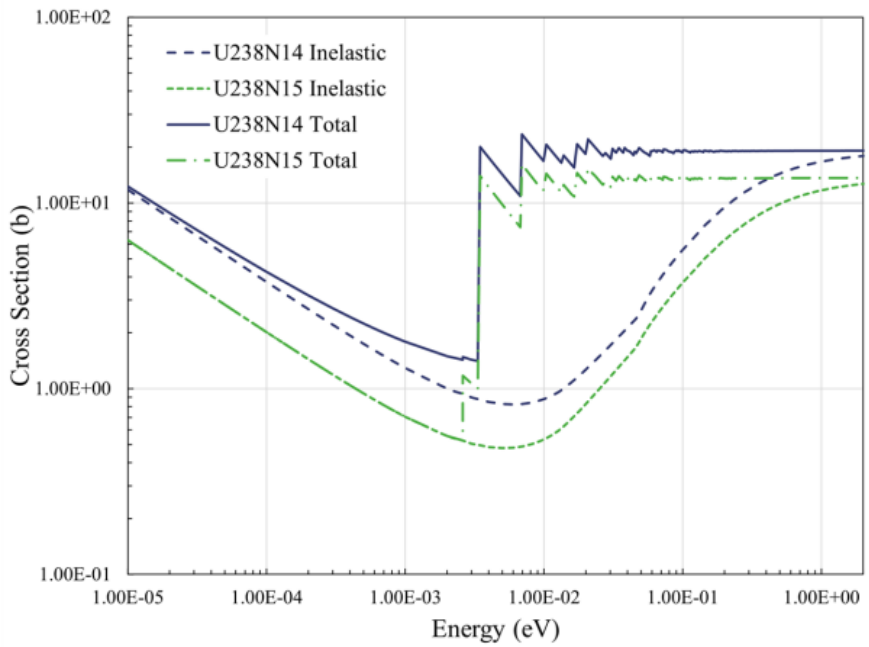


Figure 1. Thermal neutron scattering cross section for TSL evaluation of uranium mononitride at 293.6 K for ENDF/B-VIII.1. Evaluations for isotopic compositions of 238U-14N and 238U-15N were generated using ab initio lattice dynamics with the same forcefield as the ENDF/B-VIII.0 TSL evaluation (Wormald et al. 2020).

Significance

TSLs of moderator and reflector materials are essential nuclear data for predicting criticality and power distributions of fission systems operating with a thermal neutron spectra. In modern ENDF evaluations, high-fidelity TSLs are generated from ab initio methods. These evaluations are contributed to the ENDF/B database as part of the ongoing collaboration between naval reactors and the DOE Nuclear Criticality Safety Program. The use of ML potentials and AIMD techniques represents an effort to include the anharmonic effects of temperature on the TSL that are absent in ENDF/B-VIII.0 evaluations for crystalline materials generated with ab initio lattice dynamics in the harmonic approximation. The MLP approach for ZrHx builds upon AIMD based evaluations contributed to the ENDF/B-VIII.1 pre-release. This approach also has potential for use in other advanced moderators such as YHx.

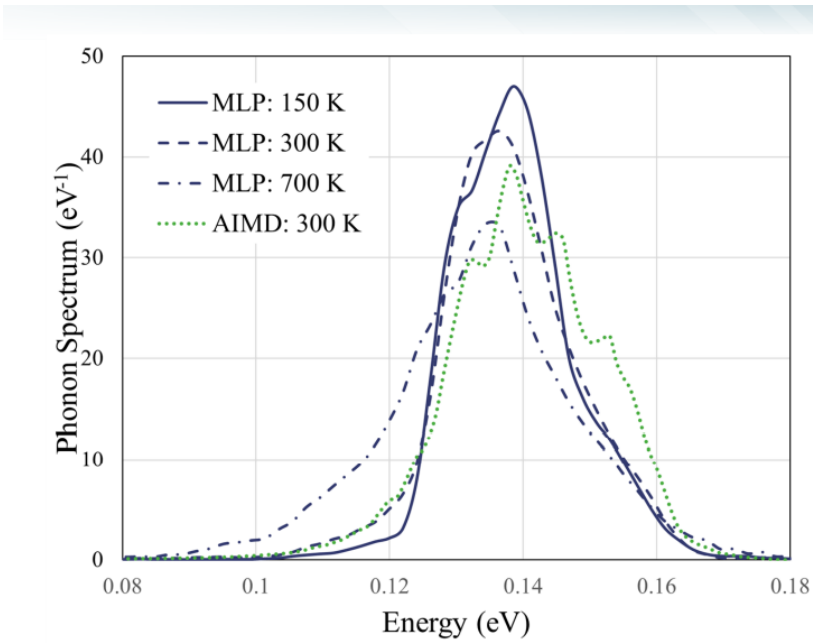


Figure 2. Hydrogen phonon spectra of ZrH2 predicted with a MLP as function of temperature. The MLP phonon spectra is compared to the AIMD spectra used to generate the ENDF/B-VIII.1 TSL. The MLP calculations demonstrate softening and broadening of the phonon spectrum due to hydrogen anharmonicity at elevated temperatures.

Key Publications

- Brown, D. A., et al. 2018. "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," *Nuclear Data Sheets*, 148:1–142. https://doi.org/10.1016/j.nds.2018.02.001.
- Wormald, J. L., A. A. Hawari, and M. L. Zerkle. 2020. "Impact of Magnetic Structure and Thermal Effects on Vibrational Excitations and Neutron Scattering in Uranium Mononitride," *Annals of Nuclear Energy*, 143:107447. https://doi.org/10.1016/j.anucene.2020.107447.
- Wormald, J. L., M. L. Zerkle, and J. C. Holmes. 2021. "Generation of the TSL for Zirconium Hydrides from Ab Initio Methods," *Journal of Nuclear Engineering*, 2(2):105–113. https://doi.org/10.3390/jne2020011.
- Zerkle, M. L., J. C. Holmes, and J. L. Wormald. 2021. "RE-EVALUATION OF THE TSL FOR YTTRIUM HYDRIDE," *EPJ Web of Conferences*, 247:09015. https://doi.org/10.1051/epjconf/202124709015.

Sponsor/Program

Nuclear Science and Technology

A.81. Thermochemically Informed Mass Transport Modeling in BISON

Report Participants

Max Poschmann,[1] Markus H.A. Piro,[1] Srdjan Simunovic[2]

1 Ontario Tech University

2 Oak Ridge National Laboratory

Scientific Achievement

A new formulation for redistribution of constituents in nuclear fuel has been developed that can incorporate the contributions from fission products. The formulation is based on the thermodynamic driving forces derived from the generalized chemical potential that includes effects of composition and temperature.

Significance

The redistribution model can readily account for the composition changes due to the generation of fission products while using only a limited set of transport coefficients. The model has been applied to UO2 and U-Pu-Zr fuels. The formulation has been employed to elucidate the effects of burnup on the oxidation of UO2 fuel in operation. In U-Pu-Zr fuel, it has been used to study the role of fission products in forming a region of decreased Zr concentration.

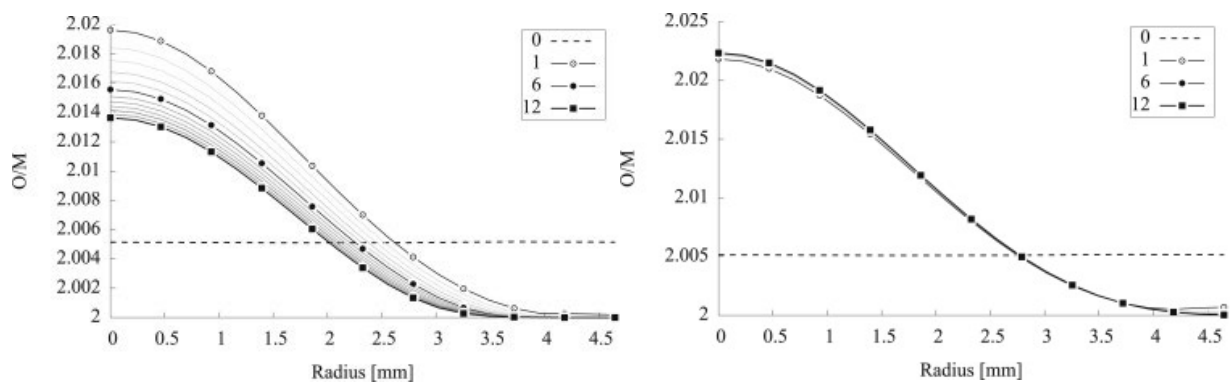


Figure 1. Simulated oxygen-to-metal ratio in UO2 fuel during operation without considering the chemical effects of fission products (top) and with fission products included (bottom). The numbers in the legend refer to months in-reactor.

Key Publications

- Simunovic, S., T. M. Besmann, E. Moore, M. Poschmann, M. H. Piro, K. T. Clarno, J. W. McMurray, and W. A. Wieselquist. 2020. "Modeling and simulation of oxygen transport in high burnup LWR fuel," *Journal of Nuclear Materials*, 538:152194. https://doi.org/10.1016/j.jnucmat.2020.152194.
- Poschmann, M., M. H. A Piro, T. M. Besmann, K. T. Clarno, and S. Simunovic. 2021. "Thermochemically-Informed Mass Transport Model for Interdiffusion of Uand Zr in Irradiated U-Pu-Zr Fuel with Fission Products," *Journal of Nuclear Materials*, 554:153089. https://doi.org/10.1016/j.jnucmat.2021.153089.

Sponsor/Program

NEAMS

A.82. Thermochemically Informed Transport of Palladium Through TRISO Fuel Particles

Report Participants

Bernard. W.N. Fitzpatrick,[1] Max Poschmann,[1] Theodore M. Besmann,[2] Srdjan Simunovic,[3] Markus H.A. Piro[1]

1 Ontario Tech University

2 University of South Carolina

3 Oak Ridge National Laboratory

Scientific Achievement

This work is a framework for modeling transport of Pd through TRISO particle kernels and outer layers. The framework is implemented in MOOSE-BISON coupled with the thermodynamics code Thermochimica. The models used to simulate UCO fuel and fission products in the TRISO particle can solve for systems containing the chemical elements U, O, C, Pu, Nd, Pr, Ce, La, Ba, Cs, Xe, I, Te, Ag, Pd, Rh, Ru, Tc, Mo, Zr, Y, Rb, and Ar. For the purposes of this demonstration, U, O, C, Pd, and the noble metal system Rh, Ru, Mo, Ag are examined here.

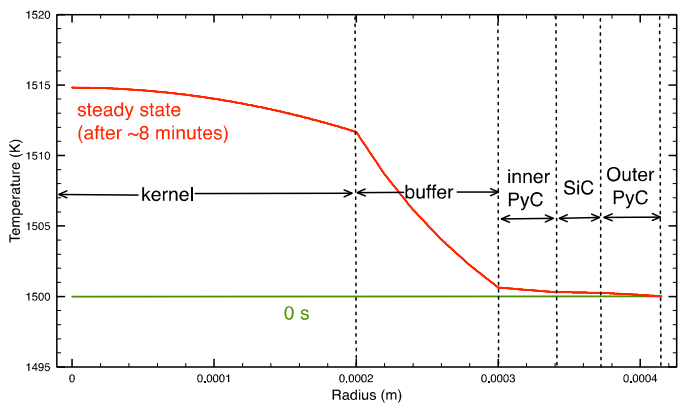


Figure 1. The particle quickly develops a steady-state temperature profile ranging from 1500 K on the periphery to 1515 K in the center of the kernel.

Significance

This is the first time thermochemistry in TRISO fuel has been coupled with fuel performance, and the first time thermochemical models have been used to predict fission product transport. In the current implementation, due to a lack of diffusivity data for Pd, fictive diffusion coefficients are used. Pd follows the chemical potential gradient, moving both into the center of the kernel and through the outer layers.

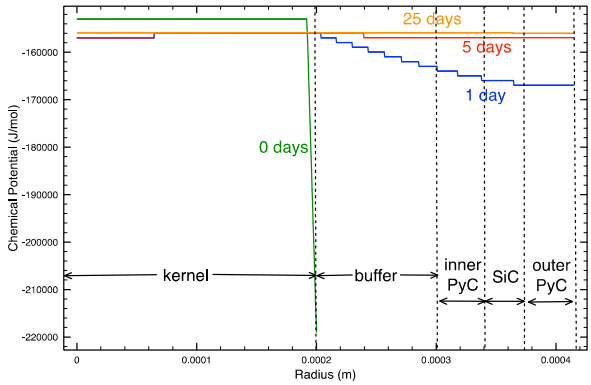


Figure 2. Chemical potential, driven by the composition and the temperature profile becomes more horizontal as Pd transports along the chemical potential gradient.

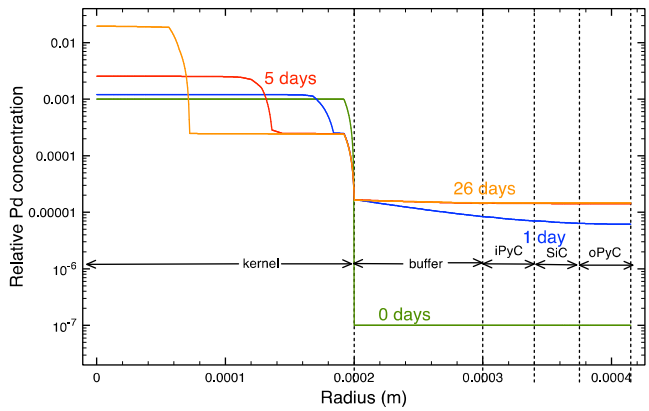


Figure 3. Pd is transported by the temperature gradient into the kernel, but also out into the outer layers of the particle.

Key Publications

- Fitzpatrick, B. W. N., M. Poschmann, T. M. Besmann, S. Simunovic, and M. H. A. Piro. ND. "Thermochemically-Informed Transport of Fission Products Through TRISO Fuel Particles," in progress.
- Fitzpatrick, B. W. N., M. Poschmann, T. M. Besmann, S. Simunovic, and M. H. A. Piro. 2020. "Thermochemically-Informed Transport of Palladium Through TRISO Fuel Particles," The Nuclear Materials Conference, Ghent, Belgium, October 26–29, 2020. https://www.elsevier.com/events/conferences/the-nuclear-materials-conference.

Sponsor/Program

NEAMS

A.83. Transient VERA/Shift Simulation of Rod Worth Measurement

Report Participants

Mark Roberts,[1] Andrew Godfrey,[2] Gary Wolfram[3]

1 Naval Nuclear Laboratory

2 Oak Ridge National Laboratory

3 Pacific Northwest National Laboratory / TVA

Scientific Achievement

The goal of the project is to explicitly model the Dynamic Reactivity Rod Worth Measurement (DRRWM) process using VERA. Simulating the DRRWM process involves moving a control rod bank and calculating detector response based on that change. This will be accomplished by simulating the transient using transient MPACT (the transport solver included in VERA) and calculating detector response with Shift (the Monte Carlo solver included in VERA, which can be used for detector response calculations). The simulated results would then be compared to measured data for the same procedure.

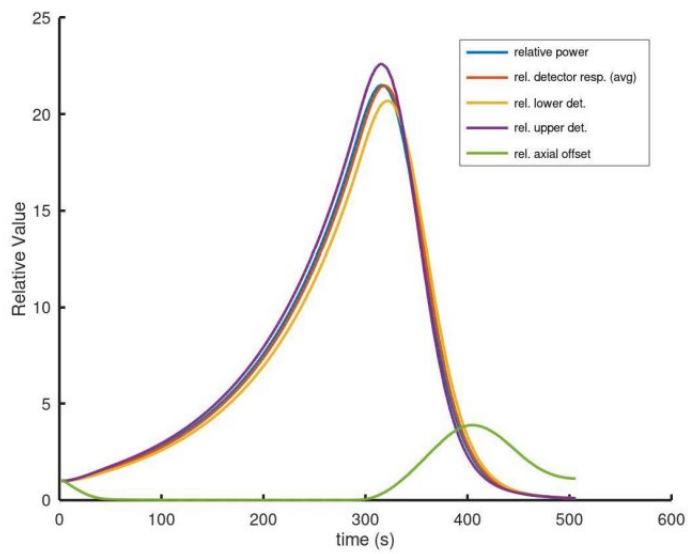


Figure 1. Processed transient data showing estimated detector response (relative). Purple shows the upper detector, yellow shows the lower detector, and orange is the combined signal. Blue shows relative change in power, and green shows the axial offset for reference.

Significance

Work is still in progress. To date, work has shown the DRWM transient can be simulated in VERA, and seperately, a steady-state Shift calculation can calculate detector response. A pin-level adjoint calculation is also performed when Shift is run, and results have shown this can be combined with the transient VERA calculation to approximate detector response. Comparison to measured data is still in progress.

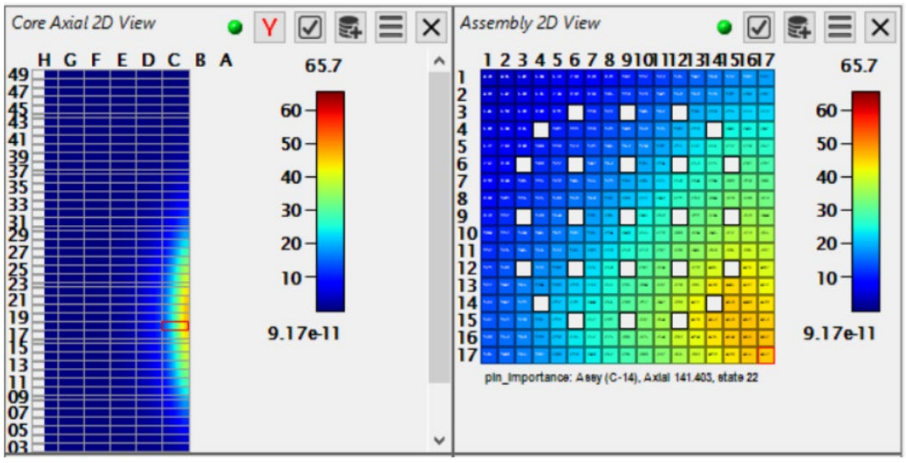


Figure 2. Per-pin relative contribution to lower detector signal for assembly C-14. Axial plot (left) shows the outer row of pins, and radial Figure (right) shows assembly at 19th plane.

Key Publications

None.

Sponsor/Program

Nuclear Science and Technology and the Consortium for Advanced Simulation of Light Water Reactors (CASL) collaboration

A.84. Uncertainty Quantification of BWR Progression Problems for the VERA Core Simulator

Report Participants

Travis Mui,[1] Connor Pigg,[1] Tomasz Kozlowski[1]

1 University of Illinois at Urbana-Champaign

Scientific Achievement

The objective of this project is to enhance the capabilities of the state-of-the-art advanced modeling and simulation code package VERA, developed under the Consortium for Advanced Simulation of Light Water Reactors (CASL), a Department of Energy innovation hub, to support the detailed modeling and simulation of BWRs. Such capabilities will play a vital role not only for improved reactivity and thermal margin predictions but also for continued advancement of new fuel products and designs, such as accident tolerant fuel (ATF) and their deployment to current operating BWRs. A set of progression problems will be developed to define a set of technical achievements in which code capability will be demonstrated and validated. Our work will supplement verification and validation activities with additional UQ and sensitivity analysis to assess the need for further model development.

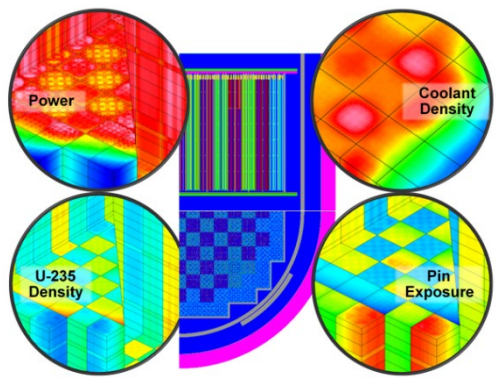


Figure 1. Graphical representation of high-fidelity simulation capability of VERA-CS.

Significance

This project will provide a key assessment of the baseline simulation capability to perform high-fidelity modeling of BWR core designs. It is expected that there will be a significant additional contribution of uncertainty attributed to two-phase flow modeling and its converse effects on simulating the neutronics and fuel performance physics. This work will also identify possible deficiencies in the physics models. This work in progress began in FY-21 with the analysis of the 2D progression problems and will continue through FY-22 to assess the 3D progression problems. Work is underway to adapt and deploy the Transient Analysis PackagE (TAPE) for the INL's HPC Center environment to work with sampling of the larger 3D models. TAPE was developed at University of Illinois at Urbana-Champaign for use with VERA-CS to allow for UQ and sensitivity analysis study.

Key Publications

- Mui, T., K. Borowiec, and T. Kozlowski. 2021. "Sensitivity and Uncertainty Analysis of VERA with BWR Progression Problems, Task 1: Sensitivity and Uncertainty Analysis of BWR 2D Progression Problems," CASL Technical Report.

Sponsor/Program

CASL, supported on DE-FOA-0001817

A.85. Unstructured Neutron Transport on HPC Architectures

Report Participants

William C. Dawn[1]

[1]North Carolina State University

Scientific Achievement

Many multiphysics simulation methods such as those in MOOSE require solutions on an unstructured mesh. Solving the neutron transport equation on an unstructured mesh is a notoriously challenging problem but has been successfully demonstrated in the Rattlesnake computer program developed by INL. By investigating the properties and performance of the equations solved in Rattlesnake, we can improve computational performance on HPC architectures. The computers available at INL are important for this work because they prioritize CPU computing with many cores compared to HPC environments available at other institutions. The computing architectures available at INL closely resemble the computing clusters used in the commercial nuclear industry.

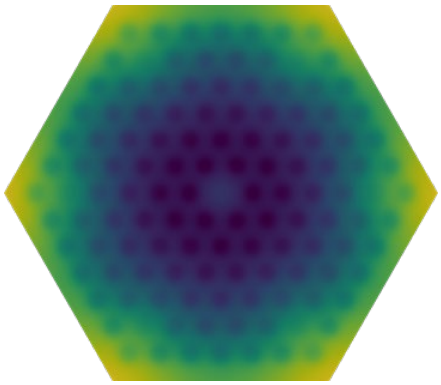


Figure 1. Fast flux in sample assembly calculated with low-order method.

Significance

This work is ongoing. To date, we have investigated the performance of Rattlesnake for certain fast-reactor systems, but more general research considering other reactors and more general transport problems would lead to a broader applicability of the findings. By investigating the algorithms in Rattlesnake and comparing alternatives, we can determine how to achieve optimal performance on a variety of architectures including other HPC environments and smaller commercial computing clusters.

Key Publications

- Dawn, W. C., J. Ortensi, M. D., DeHart, and S. P. Palmtag. 2020. "Comparison of Generation of Higher-Order Neutron Scattering Cross Sections," INL/EXT-19-54899, Idaho National Laboratory. https://doi.org/10.2172/1593864.
- Dawn, W. C. 2020. "An Analytic Benchmark for the Solution to the Isotopic Fission Spectrum Mixture Problem," INL/EXT-19-54998, Idaho National Laboratory. https://doi.org/10.2172/1593873.
- Dawn, W. C. and S. Palmtag. "Efficient Solution of the Neutron Transport Equation on Unstructured Meshes using Modern Supercomputing Architectures," in progress.

Sponsor/Program

NEAMS

A.86. Updated As-Run Analysis Approach for Shipping Calculations to HFEH

Report Participants

Emory Colvin,[1] Todd S. Palmer,[1] Joshua Peterson-Droogh,[2] Jason Brookman,[2] Austin Carter,[2] Angelica Mata Cruz,[2] Bryon Curnutt,[2] Connie Hill,[2] Chris Murdock[2]

1 Oregon State University

2 Idaho National Laboratory

Scientific Achievement

This project seeks to speed up the as-run analysis of experiment source term calculations that must be performed post-irradiation to account for effects of actual operation (exact timing of shutdowns, power changes mid-cycle, etc.) that were not included in the pre-irradiation projection calculations. Current analyses use MCNP and SCALE (specifically, ORIGEN uses COUPLE to incorporate neutron flux spectra) for both sets of calculation, which have significant computing requirements. This work seeks to save the libraries generated by COUPLE in the projections with a hidden SCALE code called OBIWAN to interpolate between existing libraries as needed for the as-run. Using this approach, we can eliminate MCNP from the as-run, significantly speeding the calculations. This will be incorporated into the MOAA code used to pass information between MCNP and SCALE.

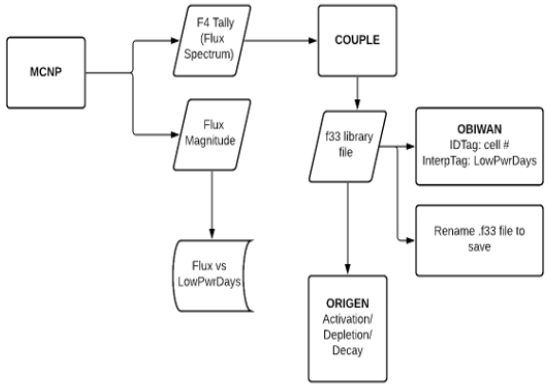


Figure 1. Work flow to save libraries during projection analyses.

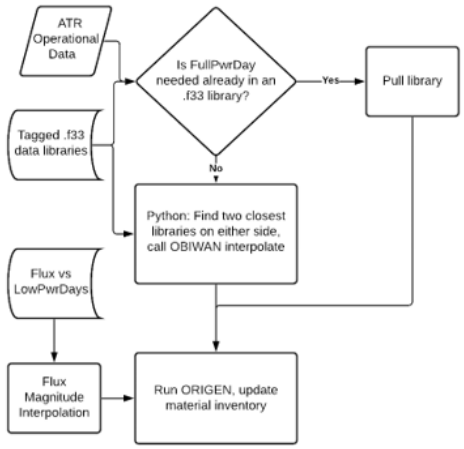


Figure 2. Work flow to use saved libraries in as-run analyses.

Significance

This is still very early in the process, but preliminary OBIWAN use on local machines is promising for its usefulness.

Key Publications

It is still too early for any specific publications/presentations to be planned.

Sponsor/Program

ATR Nuclear Irradiation Experiment Neutronic Analysis Group

A.87. Validation of the VERA for the NPP Krško Calculations

Report Participants

Marjan Kromar[1]

1 Jožef Stefan Institute

Scientific Achievement

The VERA code will be used for the scientific studies of the neutron transport inside PWR cores and ex-core regions. VERA will be validated by performing detailed pin-by-pin depletion of all completed 30 Nuclear power plant (NPP) Krško fuel cycles. NPP Krško is a two-loop Westinghouse PWR plant located in Slovenia. Results will be compared to the in-house CORD-2 system and in-core measurements performed periodically on the plant. VERA will be used to study sensitivity of calculation models applied to the typical PWR core calculation. More sophisticated models may be needed in some particular cases, or possible simplified models could be applied to yield better or similar accuracy with lower computer resources demand. I will perform some sensitivity analysis of the grid and energy mesh in order to speed up the calculations. With validated core models ex-core calculations will be performed. Results will be compared to the ADVANTG/MCNP calculations with sources determined from the CORD-2 calculations. For validation purposes a comparison to the dosimetry data from the NPP Krško ex-vessel neutron dosimetry system will be performed. A sensitivity analysis will provide information about the necessary level of model details. With validated model response functions of the ex-core neutron detectors will be studied as a function of inserted control rods. Impact of the core weighting factors will be examined within the process of control rod worth determination by the "rod insertion method," which is regularly applied in the NPP Krško post-refueling tests.

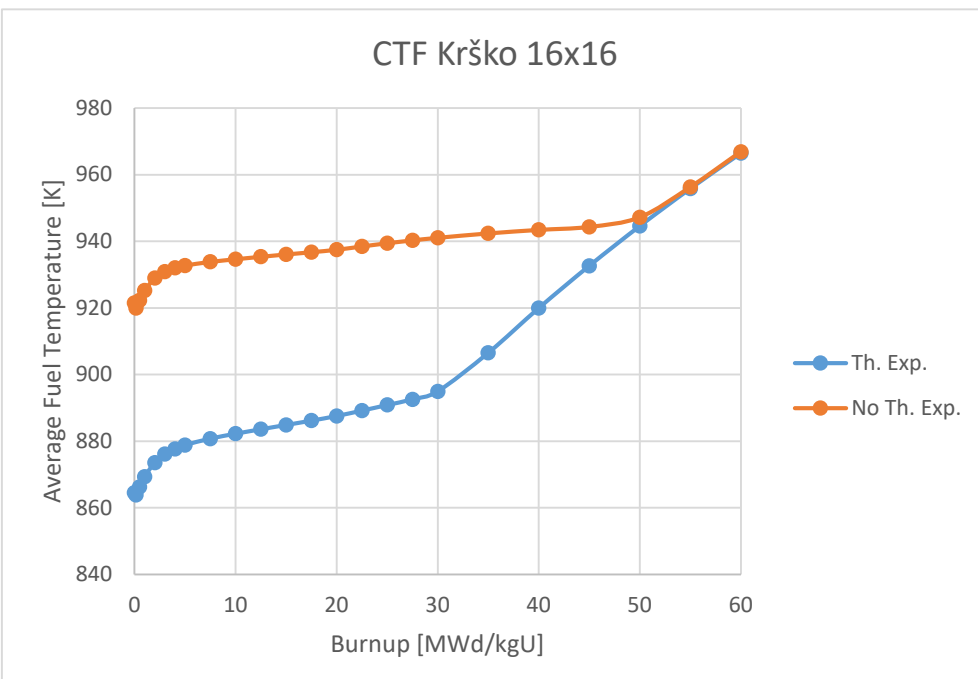


Figure 1. NPP Krško 16x16 fuel average temperature vs. burnup generated by the CTF.

Significance

Initial calculations performed on the fuel assembly level has been completed. Comparison with the Serpent-Finix calculations has indicated some deficiencies of the CTF code application. It is intended to replace CTF fuel temperatures with temperature tables generated by BISON. Comparing the application of both approaches to the neutron transport and burnup calculations on the reactor core level will provide valuable information on the way the VERA simulator should be assembled for the complete VERA validation on all 30 NPP Krško fuel cycles.

Key Publications

Only the initial work has been performed so far. It is expected to publish the results when the work progresses further.

Sponsor/Program

CASL (VERA)

A.88. VERA BWR Project

Report Participants

Scott Palmtag,[1] Chase Lawing,[1] Khaldoon Al-Dawood,[1] Mehdi Asgari[2]

1 North Carolina State University

2 Oak Ridge National Laboratory

Scientific Achievement

The VERA computing suite was developed under the CASL program to advance the state-of-the-art in the modeling and simulating LWRs. The ability to model PWRs using advanced coupled multiphysics computational tools was developed, and results were validated for over 100 cycles of PWRs. This current project is to develop and extend the VERA tools to BWRs and apply the tools to analyze the BWR fleet of reactors operated by Exelon Nuclear Generation. The results will be used to improve the eigenvalue and thermal limit predictability in BWR reactors to improve cycle length and economic output of BWRs.

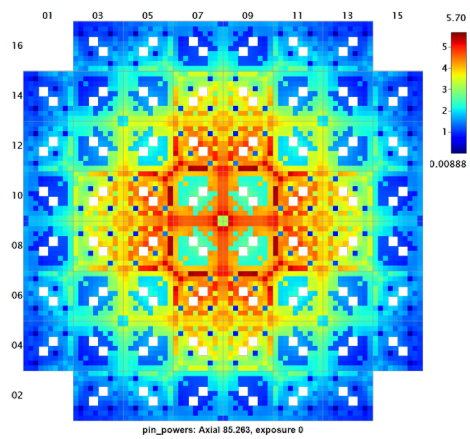


Figure 1. Radial 2D pin powers BWR mini-core.

Significance

The VERA suite offers significantly advanced modeling and simulation capability over existing industry simulation tools. The advanced capability includes detailed multigroup neutron transport for the entire core, detailed subchannel TH solution over every fuel rod, and detailed pin-by-pin fuel temperature and depletion solutions.

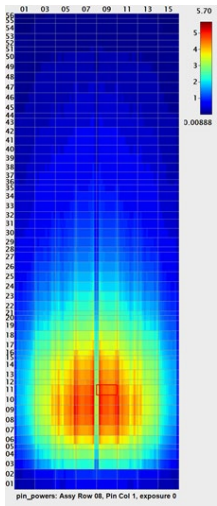


Figure 2. Axial pin powers BWR mini-core.

These features of VERA should yield substantial improvement over existing industry predictions of modeling void and depletion parameters on a rod-by-rod basis instead of a bundle-average basis and detailed modeling of different bypass flow regions. This enables a more rigorous calculation within the bundle power distribution. This is especially important in the presence of large power gradients such as occurs with the insertion of control blades. The feedback of the radial void distribution, particularly at high void, is expected to have a significant impact on calculated results. In addition, it is expected that the elimination of history models in the cross-section generation, and the inclusion of radial void distribution within bundles will improve eigenvalue and detector predictions.

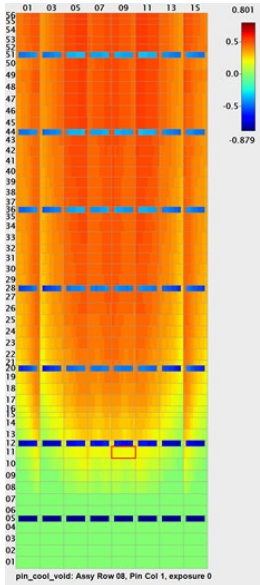


Figure 3. Axial void distribution BWR mini-core.

Key Publications

- Lawing, C., S. Palmtag, and M. Asgari. 2020. "BWR Progression Problems," ORNL/TM-2020/1792, Oak Ridge National Laboratory.
- Additional publications (including journal papers) are in progress.

Sponsor/Program

DOE FOA "Modeling and Analysis of Exelon BWRs for Eigenvalue & Thermal Limits Predictability"

A.89. VERA Support

Report Participants

Erik Walker[1]

1 Oak Ridge National Laboratory

Scientific Achievement

Supporting VERA and the VERA Users Group will occasionally require running full-core multi-cycle depletion cases that require large HPC capabilities.

Significance

The cases that are run can be used for either benchmarking or code verification and validation as well as testing new features and bug fixes on large, full-core problems. These resources were used last year to demonstrate a new generalized detector edits capability that was added to VERA.

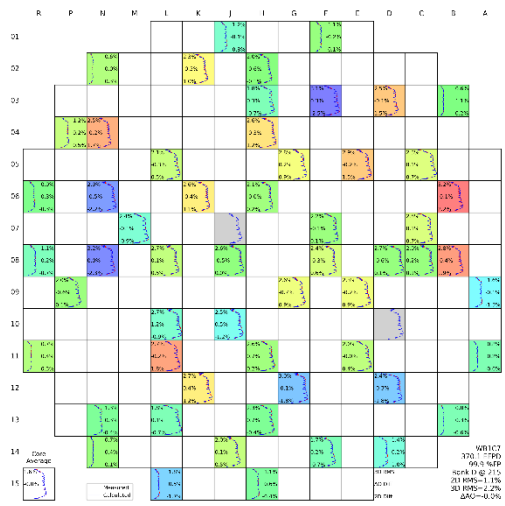


Figure 1. EOC detector map comparison.

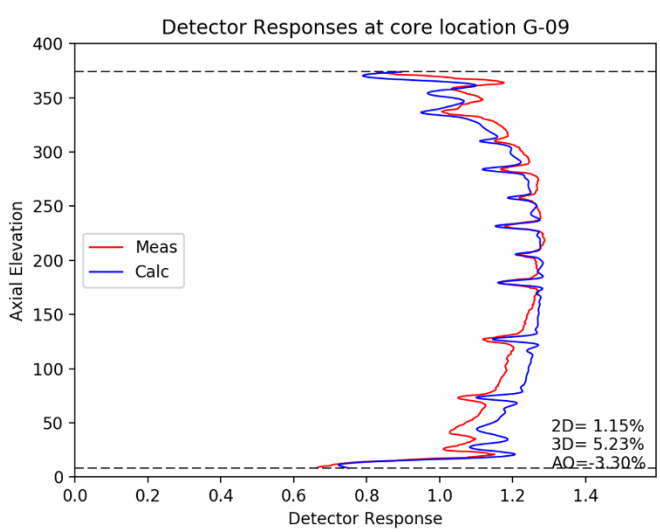


Figure 2. Single assembly comparison between MPACT and measurement.

Key Publications

- Walker, E., S. Stimpson, B. Collins, A. Godfrey, and J. Eller. 2021. "Implementation of Generalized Incore Detector Responses in MPACT," M&C 2021, Raleigh, North Carolina.

Sponsor/Program

NEAMS, SCALE

A.90. VERA Users Group

Report Participants

Brendan Kochunas,[1] Sooyoung Choi[1]
1 University of Michigan

Scientific Achievement

The VERA user's group (VUG) project involves several members from several institutions. This short report only covers those aspects of the work performed by people at University of Michigan. Under the VUG, we performed additional benchmark calculations for the APR-1400 reactor design as part of an international collaboration performed under the I-NERI program in collaboration with ORNL's, Argonne National Laboratory, North Carolina State University, KAERI, Seoul National University ,and Ulsan National Institute of Science and Technology. The scientific achievement is the verification of several high-fidelity whole-core simulation codes for an advanced LWR design that is being built with new plants coming online around the world.

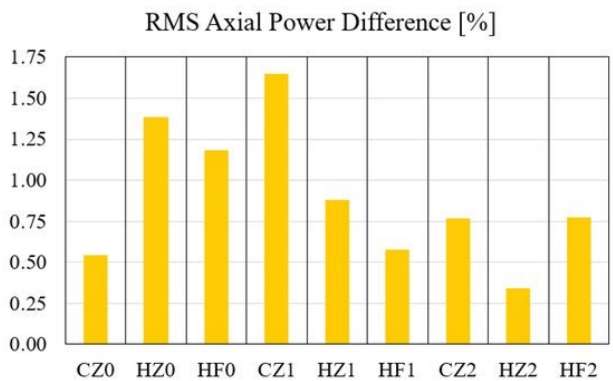


Figure 1. RMS of axial power differences for 3D APR1400 at beginning of life.

Significance

The significance of this work is that we have extended the application base of the VERA tools to include another advanced reactor design, the APR-1400 that was designed in South Korea. This is significant because there a few plants already built and operating in South Korea and the United Arab Emirates, and more under construction in these countries, as well as units planned for deployment in the United Kingdom.

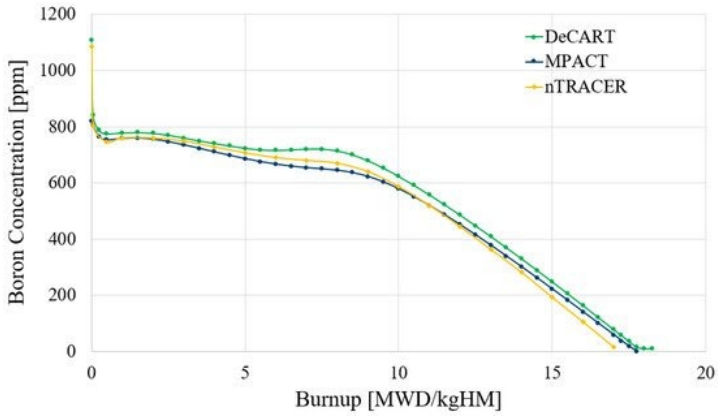


Figure 2. 3-D core depletion results in comparison to solutions generated by other benchmark participants.

Key Publications

- Barr, K., S. Choi, J. Kang, and B. Kochunas. 2021. "Verification of MPACT for the APR1400 Benchmark," *Energies*, 14(13):3831. https://doi.org/10.3390/en14133831/
- Barr, K., S. Choi, and B. Kochunas. 2021. "Verification of MPACT and VERA-CS for the APR1400 Benchmark," Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021). American Nuclear Society. https://dx.doi.org/10.13182/M&C21-33686.

Sponsor/Program

Department of Energy, CASL, NEAMS

A.91. VERA Users Group

Report Participants

Andrew Godfrey,[1] Mark Baird,[1] Tara Pandya[1]

1 Oak Ridge National Laboratory

Scientific Achievement

The VERA Users Group (VUG) provides access and support for VERA (developed by the Consortium for Advanced Simulation of Light Water Reactors [CASL]) to organizations in the U.S. commercial nuclear power industry. The VUG is responsible for sustaining the use of VERA through industry engagement for the post-CASL period by: (1) successful deployment and implementation of VERA by the nuclear industry, including facilitating software licenses, (2) sustainability of VERA by providing software maintenance, SQA, training, code support, and HPC access for users of LWR applications, (3) building on current CASL accomplishments and drive new innovations for the LWR fleet through sharing of user application experiences and feedback, (4) promoting industry participation in the DOE GAIN and FOA funding opportunities, and (5) representing LWR stakeholders in NEAMS (needs and requirements).

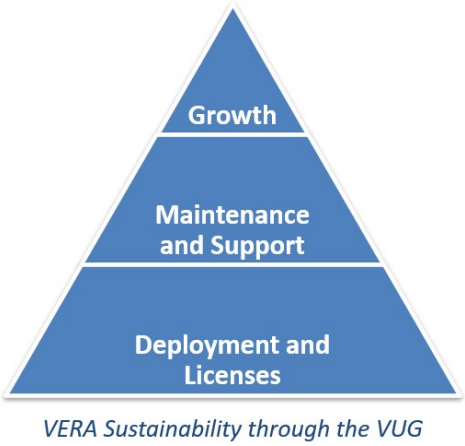


Figure 1. VUG sustains VERA for U.S. commercial power industry.

Significance

INL provided access to VUG members on both Lemhi and Sawtooth. The VUG staff have been providing VERA builds on those machines, as well as maintaining and developing new software, fixing bugs, supporting users, and testing new release candidates on those machines. This activity has allowed easy, direct access of the CASL-developed tools for the commericial power industry.

Figure 2. Sawtooth provides VUG members with easy, direct access to VERA.

Key Publications

While some publications have been produced tangentially by users, there are no direct publication from the VUG as it is mainly a support and maintenance activity.

Sponsor/Program

VERA Users Group

A.92. Westinghouse Advanced Microreactor Simulation

Report Participants

Cao Liping[1]

1 Westinghouse Electric Company, LLC

Scientific Achievement

The MOOSE-based code suites will be used for the coupled multiphysics modeling and analysis of the Westinghouse eVinci heat-pipe reactor, in particular, the coupled simulation of the reactor core. This work will be performed under the DOE-funded Advanced Nuclear Technology Development (DE-FOA-0001817 and DE_FOA_0002271) and the Advanced Research Projects Agency-Energy (ARPA-E) (DE-AR-0001026) programs. The code performance will be assessed and validated in simulating the eVinci system. Based on the assessment results, this code may potentially be applied to the modeling and simulation activities supporting the licensing application and process for the eVinci microreactor.

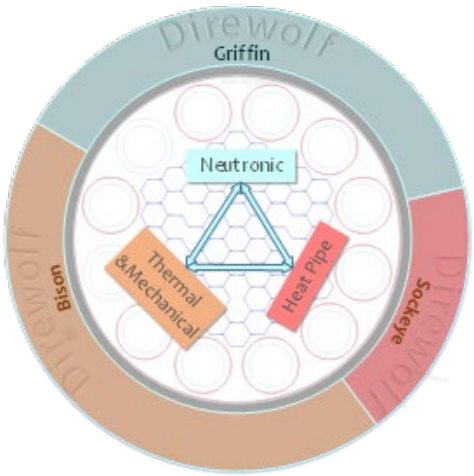


Figure 1. Coupled multiphysics simulation of microreactor.

Significance

The coupling of analysis codes for simulating the highly integrated advanced reactor systems, for example the eVinci microreactor design, is necessary to capture the feedback among the complicated physical phenomena. In particular, it plays a critical role in performing the safety studies with significantly enhanced accuracy and robustness, thus enabling a reliable and viable design to be licensed for commercial deployment. The commercialization of the advanced microreactor will provide safe, clean, and affordable nuclear energy to compete with alternative sources of energy sources on the market.

Key Publications

It is still too early for any specific publications/presentations to be planned. There are no publications yet, but ultimately multiple submittal reports to the regulators are expected to support the licensing approval of the eVinci heat-pipe reactor.

Sponsor/Program

Industry (Westinghouse), NEAMS, CASL, and Department of Energy Advanced Nuclear Technology Development program.

A.93. Auto-Machine-Learning Applications for Nuclear Reactors: Transient Identification, Model Redundancy, and Security

Report Participants

Pedro Mena,[1] Leslie Kerby,[1] R.A. Borrelli[2]

1 Idaho State University

2 University of Idaho

Scientific Achievement

The purpose of this project is to develop a ML model that can correctly identify a transient event occurring with a nuclear reactor using an AutoML package called TPOT.

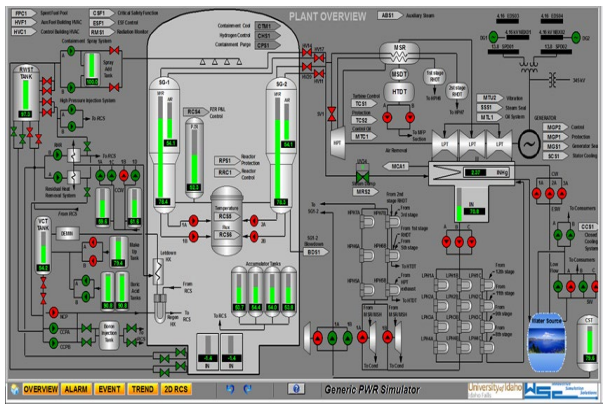


Figure 1. GPWR simulator interface from Center for Advanced Energy Studies (CAES).

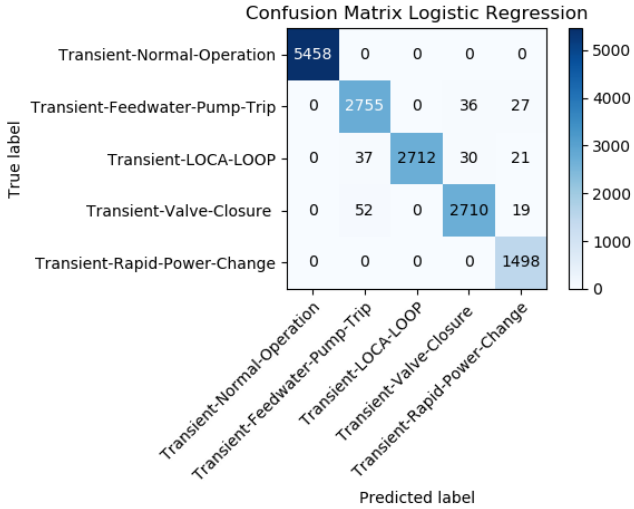


Figure 2. Confusion matrix from linear regression model produced from first publication.

Significance

The hope for this project is that it contributes to the effort to incorporate artifical intelligence in nuclear safety. This would improve safety at plants, by allowing for quicker diagnosis of issues with a reactor, quicker information avalaibility, and potenially help with the public perception of nuclear power.

Key Publications

We have yet to publish any journal articles with worked that made use of HPC. We do however plan to publish at least one article in the coming year.

Sponsor/Program

John A. Koudelka, INL Applied Visualization Laboratory

A.94. Computational Analysis and Experimental Validation of Advanced Heat Exchanger Configuration for Nuclear Application

Report Participants

SuJong Yoon,[1] Piyush Sabharwall,[1] Scott Wahlquist,[2,3] Kyle Schroeder,[2,3] Amir Ali[2,3]

1 Idaho National Laboratory

2 Idaho State University

3 Center for Advanced Energy Studies

Scientific Achievement

The project objective is to investigate a novel heat exchanger technology's TH performance numerically and experimentally for diverse applications, including nuclear. The project's phase one was completed by conducting design optimization, numerically under laminar flow conditions, and the results were very promising [1,2]. The thermal efficiency $(h = \frac{\frac{Nu}{Nu_o}}{\frac{f}{f_o}})$ was investigated over wide range of geometrical and flow parameters. Multiple models for the heat transfer and pressure drop were developed. These models are essential for further modeling activities investigating transient analysis using RELAP5-3d.

An experimental facility is currently under construction at Center for Advanced Energy Studies (CAES) to conduct validation experiments. A new graduate student pursuing his master's degree has been hired to conduct the experiments and numerical analysis under turbulent flow conditions.

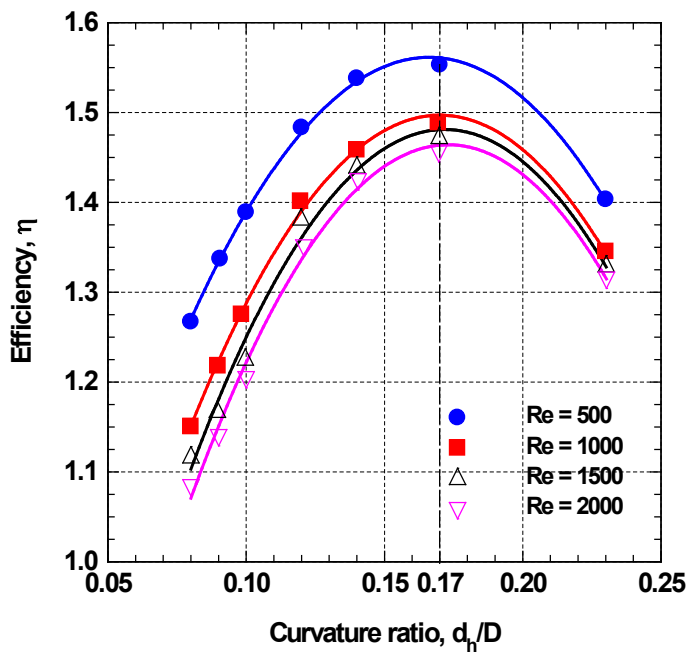


Figure 1. The thermal performance efficiency of the oval-twisted helical tube as a function of curvature ratio for various Reynolds numbers.

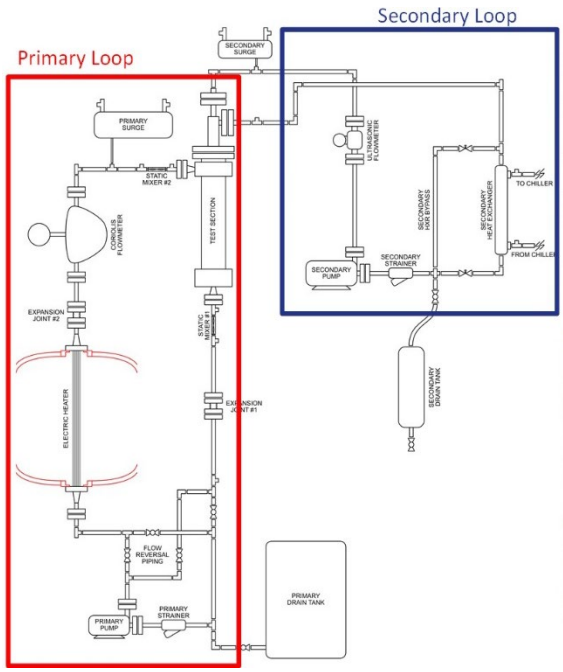


Figure 2. The heat transfer performance facility under construction in CAES.

Significance

This project aims to develop an innovative heat exchanger (HX) technology to improve the performance and increase the compactness over the existing helical tube HX technology for in-vessel intermediate heat exchanger (IHX) and once-through steam generator (SG) for molten-salt-cooled and light-water SMRs, respectively. The new HX enables to self-reduce or eliminate the concerns of flow-induced vibration and induced thermal stresses. The proposed project also seeks to develop and validate hydrodynamic and heat transfer models under prototypical and scaled SMR conditions numerically and experimentally.

These models will be implemented in an extensive safety analysis investigating multiple accident scenarios, including tube rupture loss-of-coolant, coolant flow rate and temperature fluctuation, and partial tube blockage due to fouling. These scenarios would significantly impact the structural integrity of the HX tubes through highly induced thermal stresses, lead to HX failure, and result in unsafe SMR operation. All analyses of the new HX will be compared with the helical coil tube HX (circular cross-sectional flow area) under the same conditions for improvement quantification. The project activities include developing highly compact and efficient technology and addressing gaps in operation safety for in-vessel IHX and SG to accelerate the development and deployment of multiple SMRs technologies.

Key Publications

- Wahlquist, S., S. -J. Yoon, P. Sabharwall, and A. Ali. 2020. “Novel Heat Exchanger Configuration for Enhanced Heat Transfer for Nuclear Applications,” 2020 American Nuclear Society Winter Meeting.
- Wahlquist, S., A. Ali, S. -J. Yoon, and P. Sabharwall. “Laminar Flow Heat Transfer in Helical Oval-Twisted Tube Heat Exchangers,” Submitted for publication, Frontiers in Heat and Mass Transfer journal.

Sponsor/Program

None Reported.

A.95. Considerations for Component Isolation of Conceptual Advanced Reactors

Report Participants

Samyog Shrestha,[1] Efe G. Kurt,[2] Arun Prakash,[1] Ayhan Irfanoglu[1]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

Implementation of component isolation in nuclear industry is challenging due to gaps in research and the lack of specific guidelines. In this study, parameters affecting component-level isolation of advanced reactor vessels are identified based on a representative numerical model with explicit consideration of nonlinear soil-structure interaction (SSI). The objective of this study is to evaluate the effectiveness of, and to identify potential limitations of, using conventional friction pendulum bearings to seismically isolate vessels. It is found that slender vessels or components are particularly vulnerable to rotational accelerations at the isolation interface, which are caused by rotation of the sub-structure and by excitation of higher modes in the horizontal direction of the seismically isolated system. Component isolation is found to be more effective for relatively stiffer vessels and at sites with stiff soil properties. Considering that conventional isolators are deficient in resisting axial tension, it is observed that the optimum location for supporting a component to achieve seismic isolation is at a cross-sectional plane passing through the center of mass of the vessel. These findings are corroborated by numerous response simulations (using MASTODON) of seismically isolated reactor vessels at different nuclear sites subject to a variety of ground motions.

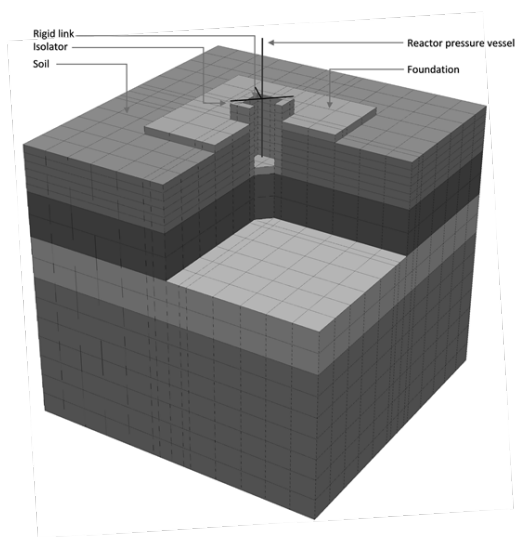


Figure 1. Cutaway view of component isolation model.

Significance

The number of operating nuclear reactors in the United States decreased from 104 in 2012 to 94 in 2020. The nuclear sector had solely relied on traditional large reactors whose growth has been hindered by concerns about public safety, large capital investment, and negative public perception. A new generation of advanced nuclear reactors is being proposed to be smaller and modular with passive safety features to counteract the concerns of previous generation of large reactors. Ensuring modularity, safety, and economic feasibility of power plants are current challenges faced by the nuclear industry. Seismic isolation of components within a nuclear facility has potential benefits in aspects of modularization (achieved by site-independent standardization of nuclear components), safety (achieved by reduced seismic demand) and economy (achieved by reduction in wall thickness of components). But, the nuclear industry lacks research and specific guidelines on component isolation. This study aims to fill that research gap and solve real-life problems in nuclear industry by evaluating the effectiveness of and identifying potential limitations of using conventional friction pendulum bearings to seismically isolate reactor vessels.

Key Publications

- Shrestha S., E. Kurt, A. Prakash, and A. Irfanoglu. ND. "On component isolation of conceptual advanced reactors." *Computer-Aided Civil and Infrastructure Engineering*, under review.

Sponsor/Program

INL - Purdue

A.96. Economics of Small Modular Reactors Considering Below-Ground Siting and Seismic Isolation

Report Participants

Samyog Shrestha,[1] Efe G. Kurt,[2] Arun Prakash,[1] Ayhan Irfanoglu[1]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

Current literature on the economics of SMRs disregards design factors such as below-ground siting and seismic isolation despite the life-cycle cost of the plant being impacted by such factors. The effect of embedding a generic SMR building on the life-cycle cost of the plant is investigated for two U.S. NPP sites. The investigation uses results from nonlinear SSI analysis of the generic SMR building at each site to develop component-level seismic hazard plot (exceedance of acceleration demand in the component) for the corresponding site. It is observed that the component-level seismic hazard decreases for the embedded SMR compared to surface-mounted except when the fundamental mode of the component aligns with that of the embedded structure. For long-period components, the exceedance rate of acceleration demand is significantly low for the two sites considered, thus making seismic isolation an attractive proposition. Seismic isolation can improve standardization of structures and components across project size and site location which in turn maximizes the extent and degree of modularization in SMRs, thus reducing construction time and cost.

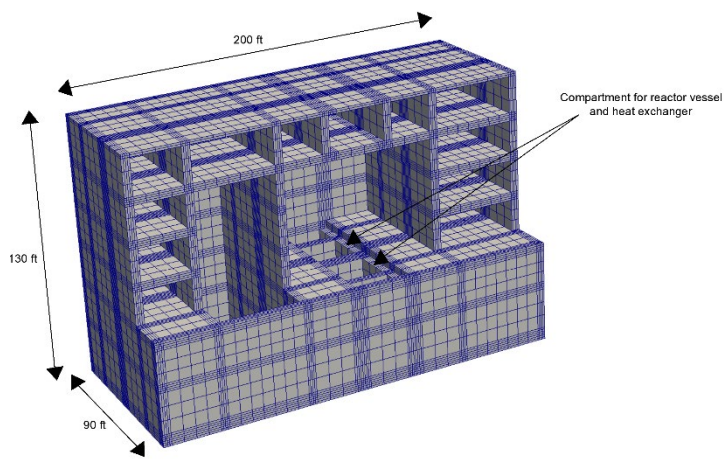


Figure 1. Cutaway view of reactor building model.

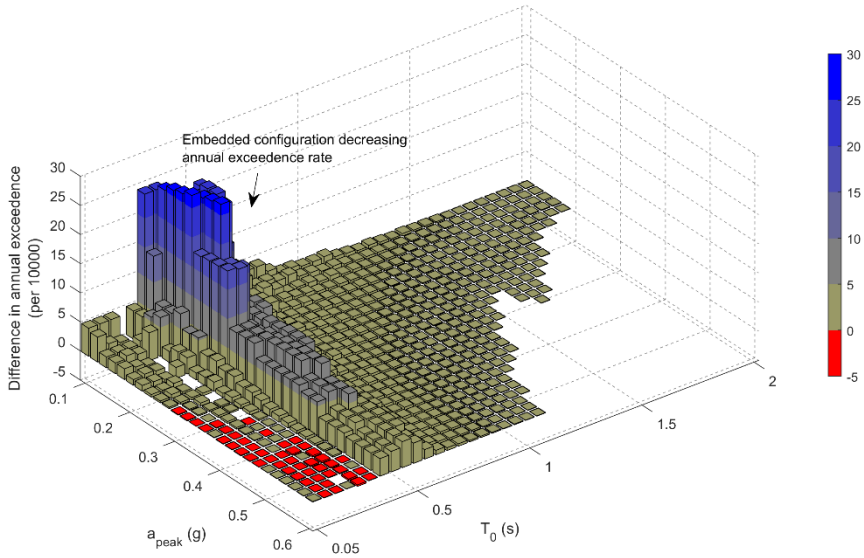


Figure 2. Difference in component-level hazard for excitation along East-West direction in Palisades site.

Significance

The contribution of nuclear energy to the total electricity generation in the United States has stayed constant at about 20% for over a decade. During this time, the nuclear sector has solely relied on traditional large reactors (LR) whose growth has been hindered by concerns about public safety, large capital investment, and negative public perception. As an alternative, SMR have been proposed as a "game changer" for nuclear industry. They differ from LRs in their size and modularity. Their smaller size allows the use of passive features ensuring post-accident safety of the modules without operator action or power. Smaller size also reduces capital cost and financing challenges.

Moreover, the design of SMRs is believed to produce favorable public perception from their visually appealing architecture in contrast to traditional LRs with massive cooling towers. Therefore, SMRs have potential for future deployment making their economic viability an important subject of research. But, there are other factors not directly considered within the investment evaluation although they influence cost over the life cycle of the plant. Such external factors include public acceptance, technical siting constraints, design robustness, historical and political aspects, supply chain risk, construction phase risks, time-to-market, impact on employment, and electric grid vulnerability. In this study, two structural design related factors which are disregarded in the current discussion on SMR economics are investigated to better understand the economic potential of SMRs.

Key Publications

No publication yet but submitted a report to INL.

Sponsor/Program

INL - Purdue

A.97. Full-Core Monitoring of Fuel Performance in LWRs

Report Participants

Koroush Shirvan,[1] Yifeng Che,[1] Joseph Yurko,[2]

1 Massachusetts Institute of Technology

2 University of Pittsburgh

Scientific Achievement

Realistic modeling of a reactor core is essential to ensure no violation of safety standards, enhance the operational flexibility, and optimize the neutron economy thereby fuel consumption. For such reason, full-core monitoring of the fuel response is favored over the peak-rod analysis to more accurately capture the most limiting behavior. A full-core simulation requires simulating thousands of independent fuel rods, which inevitably induces high computational cost. To alleviate the computational burden, ML techniques can be employed to effectively reduce the total number of necessary code runs. The constructed surrogates not only reproduce the full-core response precisely but also drive down the computational cost from days down to seconds, enabling tight coupling of fuel performance feedbacks into the core design procedure.

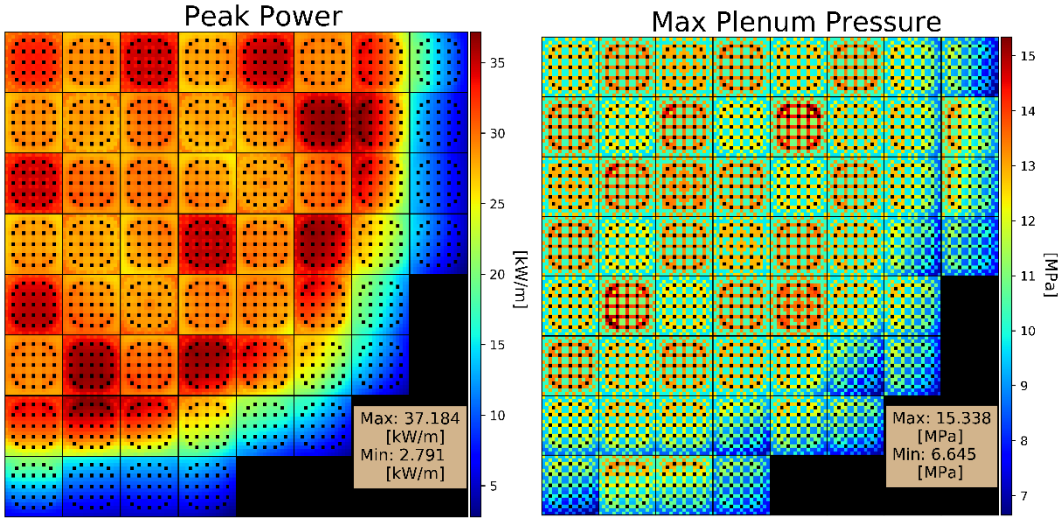


Figure 1. Full-core fuel performance modeling of a prototypical PWR core.

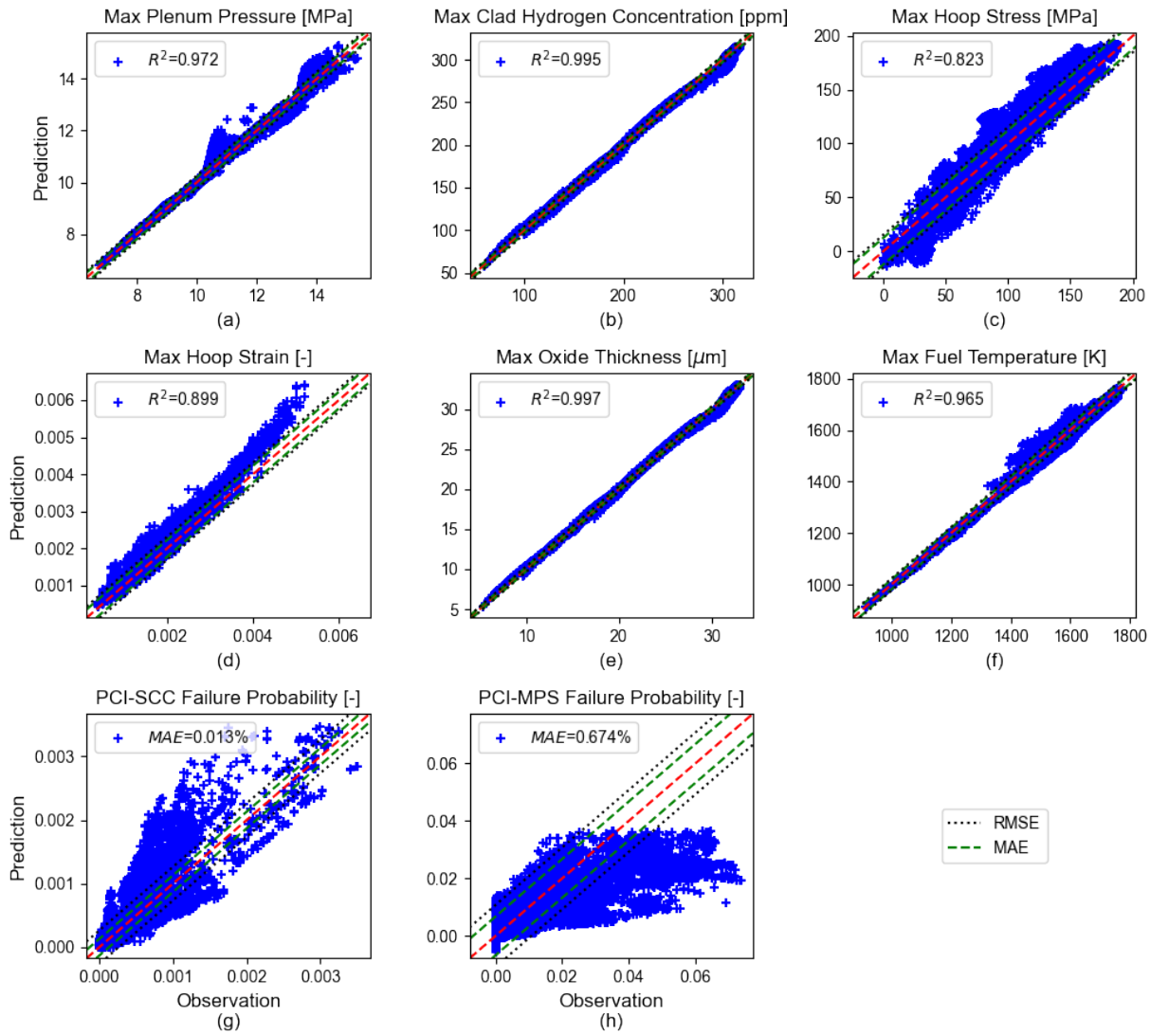


Figure 2. Predicted versus true values for the two-cycle rods in a prototypical PWR core.

Significance

This work demonstrated methodologies for full-core surrogate construction on both standards PWR cores and HB cores. Machine learning-assisted surrogates are constructed for the full-core fuel performance modeling, and Figure 1 shows the predictive performance on three standard PWR cores. The fast-running surrogates provided in the current work enables tight coupling of neutronics, thermal-hydraulics, and fuel performance during reactor core design. More importantly, automated core loading pattern design with modern optimization methods becomes possible with the existance of these fast-running full-core surrogates.

Key Publications

- Che, Y., J. Yurko, and K. Shirvan. ND. "Machine learning-assisted surrogate construction for full-core fuel performance analysis," *Annals of Nuclear Energy*, under review.

Sponsor/Program

None.

A.98. CFD-Informed Design Optimization for VTR Lead Test Vehicle

Report Participants

S. Jun Kim,[1] Cetin Unal[1]

1 Los Alamos National Laboratory

Scientific Achievement

Experimental test vehicle is one of most critical components in the VTR system. A conceptual design of VTR test vehicle is being designed and developed by Los Alamos National Laboratory. In this project, we have utilized a 1D system code (TRACE-Pb) and 3D computational fluid dynamic (CFD) model to optimize the conceptual design of the test vehicle while meeting thermal hydraulic requirement for the irradiation material test. A wide range of design parameters is evaluated using coupled calculation of neutronic and thermal hydraulic model. After several scoping study and design iterations in the pre-conceptual stage, a CFD-informed design maturation is demonstrated, and down-selected baseline design is proposed. A special mesh treatment and detailed fission and gamma heating model are employed into the simulation to capture the thermal hydraulic characteristics in the test vehicle at the desired operation window. In addition, detailed 3D local simulation result from the current CFD simulation shed a light on the design maturation insight to effectively meet the requirements.

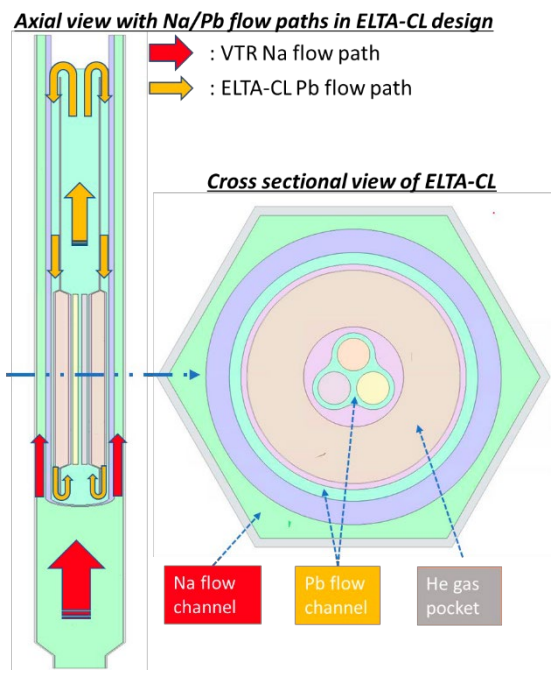


Figure 1. A schematic diagram of the proposed test vehicle design with primary (Pb) and secondary (Na) coolant flow path.

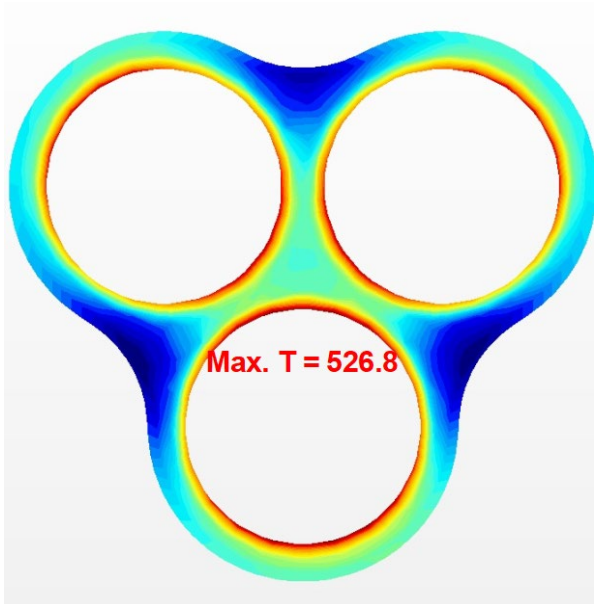


Figure 2. Estimated Pb temperature in the CFD modeling.

Significance

This work provides a perfect example of CFD-informed design maturation process for the VTR experimental test vehicle activity and will play a stepping stone role in deploying lead test vehicle for the irraidation material testing when the VTR is fully contructed and operational. Perfoming CFD-based parametric study indicates useful design insignts, such as relationship bewteen secondary Na mass flow rate and primary Pb maximum temperature and the effect of downcomer gap thickness on the gamma heating magnitute in the downcomer structures and associated Pb temperature. With the proposed modeling work, the following questions associated to test vehicle's performance and requriment can be answered: (1) what is the total gamma heating in VTR test vehicle?, (2) what is the reasonable gap material in the downcomer double walls for accpetable thermal management?, and (3) what is the Pb's thermal hydraulic characterisics (velocity and temp) in the test article.

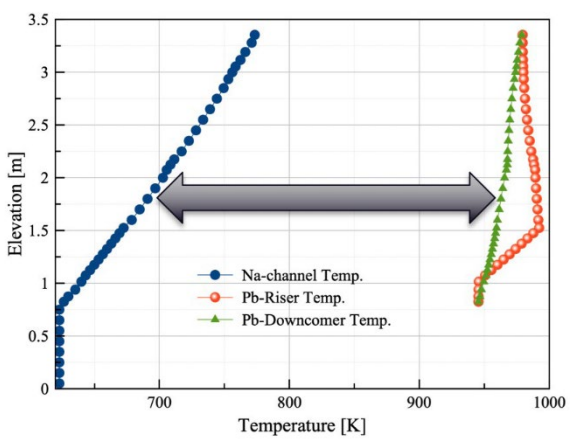


Figure 3. Thermal profiles with He gap design.

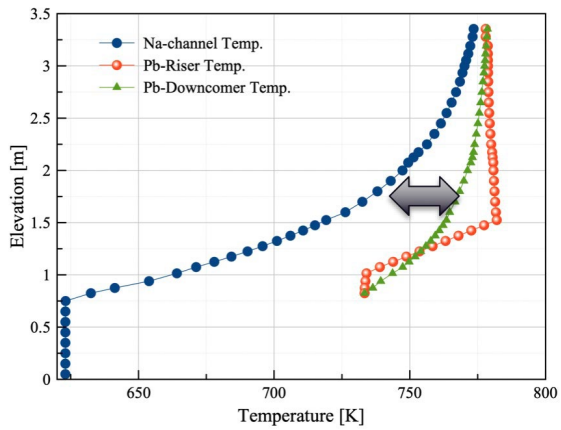


Figure 4. Improved thermal profile with Na gap design.

Key Publications

- Unal, C., et al. "Final report on the VTR Extended Length Test Assembly-Cartridge Lead (ELTA-CL) Pre-conceptual Design," LA-CP-20-20615, Los Alamos National Laboratory.
- Jun Kim, S., et al. 2021. "A conceptual design for experimental test vehicle for VTR and design optimization using multi-physics TH analysis." 2021 ANS Annual virtual meeting, June 14–17.

Sponsor/Program

None.

A.99. HFEF-14SS Cask Drop Analysis

Report Participants

Nathan Seaver[1]

1 Walsh Engineering Services

Scientific Achievement

The Materials and Fuels Complex (MFC) at the INL makes use of shielded containers to transport radioactive payloads out of commerce within MFC or to other INL destinations. Among these casks is the Hot Fuel Examination Facility (HFEF)-14 cask. This cask is one of the primary conveyances used at MFC and other INL facilities for transportation of radioactive materials within or between INL facilities. The existing (and only) HFEF-14 cask is currently experiencing demand such that a second cask is necessary. As a result, a second, functionally equivalent cask is required. This second cask will be primarily made from type 304 stainless steel, whereas the existing cask is made primarily from plain carbon steel. A finite element model of the HFEF-14ss cask was created in Abaqus CAE for analysis with the explicit solver. Thirteen different drop scenarios are considered to ensure the radioactive payload will remain within the confines of the cask, and no direct radiation shine paths are created from a drop at 40 feet above an unyielding surface.

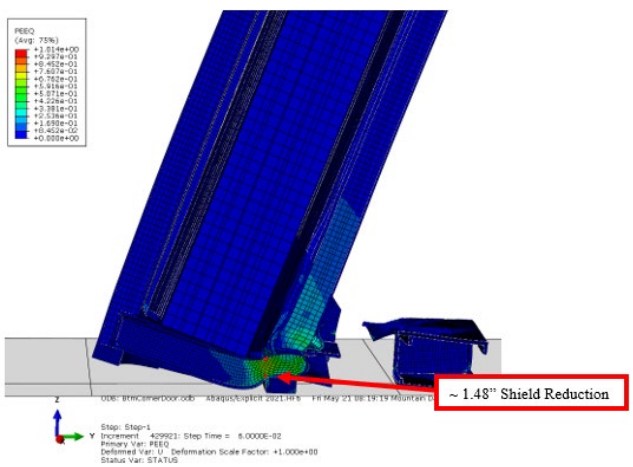


Figure 1. Bottom corner drop plastic strain in lower structures.

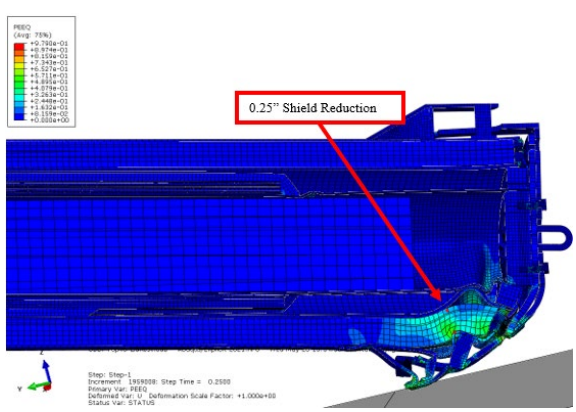


Figure 2. Top corner drop plastic strain in upper structures.

Significance

In all cases the payload is shown to remain contained within the confines of the cask, the lid and door structures remain sufficiently in place to not create a direct (unshielded) shine path, and there is not a reduction in shielding greater than 50% by thickness. The lead shielding experiences plastic strains but does not displace or deform sufficiently to reduce the shielding thickness by more than 50%. Thus, demonstrating safe and functional performance equivalent to the carbon steel cask currently in use.

Key Publications

It is not anticipated that a national publication will result from this work. However, a documented report is in progress to document the performance of the cask as it has been evaluated for future reference.

Sponsor/Program

MFC/HFEF-14 Cask

A.100. Fast Modular Reactor Conceptual Design with Verifications of Key Metrics in Fuel, Safety, and Operational Performance

Report Participants

Hangbok Choi[1]

1 General Atomics-Electromagnetic Systems (GA-EMS)

Scientific Achievement

The GA-EMS fast modular reactor (FMR) fuel design consists of UO2 pellets contained in SiC-SiC cladding. GA-EMS has designed the fuel rod such that it accommodates fuel swelling and fission gas release from the HB operation.

Significance

Existing property database of the UO2 fuel is limited by the burnup range. Internal pressure buildup may accelerate the cracking of the SiC-SiC internal layer that jeopardizes the hermeticity of the cladding. GA-EMS will develop the fuel design and analysis model using a NEAMS tool, BISON. GA-EMS will (i) evaluate the fidelity of the UO2 models under fast reactor conditions using the legacy fast reactor irradiation data, (ii) develop the dedicated GA-EMS SiC-SiC cladding models, and (iii) establish a full fuel rod model using the BISON code. The results will be evaluated for the thermal, mechanical, and chemical behavior of the fuel pellet and cladding, which will be the licensing-basis of the FMR fuel.

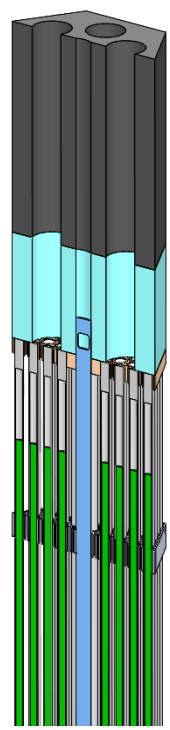


Figure 1. FMR top reflector and fuel assembly model.

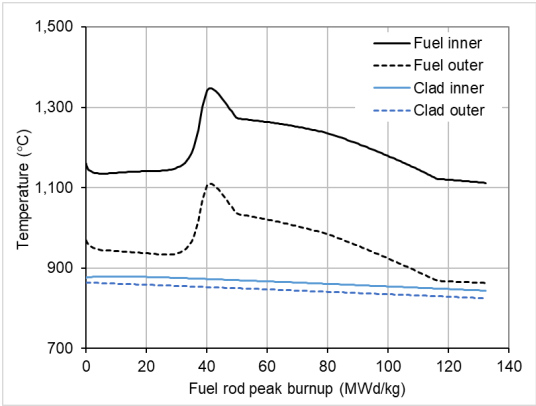


Figure 2. FMR hot rod fuel temperature.

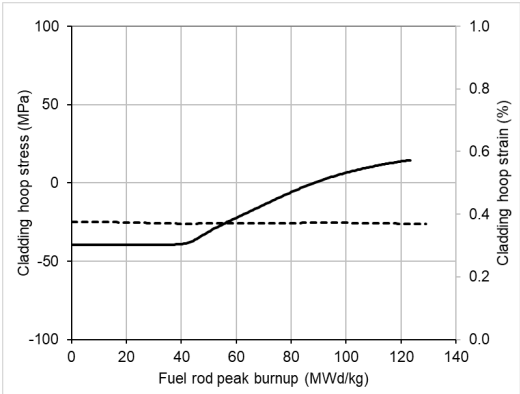


Figure 3. FMR cladding hoop stress/strain.

Key Publications

- Choi, H., et al. 2021. "The Fast Modular Reactor (FMR) - Development Plan of a New 50 MWe Gas-cooled Fast Reactor," 2021 ANS Annual Meeting, June 13-16, 2021. (To be published).

Sponsor/Program

U.S. Department of Energy Advanced Reactor Demonstration Program, Advanced Reactor Concepts 2020 (ARC-20)

A.101. Code-Coupled Modeling and Simulation of eVinci® Microreactor

Report Participants

Alex Levinsky[1]

1 Westinghouse Electric Company, LLC

Scientific Achievement

The MOOSE toolset (BISON, Rattlesnake, Sockeye, MAMMOTH, Grizzly, and RELAP7) is used for the code-coupled modeling and analysis of the Westinghouse eVinci heat-pipe reactor. This work is performed under the Meitner project (DOE ARPA-E program) and DOE FOA programs. Based on the code performance in the Meitner project, it may be decided to use these codes to perform modeling and simulation activities supporting the licensing application and process for the eVinci reactor.

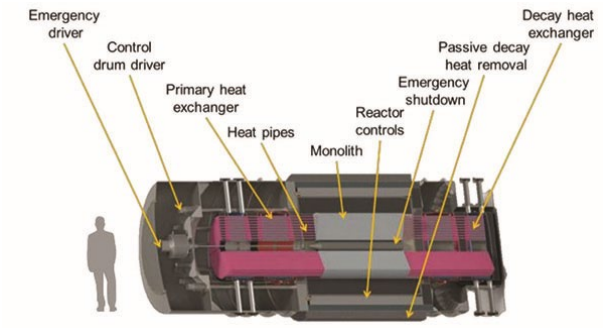


Figure 1. eVinci® microreactor sketch.

Significance

An ability to perform code-coupled simulations of the eVinci heat-pipe reactor in order to show its perfomance in transients and inherent safety features is critical for the building the first of its kind reactor.

Key Publications

- Laboure, V., J. Harter, A. Levinsky, A. Zabriskie, and L. Charlot. 2020. "Final M&S of Solid Core Block during Normal Operation," INL/LTD-20-58488, Idaho National Laboratory.

Sponsor/Program

Department of Energy, ARPA-E DOE, Los Alamos National Laboratory, INL, Argonne National Laboratory

A.102. Heat-Pipe Reactor Code-Coupled Simulations

Report Participants

Alex Levinsky,[1] Megan Durse[2]

1 Westinghouse Electric Company, LLC.

2 Westinghouse Government Services, LLC.

Scientific Achievement

The MOOSE toolset (BISON, Rattlesnake, Sockeye, MAMMOTH, Grizzly, and RELAP7) is used for the code-coupled modeling and analysis of the Westinghouse eVinci heat-pipe reactor. This work is performed under the Meitner project (DOE ARPA-E program) and DOE FOA programs. Based on the code performance in the Meitner project, it may be decided to use these codes to perform modeling and simulation activities supporting the licensing application and process for the eVinci reactor.

Significance

An ability to perform code-coupled simulations of the eVinci heat-pipe reactor in order to show its perfomance in transients and inherent safety features is critical for the building the first of its kind reactor.

Key Publications

None.

Sponsor/Program

Department of Energy, ARPA-E DOE, Los Alamos National Laboratory, INL, Argonne National Laboratory

A.103. Metal Fuel Modeling for Advanced Reactor Designs

Report Participants

John Hanson[1]

1 Oklo Inc.

Scientific Achievement

Oklo uses BISON for fuel performance simulation. The primary usage is for reactor design with BISON results informing the design of their metal fueled reactors.

In addition, BISON is used as part of an ARPA-E project on which Oklo is a participant. The project, titled "Next Generation Metal Fuel," seeks to develop metal fuel that is fabricated in a "pre-swelled" configuration with built-in porosity. This advancement would provide numerous benefits for metal-fueled reactors, including obviating the need for sodium bond, substantially simplifying fuel fabrication. BISON is used to study this pre-swelled fuel and provide insights into the expected behavior of the novel fuel form.

Oklo's access to HPC resources is used solely for accessing the BISON source code, no simulation is conducted using HPC computers, and therefore, Oklo's utilization of HPC resources is minimal.

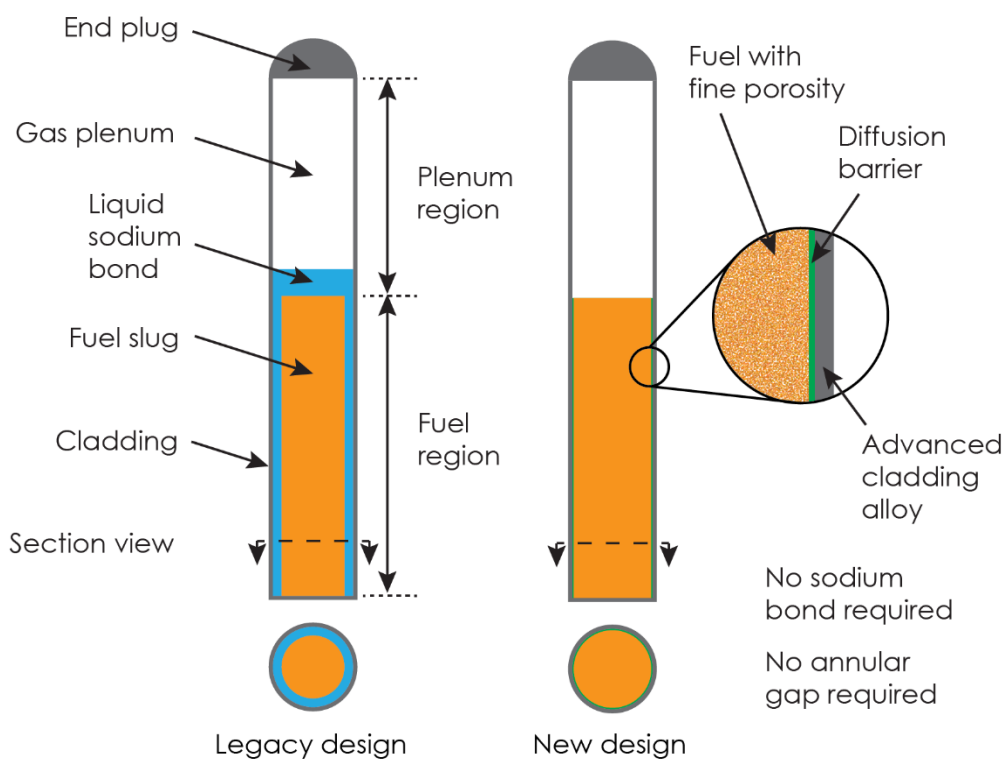


Figure 1. Nominal fuel design studied in Next Generation Metal Fuel project.

Significance

Key findings of Oklo's internal use of BISON are proprietary.

The use of BISON for the Next Generation Metal Fuel project is in progress. BISON is being used in conjuction with Marmot to study the stability and evolution of the porosity built into the "pre-swelled" fuel.

Key Publications

No publications have come of the work yet. Publications are not expected for Oklo's internal use of BISON for reactor design. Updates on the progress of the ARPA-E project have been presented regularly at ARPA-E meetings over the last year, and all milestones have been met thus far. It is expected that publications may result at the end of the project (ending CY 2021).

Sponsor/Program

Advanced Research Projects Agency-Energy (ARPA-E)

A.104. Effect of Different Point Defect Energetics in Ni80X20(X=Fe, Pd) on Contrasting Vacancy Cluster Formation from Atomistic Simulations

Report Participants

Gaurav Arora,[1] Giovanni Bonny,[2] Nicolas Castin,[2] Dilpuneet S. Aidhy[1]

1 University of Wyoming

2 Nuclear materials science institute, Belgium

Scientific Achievement

In this project, we performed MD simulations and DFT calculations in Ni-based binary concentrated alloys to study the effect of defect formation under extreme conditions. Difference in the microstructure evolution was studied for Ni-Fe and Ni-Pd, and key differences were identified in terms of defect evolution. These simulations helped us to explain the physics behind the experimental observation of limited cluster formation in Ni-Pd alloys compared to Ni-Fe alloys.

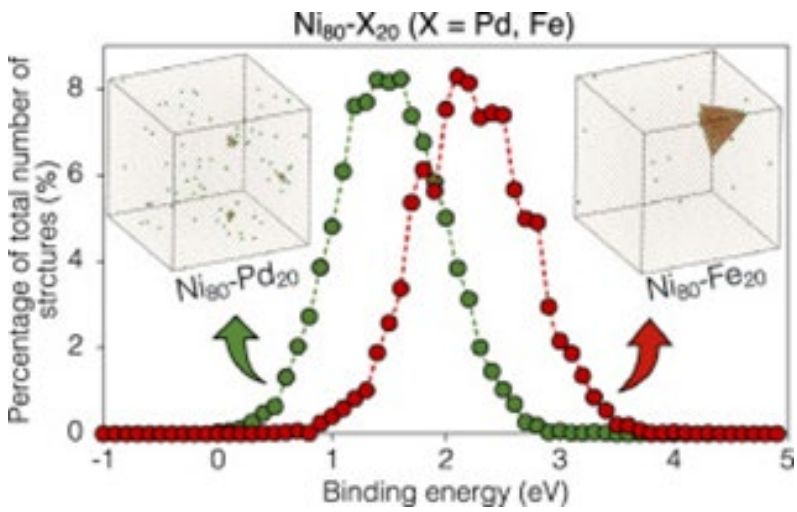


Figure 1. Difference in the binding energy between Ni-Pd and Ni-Fe illustrating its effect on defect formation.

Significance

This work showed the effect of alloy chemistry on defect energies and defect evolution. Addition of Pd lowers the migration barrier but increases the vacancy binding energy resulting in smaller cluster formation in contrast to larger cluster formation in Ni-Fe alloys due to lower vacancy binding energies.

Key Publications

- Arora, G., G. Bonny, N. Castin, and D.S. Aidhy. 2021. "Effect of different point-defect energetics in Ni80X20 (X=Fe, Pd) on contrasting vacancy cluster formation from atomistic simulations." Materialia 15, 100974. https://doi.org/10.1016/j.mtla.2020.100974.

Sponsor/Program

This work was supported as part of the Energy Dissipation to Defect Evolution, funded by U.S. DOE. SCK CEN acknowledges funding from the Euroatom research and training program 2014–2018 under grant agreement No. 755269. Computational resources were provided by ARCC at the University of Wyoming and HPC at the INL.

A.105. Fuel Pellet Microstructural Fracture Modeling

Report Participants

Janne Heikinheimo,[1] Matti Lindroos,[1] Tom Andersson,[1] Huan Liu,[2] Diogo Ribeiro Costa[2]

1 VTT Technical Research Centre of Finland Ltd

2 KTH Royal Institute of Technology, Sweden

Scientific Achievement

This project studies nuclear fuel microstructural modeling and its implications to the macroscopic models. The activity connects KTH Royal Institute of Technology's expertise in atomistic scale calculations and VTT Technical Research Centre's in macro- and mesoscale modeling. VTT studies the applicability of different models on cracking behavior and consequences to macroscopic modeling applying Z-set code for crystal plasticity and BISON code for fuel performance studies. KTH studies atomistic scale fracture parameters and related calculations for different kinds of fuels. VTT and KTH will discuss possible connection of the atomistic model parameters to microscopic scale fracture modeling. The project started in 2020. At the current state, the work focuses on fracture model development for UO2.

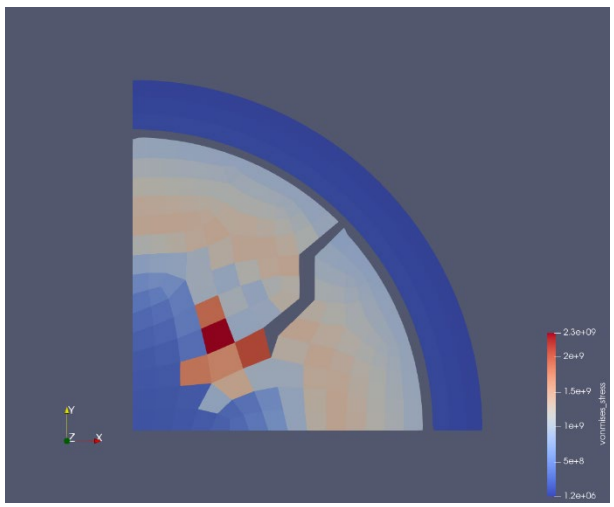


Figure 1. 2D Von Mises stress in a low-burnup UO2 fuel, where a pellet has a macroscopic crack in it (BISON).

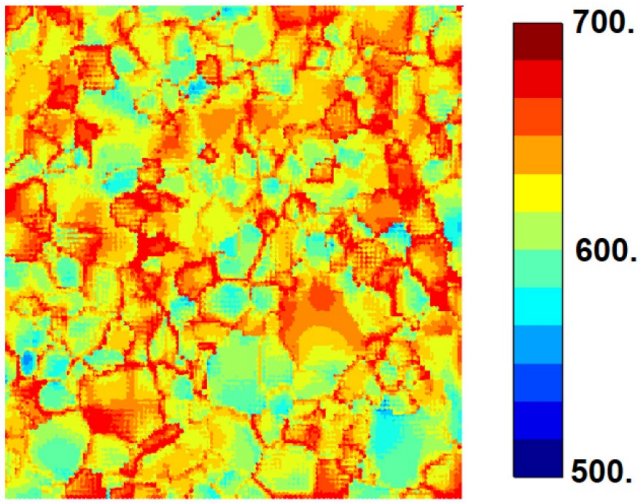


Figure 2. Von Mises stress map of the realistic microstructure under tensile loading (MPa). The crystal structure is obtained from a SEM-EBSD image of a UO2 fuel pellet.

Significance

The work is in progress. The work helps in the fuel pellet fracture model development under different conditions, and thus in better understanding of, for example, the pressure from pellet to the cladding. Currently the focus is on fresh fuel under RIA conditions. Later on the improved pellet fracturing models could be implemented and/or applied in fuel performance codes, such as BISON.

Key Publications

Publications are in process. The following publication is openly available:

- Heikinheimo, J., J. Peltonen, D. R. Costa. 2021. "Towards high-fidelity fuel pellet fracture modeling in current and new fuel designs," NKS-445, ISBN 978-87-7893-537-3.

Sponsor/Program

The project gets funding from Finnish nuclear safety programs SAFIR2022 and KYT2022 and Nordic NKS program. The project funding has stated in 2020.

A.106. Microstructural-Level Fuel Performance Modeling of U-Mo Monolithic Fuel

Report Participants

Sean Masengale,[1] Yongfeng Zhang[1]

1 University of Wisconsin, Madison

Scientific Achievement

The presence of point defects in metals is known to influence their elastic properties. This means that for fuels such as U-Mo, it is important to be able to model the effects of these point defects, as they are generated while the fuel is irradiated during fuel operation. Using MD simulations adopting the LAMMPS code, the effect of point defects in two compositions of U-Mo (U-7Mo and U-10Mo, by weight percent) are studied, along with the effect of temperature on the fuel's elastic properties. By calculating the elastic moduli of U-Mo fuels at different temperatures and with different concentrations of point defects, the influences of both point defects and temperature are elucidated.

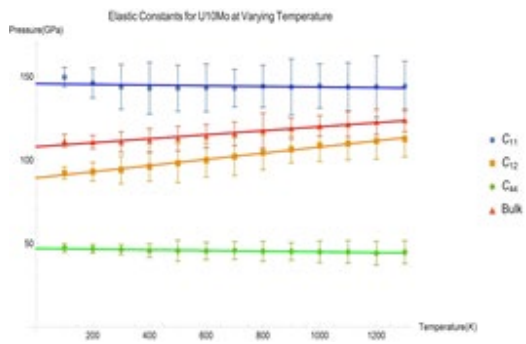


Figure 1. U-10Mo elastic properties as function of temperature.

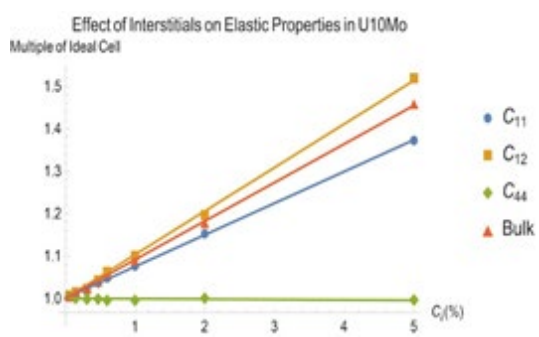


Figure 2. U-10Mo comparison of elastic properties at varying interstitial concentration to the ideal cell.

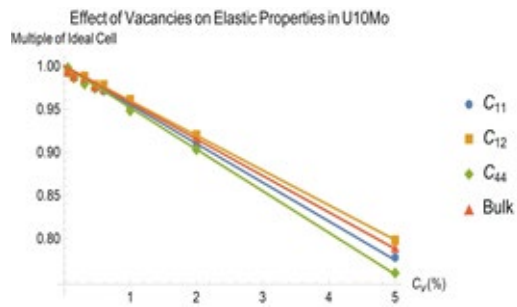


Figure 3. U-10Mo comparison of elastic properties at varying vacancy concentration to the ideal cell.

Significance

The effects of both temperature and varying concentrations of point defects can be seen in the figures above. An interesting finding is that the effect of temperature and the effect of point defects seem to be independent of each other, allowing them to be described by separate analytical models. This is illustrated in Figures 2–3, where the change in defect concentration causes the elastic moduli to change in a manner independent of temperature. Further, it is found that different types of point defects affect the elastic moduli differently. While vacancies, which are unoccupied lattice sites, decrease the elastic moduli, interstitials in general increase elastic moduli. These atomistic calculations can provide accurate data for the elastic properties of irradiated U-Mo fuel. The results are being used to develop analytical models for temperature and point defect concentration dependent elastic moduli. These models can be used in upper scale methods, such as the phase-field finite-element method, to enable multiscale fuel performance modeling, which is happening in the USHPRR program.

Key Publications

None.

Sponsor/Program

USHPRR

A.107. Simulation of Fission Gas in Uranium Oxide Nuclear Fuel

Report Participants

Sophie Blondel,[1] Dong-Uk Kim,[2] Fande Kong[3]

1 University of Tennessee

2 University of Florida

3 Idaho National Laboratory

Scientific Achievement

The objective of this project is to significantly advance the mechanistic understanding of fission gas behavior and release in UO2 nuclear fuel by developing a mesoscale simulator that takes advantage of leadership class computers. Fission gas release within UO2 nuclear fuel occurs as gas atoms diffuse through grains and arrive at GB bubbles; these GB bubbles grow and interconnect with grain edge bubbles; and grain edge tunnels grow and connect to free surfaces. In this approach, fission gas production, diffusion, clustering to form intragranular bubbles, and resolution within grains are included using spatially resolved cluster dynamics in the Xolotl code. GB migration and intergranular bubble growth and coalescence are included using the phase field method in the Marmot code. This hybrid model couples Xolotl to Marmot using the MultiApp and Transfer systems in the MOOSE framework, with Xolotl passing the arrival rate of gas atoms at GBs and intergranular bubble surfaces to Marmot and Marmot passing evolved GBs and surface positions to Xolotl.

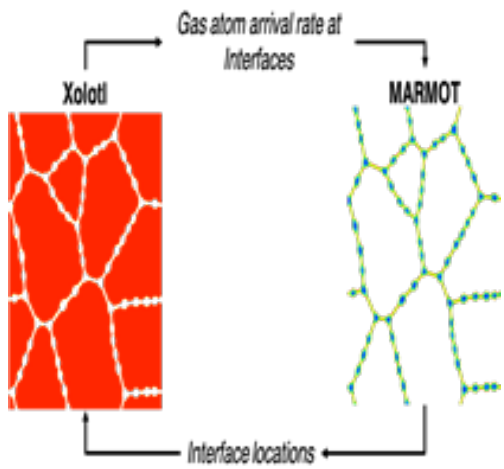


Figure 1. Schematic of the coupling between the Xolotl and Marmot codes, where Xolotl models the clustering and transport of gas atoms within the grains and Marmot models bubble growth and coalescence on GBs, as well as GB migration. Xolotl passes the flux of gas atoms reaching the interfaces (GBs and GB bubble surfaces) to Marmot, while Marmot passes the interface locations to Xolotl.

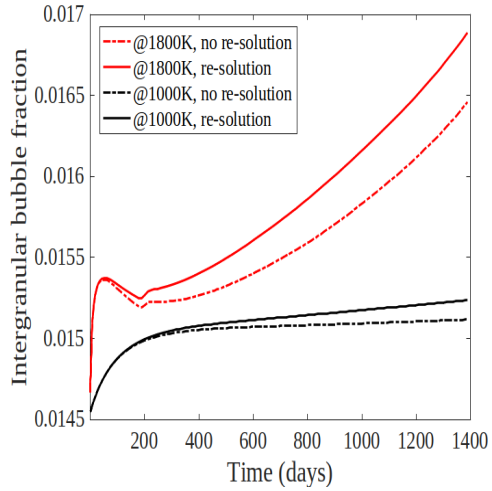


Figure 2. The evolution of the intergranular bubble fraction over time for two temperatures in a 20 μm x 20 μm 2D polycrystal of UO2 with 10 initial grains.

Significance

We have verified that the coupling is functioning correctly by comparing a result using only Marmot to a result from the hybrid model that neglects clustering and resolution. We have also shown that the hybrid model performs well numerically, with ideal or better strong scaling and near ideal weak scaling. We have used the hybrid model to investigate the impact of intragranular physics, temperature, and initial grain size on the fission gas behavior, providing a powerful means of representing many of the critical physical phenomena that influence fission gas behavior. Our hybrid model can also produce critical insights on how to improve the effective diffusivity that is currently used in fission gas release models.

Key Publications

- Kim, D. -U., S. Blondel, D. Bernholdt, F. Kong, D. Andersson, M. R. Tonks, and B. D. Wirth. "Modeling mesoscale fission gas behavior in UO2 by directly coupling the phase field method to spatially resolved cluster dynamics," submitted to *Materials Theory*.

Sponsor/Program

DOE SciDAC program

Appendix B

EDUCATION

Table of Contents

B.1. Adsorption and Surface Diffusion of Metals

Report Participants

Austin Biaggne,[1] Gregory Noble,[1] Lan Li[1,2]

1 Boise State University

2 Center for Advanced Energy Studies

Scientific Achievement

The objective of this work is to understand the adsorption and surface diffusion properties of Mo and Nb on alumina substrates. Advanced manufacturing has been shown to be a viable method to construct a high-temperature irradiation resistant thermocouple (HTIR-TC) using Mo and Nb metals. HPC resources were utilized to perform DFT calculations with the Vienna Ab-initio Simulation Package (VASP). Adsorption energies and sites on the alumina surface were determined, and surface diffusion pathways were found using nudged elastic band methods. Surface energies and diffusion energy barriers were used to calculate the diffusion pre-factors and coefficients of Mo and Nb adatoms.

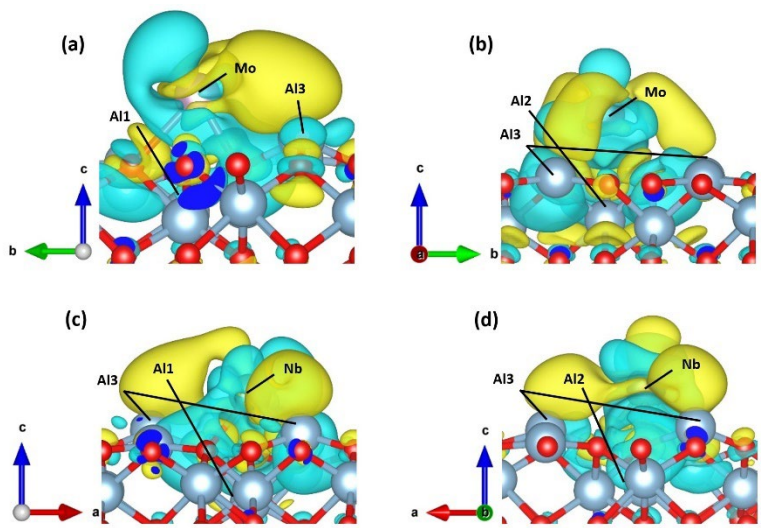


Figure 1. Charge density differences of (a–b) Mo and (c–d) Nb above the Al2O3 substrate. Yellow regions represent an accumulation of electrons, and blue regions represent a loss of electrons.

Significance

It is necessary to control the advanced manufacturing process, and this study provides atomistic insight into metal printing. In the case when Mo and Nb metals are printed together (such as for HTIR-TCs), differing diffusion rates and adsorption site competition can affect how the Mo and Nb nanoparticles form and spread on the surface. It was found that Mo and Nb preferentially adsorb to the same surface sites (shown in Figure 1), and Mo has a larger diffusion coefficient compared to Nb. Understanding these differences is crucial to the development of advanced manufacturing methods for nuclear sensors. Furthermore, results from this study can be used as inputs into larger phase field models of advanced manufacturing processes.

Key Publications

- Biaggne, A., G. Noble, and L. Li. 2021. "Adsorption and Surface Diffusion of Metals on a-Al2O3 for Advanced Manufacturing Applications," *JOM*, 73:1062–1070. https://doi.org/10.1007/s11837-021-04589-y.

Sponsor/Program

This work was supported in part through the Department of Energy Advanced Sensors and Instrumentation program under DOE Idaho Operations Office Contract DE- AC07-05ID14517

B.2. Computational Modeling of Dye Molecules

Report Participants

Austin Biaggne,[1] Lan Li[1,2]

1 Boise State University

2 Center for Advanced Energy Studies

Scientific Achievement

Dye molecules have been shown to be a viable building block for constructing excitonic devices, such as organic photovoltaics and quantum computers. Customizing dyes to tailor them for specific applications is necessary to enhance their functionality in excitonic devices. To study how substituents affect dye properties, DFT, and time dependent (TD-). DFT calculations were performed using the Gaussian 16 software to screen the effects of substituents on dye molecules, such as Cy5 (shown in Figure 1). The effects of various substituent pairs on the solubility and electronic properties were quantified and general trends were established based on the substituent's electron donating or withdrawing strength.

Significance

This project provides insight into the effects substituents have on the solublitity and electronic properties of dyes. The substition of dyes can enhance electronic properties for improved aggregation and augmented exciton coupling and dynamics. The effects of the substituents were estimated to correlate to the relative electron donating or withdrawing strength of the substituents. The results of this study can be used to select and optimize dye molecules for excitonic applications.

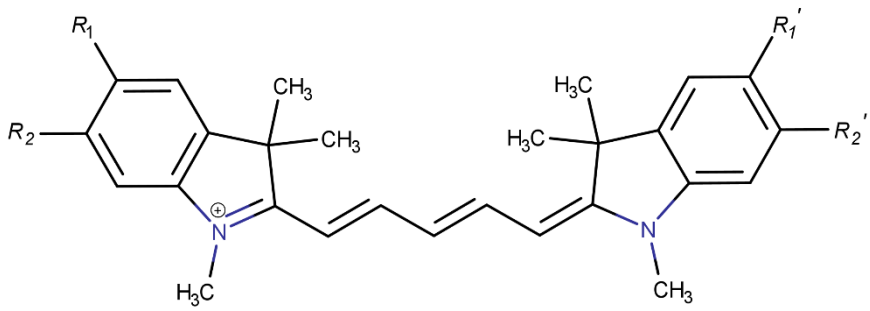


Figure 1. Molecular structure of a Cy5 dye. Substituents were placed at R1 and R2 sites.

Key Publications

- Biaggne, A., W. Knowlton, B. Yurke, J. Lee, and L. Li. 2021. "Substituent Effects on the Solubility and Electronic Properties of the Cyanine Dye Cy5: Density Functional and Time-Dependent Density Functional Theory Calculations," *Molecules*, 26(3):524. https://doi.org/10.3390/molecules26030524.

Sponsor/Program

This research was supported fully by the U.S. Department of Navy award No. N00014-19-1-2615 issued by the Office of Naval Research, except for resources provided by the HPC Center at INL that are supported by the Office of Nuclear Energy of the U.S. Department of Energy and the NSUF under Contract No. DE- AC07-05ID14517.

B.3. Effect of Soil Properties and Input Motion on Site Amplification Using Validated Nonlinear Soil Model

Report Participants

Samyog Shrestha,[1] Efe G. Kurt,[2] Kyungtae Kim,[2] Arun Prakash,[1] Ayhan Irfanoglu[1]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

Three-dimensional nonlinear site response analyses conducted in MASTODON (an open-source finite-element code capable of capturing three-dimensional nonlinear hysteretic soil response) is first validated using actual data from five earthquakes at three downhole array stations recorded in KiK-net, Japan. The same modeling approach is used to conduct site response analyses on site models of 10 NPP sites in the United States using spectrally matched near-field and far-field ground motions. The objective is to investigate the effects of soil properties and input motions on site amplification. It is found that all sites retain a definite site amplification function regardless of the input motion. The magnitude of site amplification and frequencies at which they occur depend upon soil properties, particularly the shear wave velocity profile and the constitutive relationship (strain dependent shear modulus reduction and hysteretic damping) of soil. Amplification of spectral acceleration in the vertical direction is found to be just as much as, if not more than, the amplification in the horizontal direction. Peak shear strain is found to be about 20% larger for near-field motions compared to far-field motions, whereas maximum horizontal site amplification for far-field motions is found to be consistently larger than that of near-field motions, even though the differences between the two remain within the scatter resulting from individual ground motions.

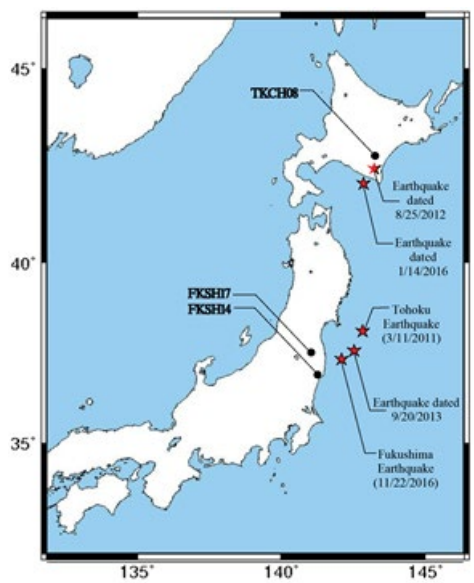


Figure 1. Map of Japan showing selected downhole array stations along with epicenters of considered earthquakes.

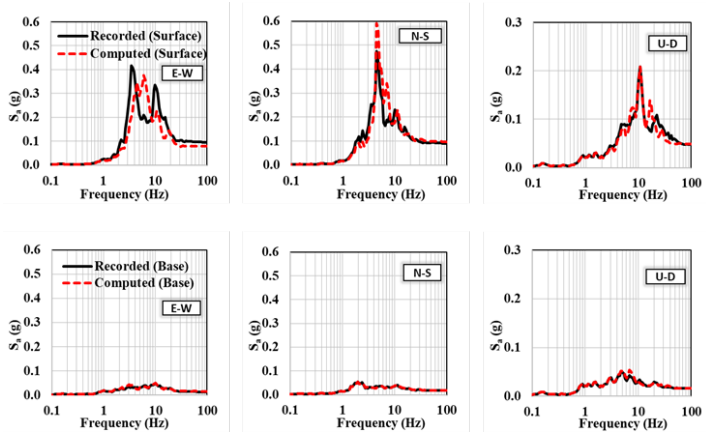


Figure 2. Comparison of 5% damped spectral acceleration for site Kawamata (FKSH17) during earthquake dated November 22, 2016.

Significance

Sets of spectrally matched ground motions are frequently used to conduct SSI analysis of nuclear facilities. But, the choice of seed motion used for spectral matching can affect the extent of site amplification. This study aims to fill the knowledge gap on how site amplification varies with the choice of near-field and far-field seed motions for spectral matching.

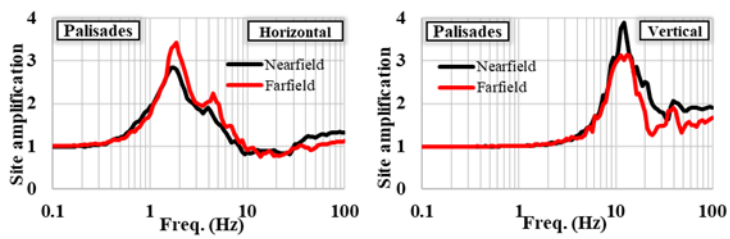


Figure 3. Mean site amplification for Palisades site.

Key Publications

- Shrestha, S., E. G. Kurt, K. Kim, A. Prakash, and A. Irfanoglu. 2021. "Effect of Soil Properties and Input Motion on Site Amplification Using Validated Nonlinear Soil Model," *Nuclear Technology*, 207(11):1639–1663. https://doi.org/10.1080/00295450.2021.1920798.

Sponsor/Program

INL - Purdue

B.4. Integrated Process Optimization for Biochemical Conversion

Report Participants

Sandra Eksioglu,[1] Dr. Qiushi Chen,[2] Dr. Mohammad S. Roni,[3] Dr. Yidong Xia[3]

1 University of Arkansas

2 Clemson University

3 Idaho National Laboratory

Scientific Achievement

The main objective is to develop analytical tools to enable a biorefinery to identify an optimal integrated process design that ensures a reliable, cost-effective, sustainable, robust, and continuous feeding of biomass feedstocks in order to achieve the design throughput of the reactor. The specific aim of the DEM part is to develop discrete element models (DEMs) to quantify and control the impact of physical and quality characteristics of biomass on the performance of the equipment used in the proposed feeding system(s), integrate the outcomes of DEMs into analytical models, and develop solution algorithms to determine optimal screen size, feed rate, buffer capacity, and location that optimize the performance of the feeding system and validate these analytical result via demonstration at INL's Process Development Unit. To achieve these outcomes several simulations have been done using LIGGGHTS software which uses DEM in the INL HPC.

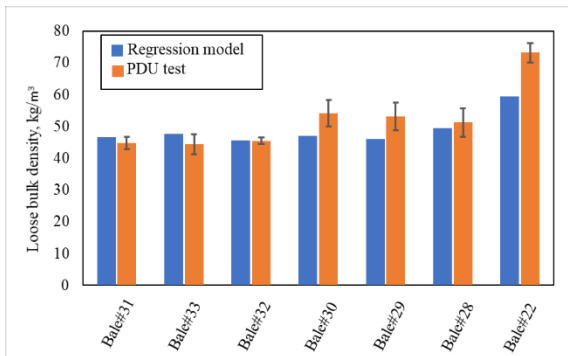


Figure 1. Validation of regression model after Grinder-1 with PDU test data at INL.

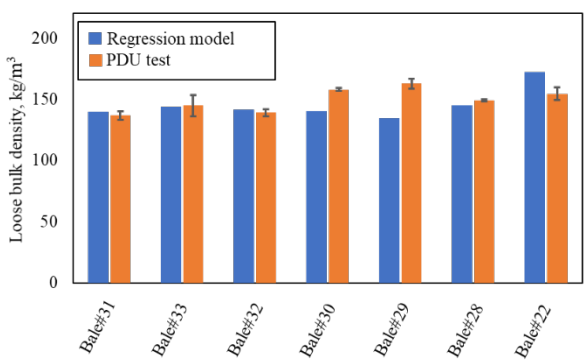


Figure 2. Validation of regression model after Grinder-2 with PDU test data at INL.

Significance

Two different regression models have been developed to predict bulk densities after two different grinders which can be used to get the particle flow rate in the system and thus helping the process optimization. To get these regression models bulk density simulations had to be performed using LIGGGHTS in INL HPC.

Grinder model has been established to predict the particle size distribution after grinding. This will help to get an idea about the particle size communition inside the grinder and what size is suitable for optimized process. Coarsegraining and other practical conditions have been considered to efficiently and accurately predict the after grinding particle sizes.

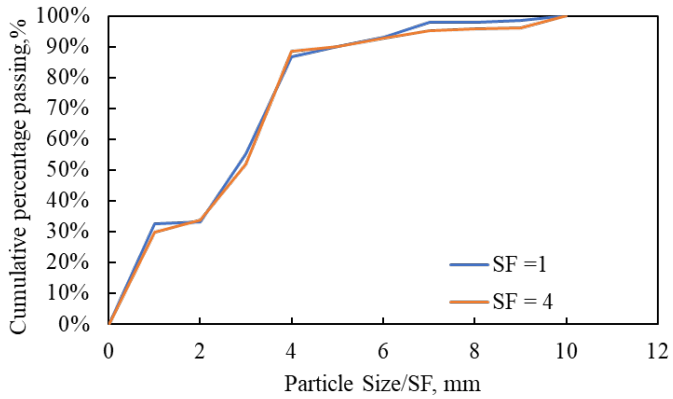


Figure 3. Grinder-2 model showing output of particle size distribution with coarse graining.

Key Publications

- "Discrete element modeling of switchgrass particle breakage in hammer mill – computational efficiency and practical considerations," 2021 ASABE Annual International Meeting, in process.

Sponsor/Program

Industry.

B.5. Modeling the Dispersal of Volcanic Ash on Mars

Report Participants

Tyler Paladino,[1] Shannon Kobs Nawotniak[1]

1 Idaho State University

Scientific Achievement

In this project, we seek to model the deposition of volcanic ash on a planet-wide scale on Mars. We seek to find correlations between ash deposition and current day hydrated regolith that blankets the Martian surface. To accomplish this, we use two pieces of software, one that simulates an explosive eruption plume in a rudimentary atmosphere (the Mars Active Tracer High-resolution Atmospheric Model (MATHAM)) and another that simulates the motion of an entire atmosphere as well as the many physical processes happening therein (the Laboratoire de Météorologie Dynamique General Circulation Model (LMD GCM)). MATHAM and the LMD GCM solve many higher order differential equations in 3D space over time and as such, benefit from being run over many CPU cores. This project is in its infancy, and as such, we have only begun to implement the two models and couple them together smoothly.

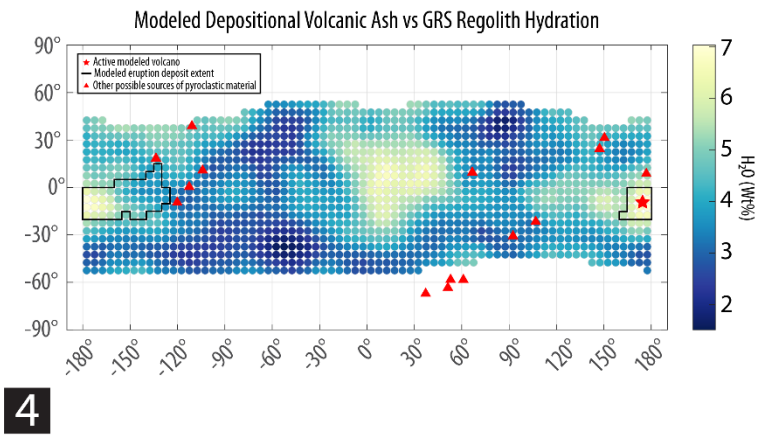


Figure 1. Map of Mars with background color corresponding to GRS hydration level. Black polygons denote modeled eruption extent. Notice good agreement between this extent and high hydration amounts. Note: This Figure only shows one single eruptive event. We will eventually compile many eruptions to get a better sense of correlation.

Significance

This work will help uncover a mystery of Mars; namely, what creates observed patterns of regolith hydration on Mars? As of now, no one hypothesis has been able to explain the patterns we see in the upper 10s of cms of regolith. If areas of high hydration are formed by explosive volcanic eruptions (which are capable of depositing much more than 10's of cms of ash), then it may be worthwhile to explore these areas as key in situ resource utilization (ISRU) zones for future manned Martian missions. To date, we have installed and run test simulations for both models, have performed sensitivity analyses on MATHAM simulations, and have begun to convert some code associated with volcanism in the LMD GCM software from serial to parallel. We are also now beginning to run final simulations with the LMD GCM and MATHAM. Preliminary results show good agreement between modeled eruptiond deposits and areas of hydrated regolith.

Key Publications

There are no publications yet as this project is in its infancy, though do we plan on publishing.

Sponsor/Program

NASA MDAP, IUC

B.6. Parallel High-Resolution Compact Partial FFT-Type Direct Algorithms for Subsurface Scattering Problems

Report Participants

Dr. Yury Gryazin,[1] Dr. Daniel Korytowski,[1] Yun Teck Lee,[1] Ron Gonzales[1]

1 Idaho State University

Scientific Achievement

This project will produce direct parallel partial FFT-type algorithms for the numerical solutions of the two- and three-dimensional Helmholtz equations. The governing equations are discretized by high-order compact finite-difference or finite-element methods. The resulting discretized system is indefinite, making the convergence of the most iterative methods deteriorate with the increase of the frequency. In this situation, the parallel direct approaches become a better alternative, especially for the systems with discontinuous and singular right-hand sides.

The focus is the efficient parallel implementation of the proposed algorithm in the shared (OpenMP) and distributed (MPI) memory environment. The complexity and scalability of the direct parallel method are investigated on scattering problems with realistic ranges of parameters in soil and mine-like targets. The results are also compared with the Krylov-type preconditioned methods developed in our previous publications.

The algorithms' implementations are written in C. The most computationally expensive portion in the algorithm is computing the discrete sine transforms of the right-hand side of the equation. This is achieved by computing the FFT of an appropriate extension of the right-hand side. The open sourced libraries FFTW are utilized for these calculations.

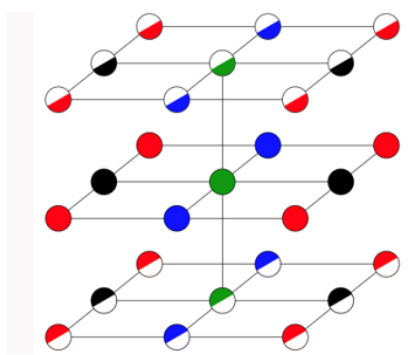


Figure 1. 27-point stencil.

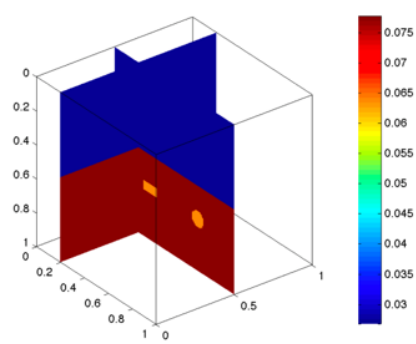


Figure 2. Subsurface inclusions.

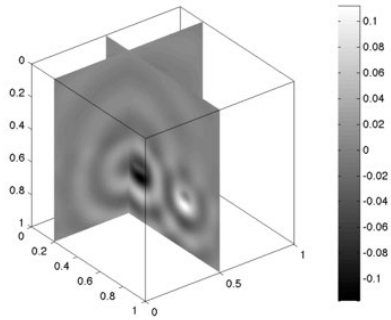


Figure 3. Wave propagation.

Significance

The work is currently in progress. It is expected to produce two more publications in addition to two doctoral dissertations. As of today, a solver for the case of variable coefficient in strictly one spatial dimension with Dirichlet boundary conditions is performing as expected on multiple test problems. The weak and strong scaling results are near optimal. The next step will introduce Neumann, Sommerfeld, and PML boundary conditions and remove the dimensional restriction on the coefficient.

Key Publications

- Gryazin, Y. G., R. G. Gonzales, and Y. T. L. Lee. 2019. "Scalable Algorithms for High-Order Approximations on Three-Dimensional Compact Stencils," *Parallel Computing*, arXiv:1912.03565, Cornell University.

Sponsor/Program

Academics, Industry

B.7. Regional Climate Modeling in the East River, Colorado

Report Participants

Will Rudisill,[1] Lejo Flores[1]

1 Boise State University

Scientific Achievement

The project aims to develop a regional climate simulation using the Weather Research and Forecasting (WRF) model for a 30-year period (1990–present). The study area is the East River Watershed in Colorado, which is the location of a DOE Watershed Function Scientific Focus Area (https://doesbr.org/research/sfa/sfa_lbl.shtml). Subsurface biogeochemical process modeling is fundamentally limited by liquid water inputs (precipiation and or snowmelt) at the top boundary. This research applied high-resolution regional climate models to replicate past precipitation conditions. The research conducted on the INL HPC system includes running the regional climate simulation and post-processing model output.

Figure 1. Study region: the East River Watershed, Colorado, USA. (Outline in yellow).

Significance

The work is still in progress. As of now, >90% of the 30-year simulation has been completed. The datasets have been shared with colleagues at the Lawrence Berkeley National Laboratory. Ultimately the dataset will be shared publicly and used by other scientists conducting research within the East River SFA. Future work will use HPC resources to (1) complete the remaining simulations and (2) post-process data outputs using parallel Dask/Xarray tools. Currently, a manuscript is in progress that will be submitted to a leading peer-reviewed journal.

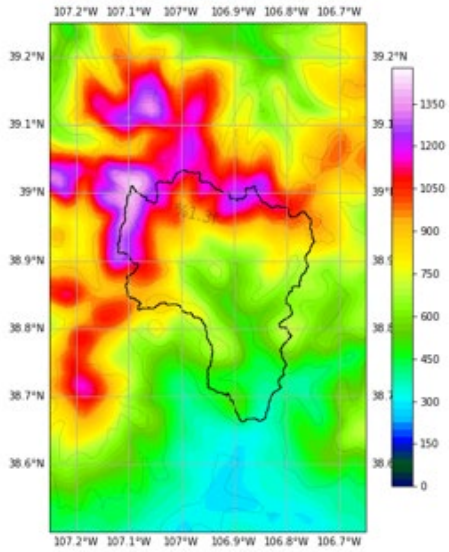


Figure 2. Example of WRF modeled precipitation for 2005. Computations were made on INL's Falcon computer.

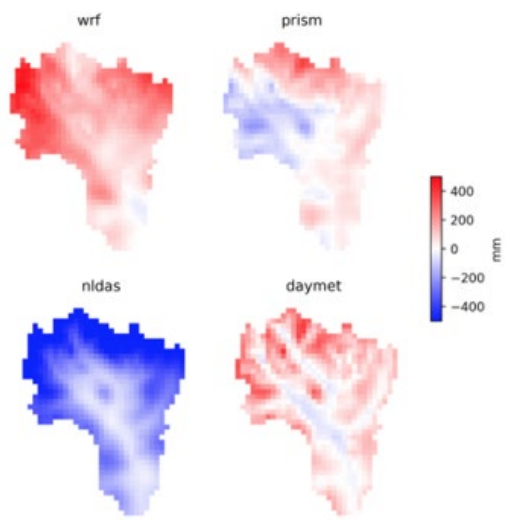


Figure 3. Comparisons between WRF simulated precipitation and other reference precipitation datasets.

Key Publications

- Rudisill, W. J., C. Nash, A. N. Flores, D. Feldman, and R. W. Carroll. 2019. "A Comparison of Dynamically Down-scaled and Interpolated Daily Meteorological Datasets in the East River, CO," Presented at American Geophysical Union Fall Meeting: San Francisco, CA, December 9, 2019–December 13, 2019.
- Rudisill, W. J. and A. N. Flores. "Evaluating dynamically downscaled precipitation fields using remote sensing, streamflow measurements, and bayesian inference." in progress.
- Rudisill, W. J. and A. N. Flores. 2020. "A Process-Aware Comparison of Mountain Precipitation Estimates in The East River Watershed," 19th Conference on Mountain Meteorology, AMS.

Sponsor/Program

Idaho University Consortium

B.8. Sensitivity Study on Parameters Influencing Soil-Structure Interaction of Embedded Structure

Report Participants

Samyog Shrestha,[1] Osama Abdelaleim,[1] Efe G. Kurt,[2] Arun Prakash,[1] Ayhan Irfanoglu[1]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

In this study, Monte Carlo method (MCM) is used to propagate uncertainties in material properties through finite element models of soil column and soil-structure system. The objective of this study is to examine the response of embedded structures to uncertainties in material properties of soil, structure, and friction coefficient in soil-structure interface. It is observed that the mean stochastic response is sensitive to variability in input ground motion rather than randomness in material properties. The mean stochastic response is found to be within 10% of the deterministic response for more than 90% of cases considered in this study. Considering realistic uncertainties in material properties, the structural response of embedded structure does not vary drastically; the coefficient of variation for roof drift ratio and roof acceleration was limited to 15% to 25% for analyses conducted in this study. The variation in stochastic response depends on the type of response monitored. Within the scope of this study, the peak velocity at the base of the embedded structure is insensitive to randomness in material properties. Uncertainties in friction coefficient at soil-structure interface is less significant than random properties of soil and structure. The roof acceleration in the embedded structure is most sensitive to randomness in soil properties particularly for site subjected to large shear strain.

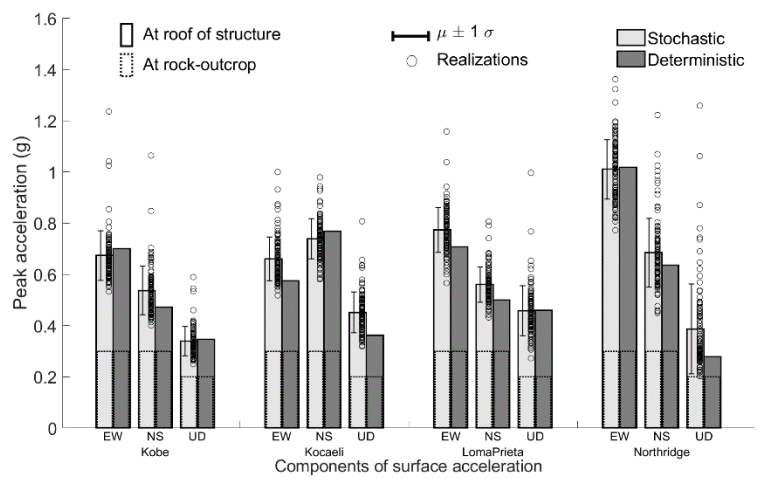


Figure 1. Peak response acceleration from SSI analyses for Palisades site.

Significance

In the past few decades, studies on stochastic SSI have been based on simplified models of beam supported on springs and dashpots representing a structure on a shallow foundation. Despite being studied from different perspective, there are still aspects such as embedded structural configuration, soil-structure interface nonlinearity, and vertical ground excitation which have not been explored in detail. The necessity to address these aspects has also been felt more recently, for example with emerging designs of critical structures such as NPPs being proposed to be constructed below-grade.

The advancement of computational capabilities have also prompted towards more realistic SSI models accounting for interface nonlinearity such as sliding and gapping in the soil-structure system which were mostly discounted in the past. In this study, reasonable range of uncertain parameters are identified from existing literature and such uncertainties are propagated through models of soil column and soil-structure system using MCM to identify their influence in the response of soil and structure from sample statistics.

Key Publications

There are no publications yet, but a report has been submitted to INL.

Sponsor/Program

INL – Purdue

B.9. Simulation of a Nonlinear Soil-Structure Interaction Observed in a Shake Table Test

Report Participants

Samyog Shrestha,[1] Efe G. Kurt,[2] Kyungtae Kim,[2] Arun Prakash,[1] Ayhan Irfanoglu[1]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

Nonlinear SSI analysis is performed to replicate experimental results from shake table test of a steel tunnel embedded in soft soil. The first among a series of 1/9 scale tests performed on a steel tunnel with 2 ft deep overburden soil embedded in a 22 ft long, 9.6 ft wide, and 15 ft high laminar box (Kim et al. 2017) is considered. A numerical model of the test is developed in the MASTODON simulation platform. It is found that the displacement, velocity, spectral acceleration at various depths in the soil, and the tunnel racking response compare well to the test data. Discrepancies between the analysis and test results are also quantified and discussed along with insights into the nonlinear SSI between the tunnel and soil in this test.

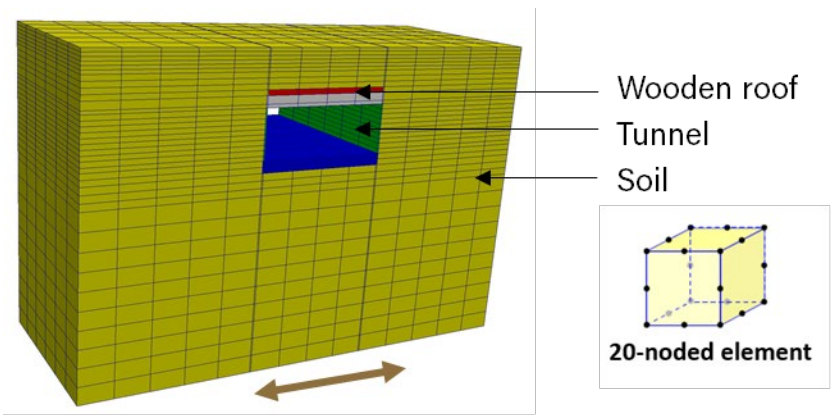


Figure 1. Tunnel – soil model in MASTODON.

Significance

Nonlinear SSI analysis methods are still evolving with an increase in computational power. To improve reliability of such analyses, they must be used to replicate experimental results which are limited in large scale. This study serves to compare numerical results against experimental data and identify potential computational challenges.

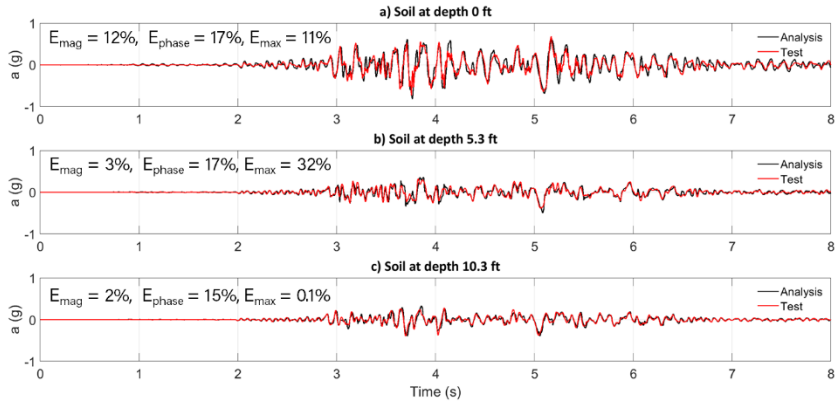


Figure 2. Comparison of response acceleration.

Key Publications

- Shrestha, S., E. Kurt, K. Kim, A. Prakash, and A. Irfanoglu. 2021. "Simulation of a nonlinear soil-structure interaction observed in a shake table test," Engineering Mechanics Institute, May 25–28, 2021.

Sponsor/Program

INL – Purdue

B.10. Temperature-Dependent Heat Capacity Effects on Volcanic Plume Fluid Mechanics and Thermodynamics

Report Participants

Meghan A. Fisher[1]

1 Idaho State University

Scientific Achievement

A volcanic plume's thermal energy is primarily used to heat entrained air. If it entrains enough air to become positively buoyant, it will rise until it is in thermal equilibrium with the surrounding atmosphere. The rate in which the plume heats the entrained air (i.e. the specific heat capacity) is thus an important driver of plume dynamics. Bulk specific heat capacity of volcanic plumes varies not only with composition but also with temperature. However, all previous volcanic plume models (0th order scaling models, 1D integral models, and 3D spatiotemporal numerical simulations) disregard the dependency specific heat has with temperature. Using a 1D integral and a 3D Navier-Stokes volcanic plume model, we have been evaluating the effect that temperature-dependent specific heat capacity has on plume buoyancy, stability, and overall rise height. Preliminary results indicate that:

- The specific heat capacity of ash varies by more than 75% across the range of plume temperatures. In more than two thirds of the plume, the temperature-dependent specific heat capacity of ash is at least 45% smaller than the constant heat capacity value of 1100 J/kgK.
- Volcanic plumes have 8–30% less initial thermal energy than estimated using constant heat capacity. This corresponds to plume heights that are 4–15% smaller. Unlike the addition of water latent heat or entrainment of ambient air, the reduction of plume height of large eruptions is about the same as the reduction of plume height of smaller eruptions.
- Temperature-dependent specific heat capacity has a larger effect on overall plume height than atmospheric moisture, ambient wind, release of latent heat due to phase transitions of water vapor, and entrainment parameterization.
- With temperature-dependent specific heat capacity, plumes more efficiently heat entrained air in the lower gas-thrust region and less efficiently heat air in the upper, convective region.
- When the plume reaches thermal equilibrium, plume temperatures will be higher
- Partial column collapse occurs at lower temperatures than previously indicated.

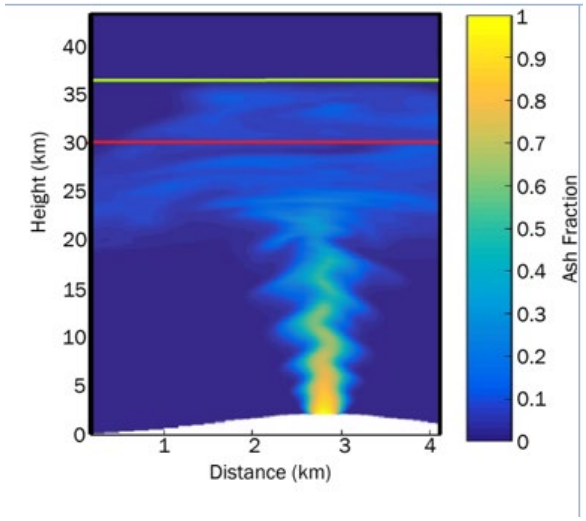


Figure 1. 2D slice of time averaged 3D volcanic plume simulated by ATHAM, the active tracer high-resolution atmospheric model.[a] The green line indicates the rise height when using temperature-independent heat capacity and the red line temperature-dependent heat capacity.

Significance

Predicting plume height and plume collapse are a vital part of volcanic hazard forecasting. This work has identified temperature variability in specific heat capacity as a significant factor governing plume rise and stability. Volcanologists have recognized that atmospheric moisture, ambient wind, and release of latent heat due to phase transitions of water vapor all have noticeable effects on plume stability and height and should be considered in plume models. Temperature variability in specific heat capacity has a larger effect than all of these other considerations and thus cannot be ignored.

As part of this work, we are releasing a volcanic thermodynamic function (volcthermf) library that calculates heat capacity, enthalpy, entropy, potential temperature, and conservation temperature for volcanic plume. The library is designed to be easily integratable with a variety of plume models used by several different research groups. It will allow these other groups to incorporate our findings into their own models with very little overhead.

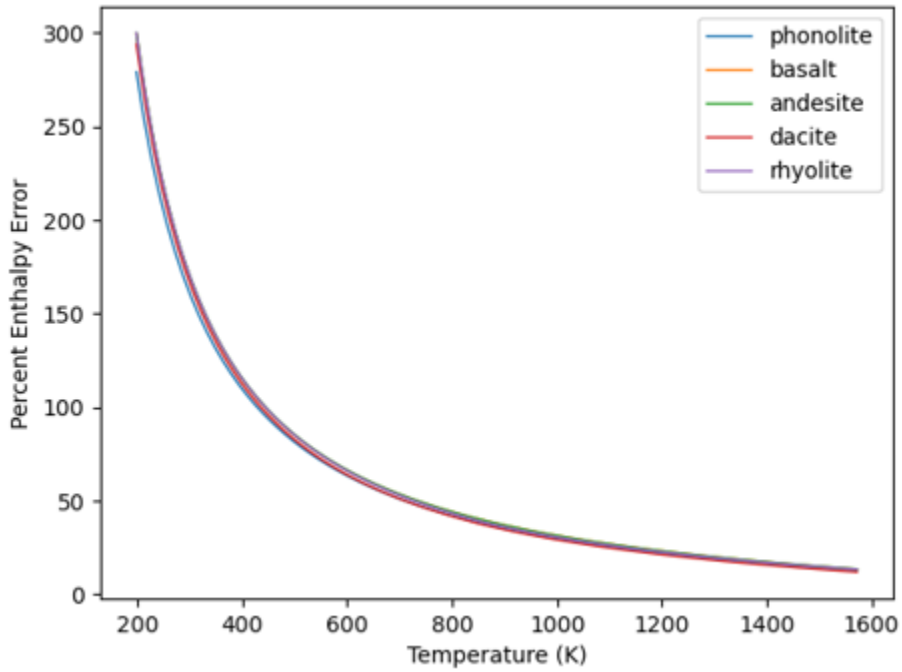


Figure 2. Percent error in total enthalpy for various volcanic ashes between temperature-dependent and temperature-independent specific heat with respect to temperature. Constant specific heat capacity is 1100 J/kgK.

Key Publications

- Fisher, M. A. and S. K. Nawotniak. NDa. "VolThermF: temperature-dependent specific heat capacity of pyroclastic rocks and volcanic gases," in progress.
- Fisher, M. A. and S. K. Nawotniak. NDb. "Thermodynamic effects on volcanic plume stability and rise height," in progress.

Sponsor/Program

IUC - The project is part of a dissertation for a Ph.D. in geoscience at Idaho State University.

[1]Oberhuber, J.M., M. Herzog, H.-F. Graf, and K. Schwanke. 1998. "Volcanic plume simulation on large scales." J. Volcanol. Geotherm. Res 87, 29–53.

Appendix C

ENERGY STORAGE

Table of Contents

C.1. Micro-Kinetic Model Identification and Uncertainty Reduction from Transient Kinetic Data

Report Participants

Adam C. Yonge,[1] Ross Kunz,[2] A.J. Medford,[1] Rebecca Fushimi[2]

1 Georgia Institute of Technology

2 Idaho National Laboratory

Scientific Achievement

A key difficulty to TAP analysis, and transient kinetic techniques in general, is the conversion of the large volume of experimental data to catalyst knowledge. For this reason, the Python program TAPsolver has been developed to improve the analysis of TAP experiments, using a combination of physical models (reaction-diffusion equation) and ML techniques (algorithmic differentiation and optimization) to robustly extract intrinsic kinetic parameters. This program utilizes algorithmic differentiation to perform PDE-constrained optimization, as well as to observe the sensitivity of kinetic parameters over time. Novel methods can easily be incorporated in the TAPsolver workflow, and the code's flexibility will allow other transient experiments to be analyzed. The second-order derivatives calculated through algorithmic differentiation have a similar level of accuracy to the first-order, allowing for confidence intervals to be constructed around the local minimum through Hessian-based analysis.

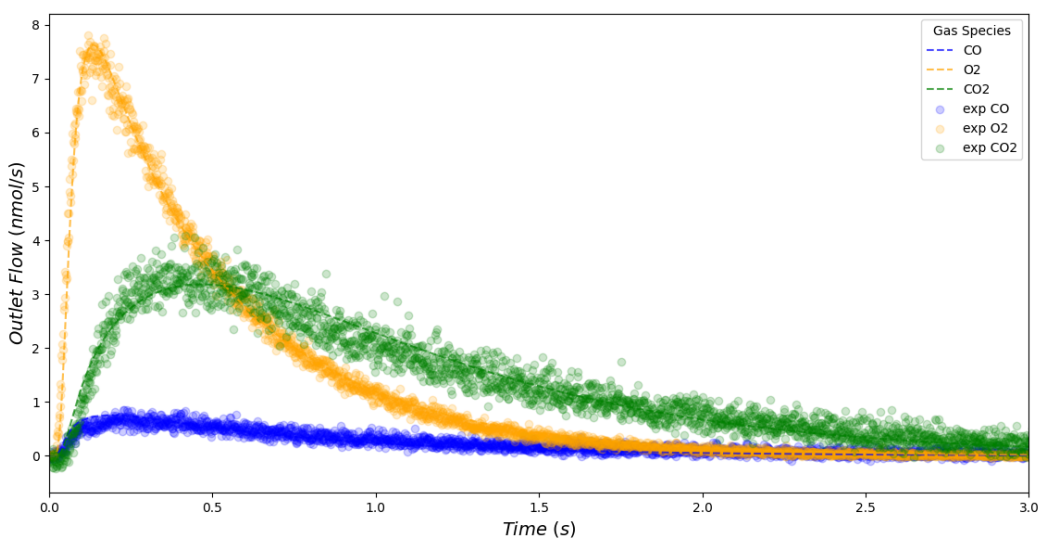


Figure 1. The results of a fitted Eley-Rideal reaction mechanism to experimental carbon monoxide oxidation data determined with TAPsolver.

Significance

Understanding the uncertainty around fitted kinetic parameters of micro-kinetic models can help guide the selection of additional experiments. TAP experiments have many adjustable initial conditions (including pulse time, intensity, surface composition, and temperature), which lead to many potential experiments. Taking an active learning approach for TAP experiments will help construct accurate and reliable top-down micro-kinetic models, leveraging the fast and information-dense nature of TAP experiments. Method development and general implementations could lead to broader accessibility and a stronger desire to use TAP experiments. Alongside the implementation of the active learning approach, the TAP experiments performed on the MnNa catalyst will aid in the identification of emergent properties found in variations of the catalyst composition.

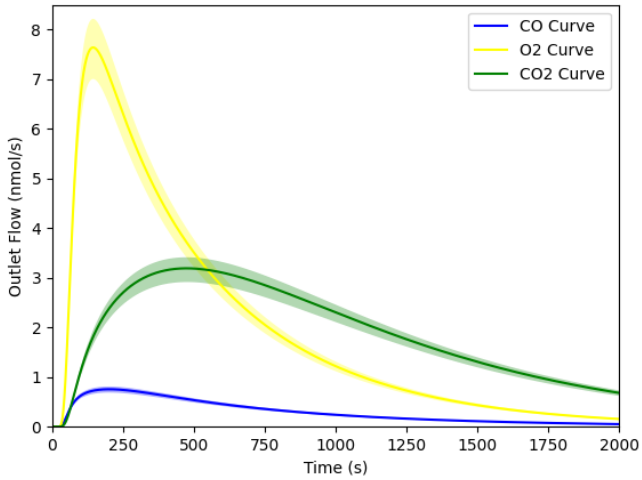


Figure 2. The propagation of pulse intensity and fitted kinetic parameter uncertainty in the forward mode.

Key Publications

- Yonge, A., M. R. Kunz, R. Batchu, Z. Fang, T. Issac, R. Fushimi, and A. J. Medford. "TAPsolver: A Python package for the simulation and analysis of TAP reactor experiments," submitted to Chemical Engineering journal.
- Kunz, M. R., A. Yonge, Z. Fang, D. Constales, R. Fushimi, and A.J. Medford. "Data Driven Reaction Mechanism Estimation via Transient Kinetics and Machine Learning," submitted to Chemical Engineering journal.

Sponsor/Program

EEST

Appendix D

OPERATIONS

Table of Contents

D.1. FPoliSolutions Risk-Informed System Engineering Method Within FPoli-AAP Platform Deployed on HPC

Report Participants

CesareFrepoli,[1] Jarrett Valeri,[1] Steve Heagy,[1] Chris Gosdin,[1] Mike Mankosa,[1] Tim Johnston[1]

1 FPoliSolutions, LLC

Scientific Achievement

FPoli Agile Application Platform (FPoli-AAP) is a digital infrastructure from which highly responsive digital solutions can be quickly deployed and customized. Specifically, for risk-informed solutions, the mission has been to develop and commercialize an integrated data/simulation management framework which will enable a rapid introduction of Risk-Informed System Analysis services for NPPs. The solutions target both the operating fleet, as well as advanced reactors under development. Within the FPoli-AAP Platform is RISE or risk-informed system engineering. The RISE service has been developed specifically to orchestrate the complexities associated with implementing a risk-informed design process in line with the proposed 10 CFR Part 53 rule as formulated in the NEI-18-04 roadmap. The objective of the new rule is to provide a generic licensing framework that is risk-informed and technology-neutral. However, its practical implementation is quite complex, and the definition of an economical and effective solution that satisfy the original intent of the LMP is non-trivial. This represents a gap, and RISE was architected to specifically close that gap. RISE is powered by the FPoli-AAP digital framework. The platform uses modern data management and simulation management tactics to orchestrate complex workflows with a generic powerful UI/UX. Several uses cases can be supported from test data management (FPoliDON), document management (FPoliDOX), and simulation management (FPoliSIM). RISE is the new service designed to automate and facilitate the workflow associated with NEI-18-04 and built within the same FPoli-AAP framework. FPoli-AAP is being deployed on the HPC for projects including INL Contract No. 254061 associated to SOW-18518.

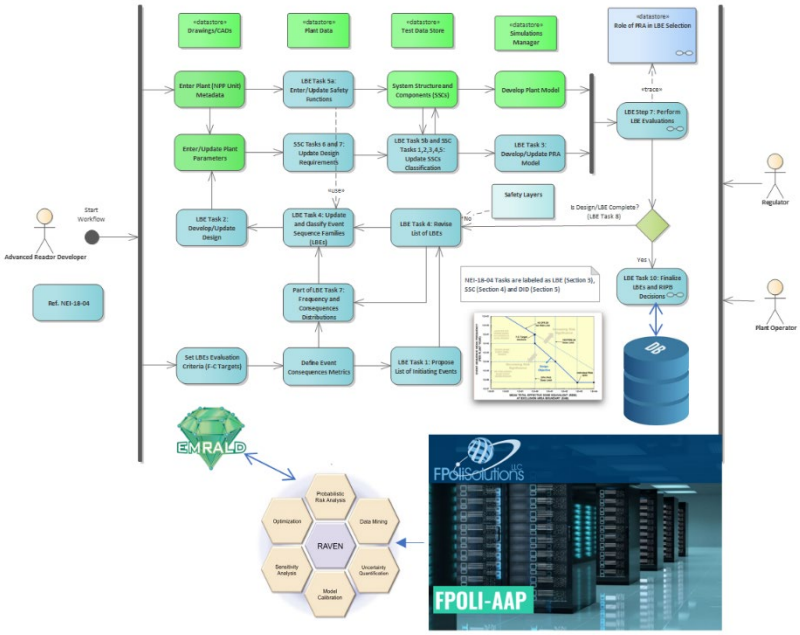


Figure 1. FPoli-AAP RISE platform: a digital solution to orchestrate complexities associated with the implementation of risk-informed design in response to NEI-18-04 (LMP).

Significance

The main goal of this project is to address specific concerns relative to the implementation of 10 CFR Part 53. FPoli will use its RISE service to orchestrate the engineering activities toward this goal. Examples of RISE usage include:

- Generate event trees
- Perform SSC classification
- Identify safety-basis events (deterministic assessment using event trees)
- Develop a practical evaluation methodology in line with the proposed 10 CFR Part 53 rule as formulated in the NEI-18-04 roadmap
- Determine defense-in-depth adequacy
- Implement enhanced automation of workflows for implementation of analysis methodology utilizing FPoli-AAP technology
- Populate selected data in FPoli-AAP platform to support digital documentation
- Post-process analysis results.

Key Publications

None.

Sponsor/Program

Industry

D.2. Smart Contingency Analysis Neural Network for In-Depth Power Grid Vulnerability Analyses

Report Participants

Sam Yang,[1] Bjorn Vaagensmith[2]

1 Florida State University

2 Idaho National Laboratory

Scientific Achievement

The second phase of our project entailed exploring various ways to enhance Smart Contingency Analysis Neural Network (SCANN), a deep-learning-based power grid contingency analysis tool developed under LDRD SEED grant. In particular, we leveraged the INL HPC Hoodoo GPUs to build and test a variety of neural networks, namely physics-informed neural networks, graph neural networks, and Bayesian neural networks. Based on this exploration, we proposed to revise the SCANN architecture as shown in Figure 1 under a new LDRD grant starting in October 2021. The revised architecture combines the existing deep neural network with a physics-informed graph neural network to solve nonlinear power flow equations, and it houses a Bayesian neural network in between for UQ.

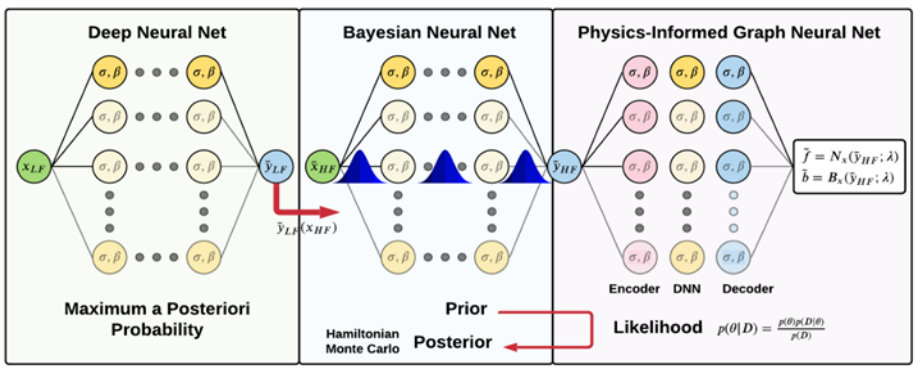


Figure 1. SCANN architecture proposed under the new LDRD grant.

Significance

The revised SCANN architecture shown in Figure 1 enables high-order grid contingency analyses with uncertainty, and this will be the first of its kind to the PIs' best knowledge. In addition to power flow data, we expect the new version of SCANN to provide insights into the effects of hybrid networks and their hyperparameters on the performance of power grid state predictions as well as challenges/limitations of our approach.

Key Publications

- Yang, S., B. Vaagensmith, and D. Patra. "SCANN: Smart Contingency Analysis Neural Network for In-Depth Power Grid Vulnerability Analyses," in preparation.

Sponsor/Program

LDRD

Appendix E

RENEWABLE ENERGRY

Table of Contents

E.1. Ab Initio Modeling of Molten Salts

Report Participants

Benjamin Beeler,[1,2] Ruchi Gakhar,[2] Gorakh Pawar,[2] Yuxiao Lin[2]

1 North Carolina State University

2 Idaho National Laboratory

Scientific Achievement

We calculated the density of the LiCl-KCl pseudo-binary molten-salt system over the entire range of compositions for a variety of temperatures in the liquid phase. In this project, ab initio molecular dynamics simulations (AIMD) were performed to establish equilibrated liquid structures, obtain the equilibrium volume, and determine the bulk modulus at each individual temperature and composition. This work provides a basis for a wide swath of thermophysical property investigation via AIMD into the LiCl-KCl molten-salt system.

Significance

Each unique molten-salt system possesses different properties and interactions and thus must be modeled uniquely. One such area for computational implementation that includes this individuality is in the selection of the van der Waals (vdW) dispersion interaction. Within the VASP, there are a number of modifications to the exchange correlation energy to account for dispersion; however, there are also individual vdW exchange correlation functionals. Both types of vdW inclusions have been previously utilized to study ionic liquids, but no standards have been developed specifically for molten salts or for the LiCl-KCl system. Establishing a given dispersion interaction was undertaken by calculating the equilibrium volume for the LiCl, LiCl-20KCl (mol percent), and KCl systems at 1100 K. Comparing a selection of the different vdW dispersion interactions is included in Figure 1.

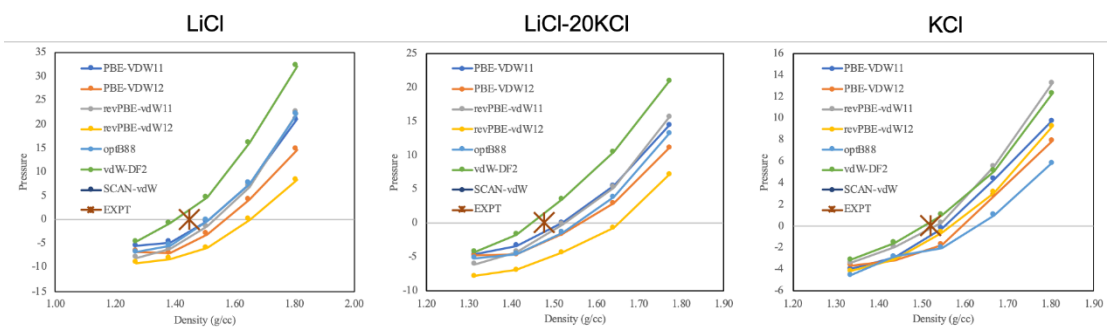


Figure 1. Comparison study of different van der Waals dispersion formulations within DFT for predicting density of the LiCl-KCl system.

This study pointed us towards the DF2 van der Waals functional, as this implementation most accurately predicted the general trends in density as a function of composition. Subsequently, the densities for the entire compositional and temperature phase space were calculated and are displayed in Figure 2. There is some noise within the data, but this is to be expected, as these are systems of approximately 200 atoms equilibrated over a period of a few picoseconds. However, this provides excellent qualitative aggreement with experimental densities, consistently and slightly underpredicting the density. The work can now serve as the basis to determine fundamental thermophysical properties of the LiCl-KCl system, such as heat capacity, themal conductivity, melting point, and viscosity.

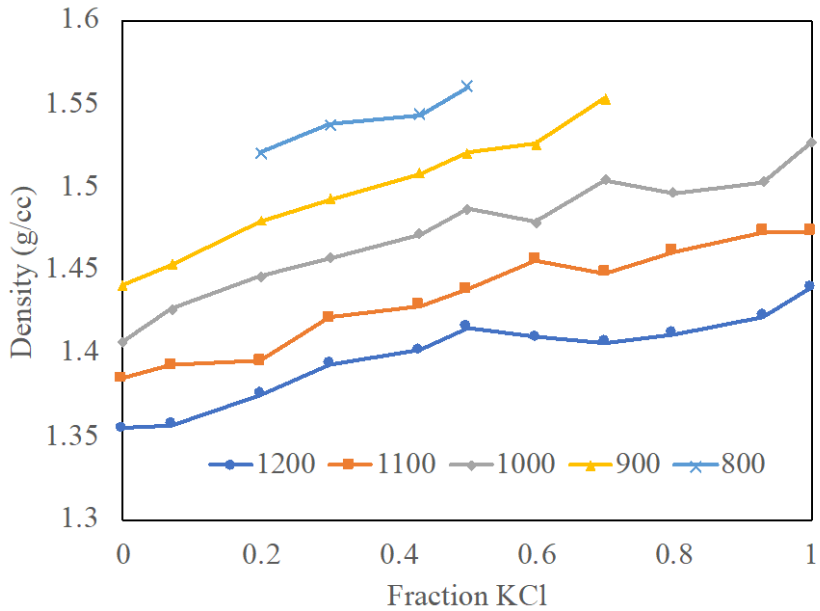


Figure 2. Density of LiCl-KCl as a function of composition and temperature.

This was the first study of its kind to systematically investigate the full scope of compositions and temperatures in the liquid phase for a molten salt.

Key Publications

Publications to be submitted.

Sponsor/Program

LDRD 20A44-041

E.2. ARPA-E High-Precision Construction Technical Support

Report Participants

Christopher J. Forsgren,[1] Donna M Delparte,[2] Christopher S. Ritter,[1] Kevin Han[3]

1 Idaho National Laboratory

2 I2IGeo LLC

1 North Carolina State University

Scientific Achievement

The objective of this work is to collect and provide drone data and technical support for digital engineering and digital twin techniques. These techniques will employ collecting drone flight data with the highest quality measurements available supporting the ARPA-E project.

Significance

Implementing a modern requirements management software tool during the development of the VTR engineering concept is anticipated to reduce the cost and schedule associated with coordinating engineering design and constructio of other VTR program activities.

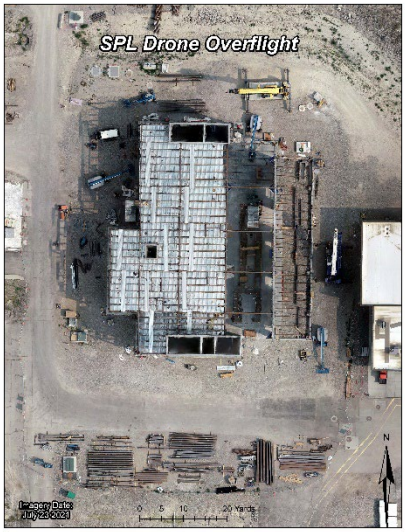


Figure 1. Drone imagery.

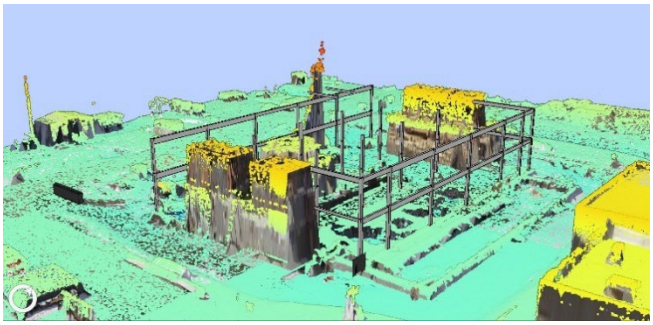


Figure 2. Data modeling.

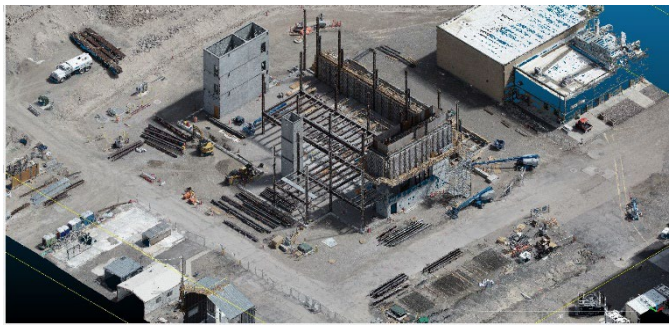


Figure 3. Point cloud with model.

Key Publications

- Forsgren, C. 2021. "Virtual Prototyping for Construction Management using Digital Engineering," Esri Annual Conference.

Sponsor/Program

Advanced Research Projects Agency-Energy (ARPA-E)

E.3. ARPA-E NAMAC Project

Report Participants

Askin Guler Yigitoglu,[1] Lee Taseseung[1]

1 Oak Ridge National Laboratory

2 Argonne National Laboratory

Scientific Achievement

I am under the resource team, which supports design team activities for the ARPA-E Development of a Nearly Autonomous Management and Control (NAMAC) System for Advanced Reactors, and my specific task is to support deployment of NAMAC Plant Simulator, NAMAC Digital Twin, and RAVEN (Risk Analysis Virtual Environment) on HPC resources and development of digital twin training database to be populated by GOTHIC simulations,.

Significance

GOTHIC input deck for EBR-II: Running of the GOTHIC simulation on Falcon Cluster for the Loss of Forced Flow scenario with the input data uncertainties (perturb by RAVEN) succeeded and 50K realizations are collected and formatted as namac_database in a shared folder to train the Digitial Twin.

Key Publications

- ARPA-E quarterly NAMAC reports are publishing by the project design team.
- Dinh, N. "Development of a Nearly Autonomous Management and Control (NAMAC) System for Advanced Reactors." https://arpa-e.energy.gov/sites/default/files/1320%20Dinh_approved.pdf.

Sponsor/Program

Frontier Observatory for Research in Geothermal Energy (FORGE)

E.4. Frontier Observatory for Research in Geothermal Energy

Report Participants

Branko Damjanac[1]

1 Itasca Consulting Group, Inc.

Scientific Achievement

Utah Frontier Observatory for Research in Geothermal Energy (FORGE) is a dedicated underground field laboratory sponsored by DOE for developing, testing, and accelerating breakthroughs in EGS technologies to advance the uptake of geothermal resources around the world. Itasca is a part of the research team. The main role of Itasca's team, in cooperation with University of Utah and INL, is to numerically simulate reservoir response to stimulation by fluid injection. The purpose of these simulations is to optimize development of the field and stimulation strategy. The numerical code, XSite, is used to simulate hydro-mechanical response of naturally fracture formation with explicit representation of pre-existing fractures during fluid injection.

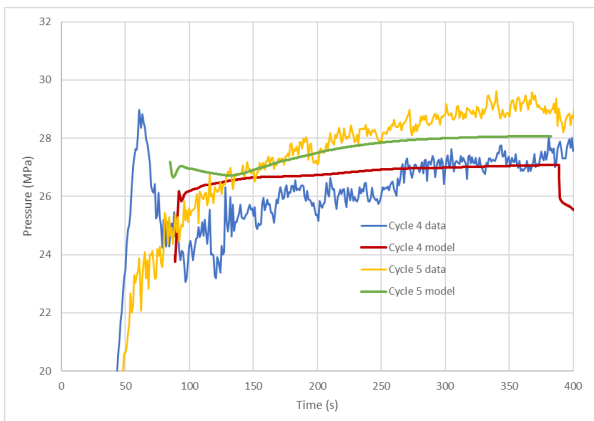


Figure 1. Cycles 4 and 5 of zone 2 in well 58-32: pressure (surface pressure) history matching during injection.

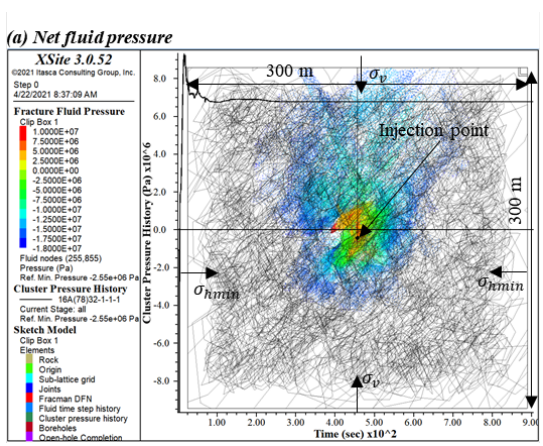


Figure 2. Simulation results of Case 1 with DFN1, 20 bpm for 15 minutes, no dilation of DFN.

Significance

The initial modeling was carried out to validate/calibrate model by matching injection pressure history during the injection tests in one of the exploratory boreholes. Subsequently, the model is used to investigate sensitivity of the stimulation effects to uncertainties in the model parameters and to different operational parameters like injection rate and fluid viscosity. The model results will be used to aid the decision in selecting the optimum reservoir stimulation strategy.

Key Publications

- Xing, P., B. Damjanac, Z. Radakovic-Guzina, A. Finnila, R. Podgorney, J. Moore, and J. McLennan. 2021. "Numerical Simulation of Hydraulic Fracturing Stimulation of the Enhanced Geothermal System Well at Utah FORGE Site," Proceedings of the 55th U.S. Rock Mechanics/Geomechanics Symposium, Houston, Texas, June 20–23, 2021, ARMA 21-1168.

Sponsor/Program

Frontier Observatory for Research in Geothermal Energy (FORGE)

E.5. Frontier Observatory for Research in Geothermal Energy

Report Participants

Aleksandr Goncharov,[1] John McLennan[1]

1 University of Utah

Scientific Achievement

We developed the enhanced geothermal system with potential prospective of successful commercial use. We used the software, XSite by Itasca Consulting Group, Inc., and performed 3-D modeling of the perforated section of the well.

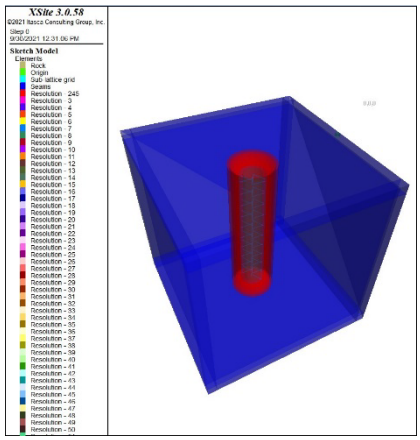


Figure 1. First version of the model.

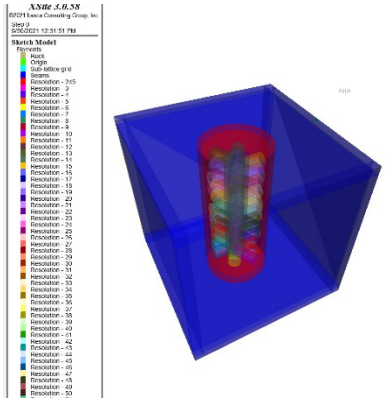


Figure 2. Second version of the model. It underwent several modifications: adding/replacing resolutions, addressing convergence and instability issues.

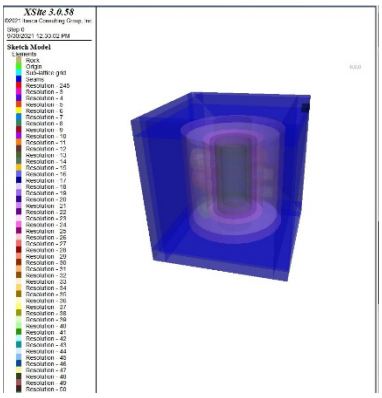


Figure 3. Third version of the model. Revised and rebuilt. The case for it is being run on HPC.

Significance

The main purpose of using INL's HPC Center was to provide the resources to build a model that could represent the near-wellbore region of the 10 ft perforated section of the Well 58-32. Numerical results obtained from running the model will assist in shaping the stimulation program and reaching the necessary level of connectivity between the injection and the production wells.

Key Publications

- A literature review paper, which will review the studies and findings related to near-wellbore effects, is currently in progress. Organizing and summarizing the work that has been done to date will help clearly identify the gaps in understanding these phenomena in the context of EGS.
- It is expected to receive conclusive results within the next several weeks. As soon as results are acquired, it is planned to discuss with the members of the Modeling and Simulation Team how these results could affect the stimulation program. After the discussion, it is planned to submit an abstract for the ARMA 2022 56th U.S. Rock Mechanics/Geomechanics Symposium. The paper is expected to cover the simulation results and their interpretation.

Sponsor/Program

Frontier Observatory for Research in Geothermal Energy (FORGE)

E.6. Historical-Dependent Contact Models for Discrete Element Modeling of Deformable Biomass Particles

Report Participants

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Scientific Achievement

In this project, we have proposed a set of hysteretic nonlinear contact models for approximating the bulk strain-hardening phenomena of granular biomass in handling and storage conditions. The resultant DEM model is implemented in LIGGGHTS-INL, a capability-extended adaptation of the LIGGGHTS package, and applied in parametric simulation studies of an axial compressibility test for milled pine chips. All the simulations were conducted using LIGGGHTS-INL on INL's Sawtooth HPC cluster. The total case number of DEM simulations for each type of model is 146705. A compute node with two Intel Xeon 8268 CPUs (24 cores per CPU, 2.90 GHz, 192 GB of RAM, and Mellanox Infiniband EDR) was assigned for each individual DEM simulation case.

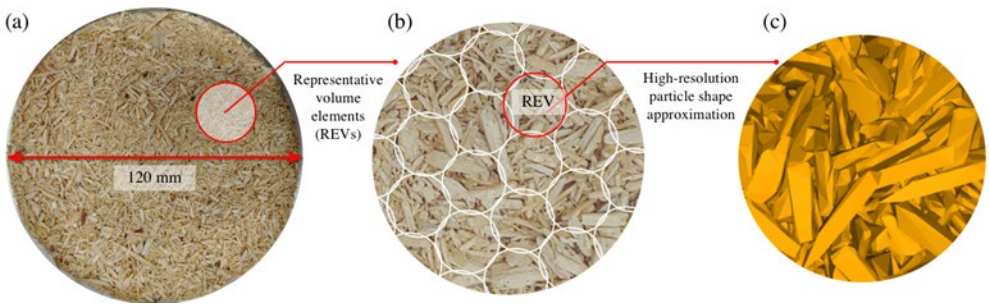

Figure 1. The illustration of representative elementary volume.

Significance

This work has introduced a monosphere DEM model that can be used to elucidate the bulk mechanical behavior of granular biomass. These contact models comprise of simple polynomial and/or exponential functions to allow for easy calibration. Though more sophisticated formulations are possible, the proposed contact models have shown reasonable accuracy for the tested biomass. The observations from our numerical simulations suggest that the proposed model is capable of capturing the bulk stress-strain behavior, especially the strain-hardening modulus, of the LALM pine chips subjected to a wide range of compressive stresses.

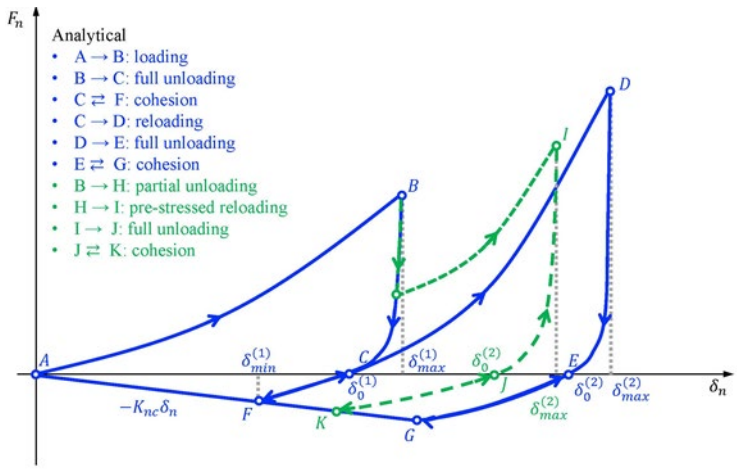

Figure 2. Schematic of a hysteretic nonlinear normal contact force-displacement model.

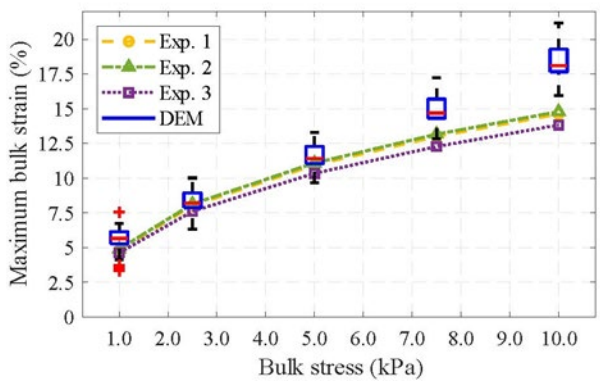

Figure 3. Comparison between the experimental data and the DEM type-II model results.

Key Publications

- Chen, F., Y. Xia, J. L. Klinger, and Q. Chen. "A set of hysteretic nonlinear contact models for DEM: theory, formulation, and application for lignocellulosic biomass," submitted to *Powder Technology*.
- Chen, F., Y. Xia, and Q. Chen. 2020. "Historical-dependent Contact Model for Discrete Element Modeling of Deformable Biomass Particles," ASABE 2021, virtual.
- Chen, F., Y. Xia, Q. Chen, and Y. Guo. 2020. "A Hysteretic Nonlinear Elastoplastic Contact Model for Discrete Element Modeling of Milled Woody Biomass," AICHE 2020, San Francisco, CA, November 16–20, 2020.

Sponsor/Program

The research is fully supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), Bioenergy Technologies Office, the Feedstock-Conversion Interface Consortium, under DOE Idaho Operations Office with Contract No. DE-AC07-05ID14517. The research used resources in the HPC Center at INL, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the NSUF under Contract No. DE-AC07-05ID14517.

E.7. Integrated Energy System Reliability Framework

Report Participants

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Scientific Achievement

Integrated Energy Systems (IESs) project is a multi-laboratory project. IES project design team develop system analysis codes and integrates in the INL GitLab Hybrid repo (https://hpcgitlab.hpc.inl.gov/hybrid) to optimize design configurations. The reliability modeling framework of IES developed at ORNL which builds of relevant probabilistic models, statistical inference of the developed models, validation of the fitted models using statistical criteria such as goodness-of-fit tests, estimating components and systems failure rates, and optimized maintenance intervals.

Significance

Reliability framework feedbacks the reliability related cost (e.g., optimum replacement interval) to the cashflow and optimization module of RAVEN(/HERON) over the reactor operational life (~60 years) for selected components and systems.

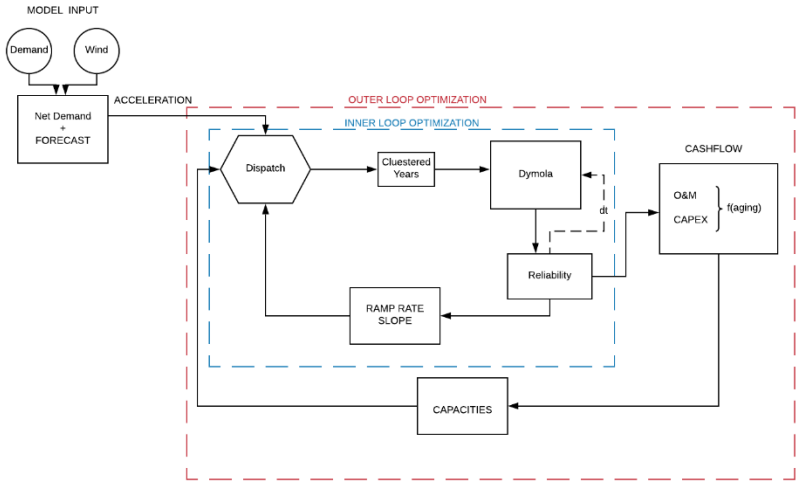

Figure 1. An overview of the interface architecture for model interactions.

Key Publications

"Dynamic Reliability Analysis Framework," Integrated Energy Systems, in progress.

Sponsor/Program

DOE, CTD-IES (cross-cutting technology development - integrated energy system)

E.8. Simulation of Stimulation at FORGE Site

Report Participants

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Scientific Achievement

A highly deviated injection well, 16A(78)-32, was drilled to a total depth of 10,987 ft at the FORGE site near Milford, Utah. The lateral tangent was maintained at 65° to the vertical. A series of injection testing was conducted in a 200 ft openhole section at the toe of this well. After a brief hiatus, stimulation by fluid injection will be carried out with three stages near the toe. Numerical modeling should be an essential tool for design and optimization of stimulation strategies that would connect the injection and production wells. These simulations use a lattice-based code, XSiteTM, which simulates fully coupled hydro-mechanical processes with explicit representation of a discrete fracture network (DFN).

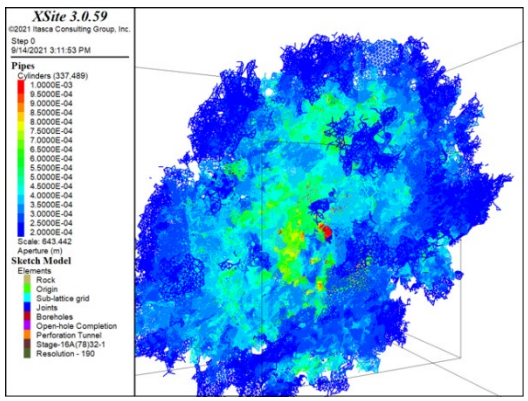

Figure 1. Stimulated fracture aperture.

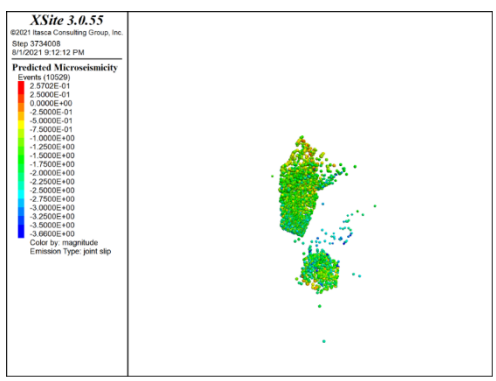

Figure 2. Microseismicity.

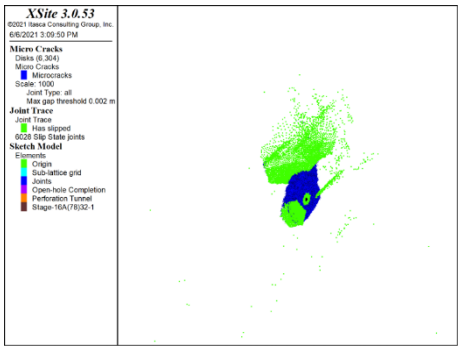

Figure 3. Slipped natural fractures.

Significance

- Numerical model is calibrated by pressure history matching with the injection tests
- Hydraulic fracture and hydro-shearing generally propagate upward from the stimulation well
- Greatest uncertainty associated with DFN in situ strength and permeability
- For permeable and only frictional DFN, stimulation with water (or slickwater) at rates 20–40 bpm will create continuous flow path of more than 150 m above the injection well even after 30 minutes of injection
- For impermeable and strong DFN, there is almost no stimulation of DFN
- For impermeable and strong DFN, stimulation with water (or slickwater) at rates 20–40 bpm will create hydraulic fracture with height greater than 70 m above the injection well even after 15 minutes of injection
- Greater viscosity fluids and injection rates appear to be more efficient in propagating hydraulic fractures and inducing hydro-shearing.

Key Publications

- Xing, P., B. Damjanac, Z. Radakovic-Guzina, A. Finnila, R. Podgorney, J. Moore, and J. McLennan. 2021. "Numerical Simulation of Hydraulic Fracturing Stimulation Enhanced Geothermal System Well at Utah Forge Site," Presented at the 55th U.S. Rock Mechanics/Geomechanics Symposium.
- Xing, P., B. Damjanac, Z. Radakovic-Guzina., A. Finnila, R. Podgorney, J. Moore, and J. McLennan. 2021. "Numerical Simulation of Injection Tests at Utah FORGE Site," Presented at the 46th Stanford Geothermal Workshop.

Sponsor/Program

FORGE

E.9. Understanding the Effects of Surface Chemistry on Electron Transport and Electrolyte Transport in MXenes

Report Participants

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Scientific Achievement

While there are some experimental studies on electrical conductivity of MXene, theoretical works are few. The density functional tight binding (DFTB) approach enables treatment of complex systems with several hundred to thousands of atoms at the quantum level. DFTB calculations with the nonequilibrium Green's functions (NEGF) technique were used to calculate in-plane transport in the MXenes (i.e., within the MXene layers) as a function of composition. All MXene compositions were found to show a linear relationship between current and voltage (Figure 1) at lower potentials, indicating their metallic character. However, their IV curves (i.e., conductivity) show different trends among different compositions. MXenes without any surface terminations (Ti3C2) show higher conductivity compared to MXenes with surface functionalization (Ti3C2O2 and Ti3C2(OH)2). Among MXenes with O and OH termination, MXenes with O surface termination have lower conductivity than OH surface termination. Conductivity changes with the ratio of O and OH on the MXene surface. IV curves and their conductivities correlate with their transmission and the electronic DOS around the Fermi level.

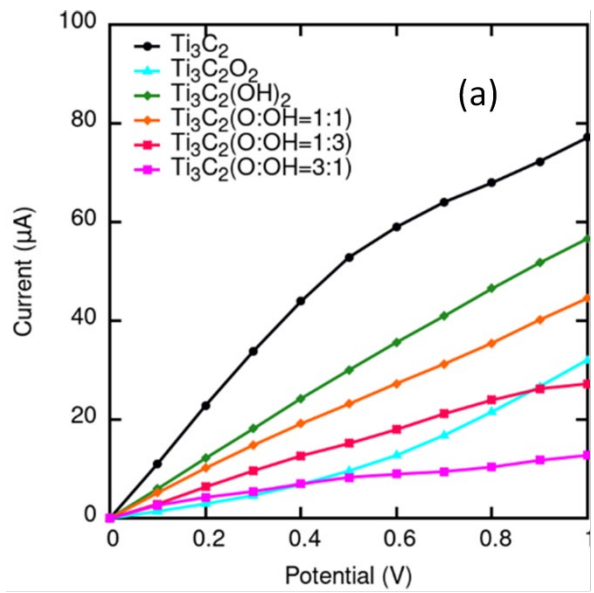

Figure 1. DFTB calculated IV curves for various MXene compositions.

Significance

MXenes are a rapidly developing class of two-dimensional materials with suitable properties for use in emerging electrochemical energy storage devices, including batteries and supercapacitors. The chemical synthesis of MXene leads to the surfaces being functionalized with different functional groups (O, OH, and F). Since MXene layers are only atomically thin, such surface functionalities can play an essential role in the electrical conductivity of MXene. Conductivity is a key for both the transport and storage of ions in MXene during their energy applications. The surface composition-dependent conductivity of the MXenes provides a path to tune their conductivity for enhanced pseudocapacitive performance.

We are also in the process of simulating effect of correlated motion in electrolytes (bulk and nanoconfinement) with various cations and effect of nuclear quantum dynamics on water Van Hove Correlation Function. In the study, we will use the molecular dynamics simulation (MD) based on DFTB as well as ab initio MD will be used as needed to understand the effect.

Key Publications

- Khanal, R. and S. Irle. 2021 "Effect of Surface Functional Groups on MXene Conductivity," 2021 MRS Fall Meeting, Boston, MA.

Sponsor/Program

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