

Laboratory Directed Research and Development

# SNAPSHOT FISCAL YEAR 2016

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Research Project Highlights  
Awards and Recognition  
Collaborations  
Doctoral Research

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# From the Director



**Mark Peters**

*Director, Idaho National Laboratory*

*Congress designated Idaho National Laboratory the nation's lead facility for nuclear energy research and development in 2005. In addition to our leadership in the core nuclear energy mission, INL has also become a world leader in national security and protecting critical infrastructure from manmade and natural threats.*

*Laboratory Directed Research and Development (LDRD) plays a vital role in helping INL fulfill its nuclear energy, broader clean energy and national security missions. LDRD investments in scientific and engineering staff, postdocs, students and collaborations enable new science, technology and engineering capabilities. In collaboration with our university, industry and other national laboratory partners, LDRD investments grow our scientific foundation and accelerate innovation and the development of solutions to energy and security challenges faced by the nation and globe.*

*INL's research and development (R&D) helps extend the lives of a nuclear reactor fleet that provides 19 percent of the nation's electricity and 63 percent of its carbon-free electricity. It allows us to improve the performance of nuclear fuel. It creates the next-generation of nuclear reactors and solves the challenges of used nuclear fuel management.*

*Our R&D allows us to better understand how to produce the clean energy needed to power our future.*

*Finally, our R&D helps us ensure global, national and homeland security by teaching us how to make critical infrastructure – from power grids to water and transportation systems – more resilient to cyberattacks.*

*This report, "Snapshot – Fiscal Year 2016 Laboratory Directed Research and Development," highlights projects that help develop future energy systems, make the world cleaner and safer, and protect our citizens and soldiers.*

*Inside you will read about cutting-edge R&D that builds INL's core capabilities, aligns with INL's strategic plan, and benefits the Department of Energy (DOE), as well as an expansive sponsor base consistent with DOE and INL missions. The R&D creates opportunities for our staff, attracts promising young scientists and engineers, and helps educate the next generation. Many LDRD projects support undergraduate and graduate students, and enhance our university and industry collaborations.*

*LDRD projects are selected on a competitive basis through rigorous peer review and management processes, and these projects build a creative environment grounded in scientific and technical excellence.*

*Over the years, science and innovation resulting from LDRD projects have benefited INL in a variety of ways: new research programs; recognition through awards, publications and patented inventions; stronger scientific and engineering talent; and new tools, instruments and capabilities. The LDRD Program is a key component of INL's ability to fulfill its nuclear energy, broader clean energy, and national security missions and serve the American people.*

*Please take a few moments to read this report and learn more about the important work being done every day at Idaho's national laboratory.*

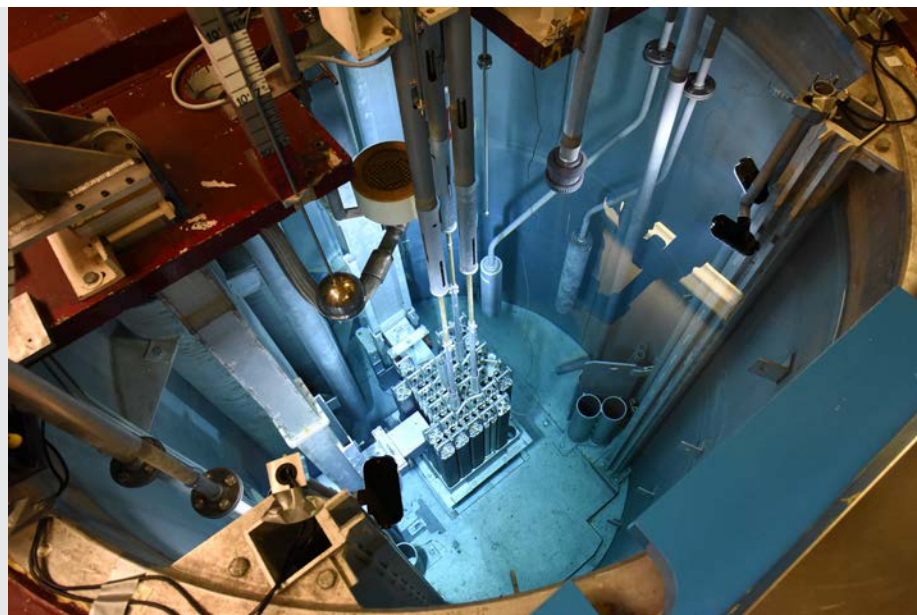
A handwritten signature in black ink that reads "Mark Peters". The signature is fluid and cursive, written in a professional style.

# Laboratory Directed Research and Development **SNAPSHOT – FISCAL YEAR 2016**



## **On the Cover**

The Neutron Radiography Reactor, located in the Hot Fuel Examination Facility at INEL's Materials and Fuels Complex.



Prepared by Idaho National Laboratory,  
Idaho Falls, Idaho 83415.

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# Introduction

## INTRODUCTION

Laboratory Directed Research and Development (LDRD) is a small but vital U.S. Department of Energy (DOE) program. Each year, the program selects a limited number of proposed research and development (R&D) projects that help Idaho National Laboratory (INL) maintain its scientific and technical vitality, enhance its ability to fulfill DOE missions, foster creativity, stimulate exploration in science and technology, serve as a proving ground for research, and support high-risk, high-value R&D. Through LDRD, INL is able to improve its distinctive capability and

enhance its ability to conduct cutting-edge R&D for its DOE and Strategic Partnership Program sponsors.

This report provides highlights from LDRD projects that were performed at INL in Fiscal Year (FY) 2016. Projects like those featured on these pages prove the value of the LDRD Program each year as they lead to new programs, intellectual property, patents, copyrights, national and international awards, and publications. The program also feeds the science and technology pipeline with scientists and engineers through undergraduate and graduate internships,

postdoc assignments, and collaborations with universities and industry across the nation.

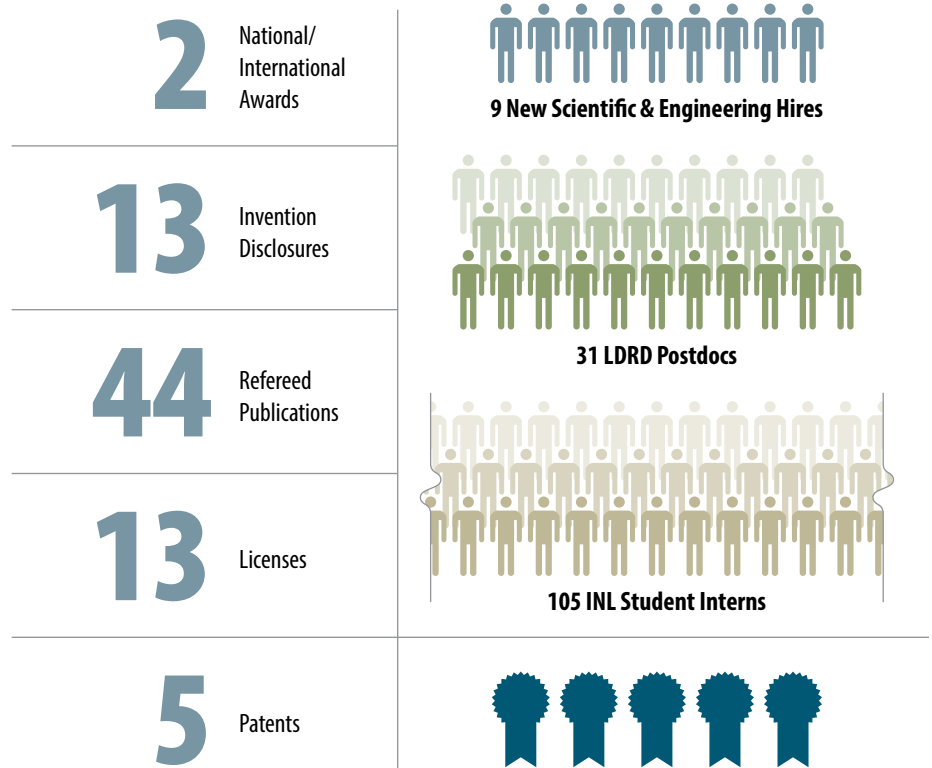
This report is a “snapshot” of research highlights that exemplify the diversity of scientific and engineering research conducted at INL, awards and recognition resulting from LDRD funding, and collaborations using LDRD funding.

Additional details about the LDRD Program can be found in a supplement to this publication entitled the *Laboratory Directed Research and Development 2016 Annual Summary Report*.<sup>\*</sup> It contains summaries of

## BENEFITS OF LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

INL consistently realizes significant benefits from the LDRD Program. The FY 2016 metrics are shown at right.

*INL's diverse LDRD portfolio explores scientific and engineering concepts to support DOE's Office of Nuclear Energy, the broader DOE, and this nation's research, development, demonstrations, and deployment of nuclear energy, clean energy, and security.*



# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

all 71 LDRD projects funded in FY 2016, including a general description of each project, a summary of the scientific or technical progress achieved during the life of each project, a brief statement describing how each project benefited the DOE and National Nuclear Security Administration missions, and relevant invention disclosures and peer-reviewed publications and presentations that resulted from the projects. The LDRD 2016 annual report also includes multiple appendices listing benefiting agencies, publications, patents, collaborations, postdocs, and interns supported by the LDRD projects.

## THE LDRD PROCESS AT IDAHO NATIONAL LABORATORY

Each year, projects are selected for inclusion in the LDRD Program through a proposal review and selection process. To select the best and most strategic of the ideas submitted, INL's associate laboratory directors responsible for various mission areas establish committees

for the focus area and for the transformational funds. These committees then review new proposals and ongoing projects. The committees are staffed by senior research and technical managers who are subject matter experts and have no conflict of interest regarding the proposed projects.

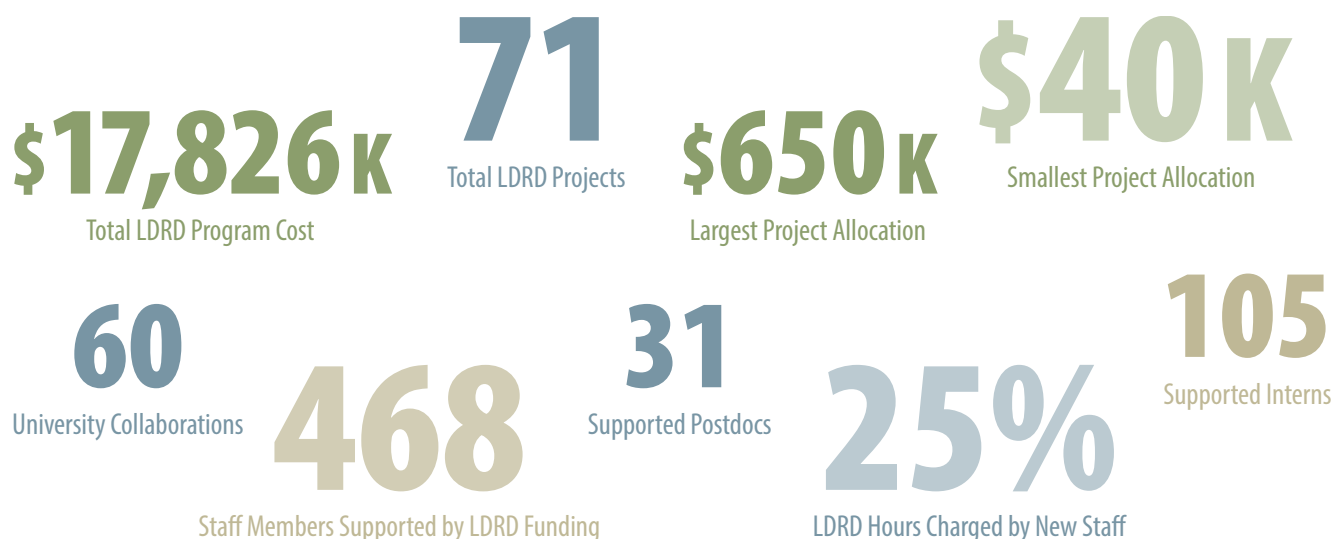
Proposals for project funding for the Strategic Initiatives R&D Fund, the Transformational R&D Fund, and the University Partnership Fund undergo two rounds of review. In the first round, the committees evaluate short preliminary proposals and select the most promising for development into full proposals. In the second round, the committees review the full proposals, as well as ongoing projects that are requesting second- or third-year funding. After the reviews are completed, the committees provide funding recommendations to the associate laboratory directors. They, in turn, present

the recommendations along with their input to INL's deputy director for Science and Technology, who develops an overall funding strategy and provides approvals for the investments. All projects selected for funding must also receive concurrence from the DOE Idaho Operations Office.

## PROJECT HIGHLIGHTS

This report summarizes 28 of the 71 LDRD projects that were conducted at INL in FY 2016. These projects represent the creativity and innovation that help the LDRD Program advance nuclear energy, enable clean energy, and secure and modernize critical infrastructure. Information about all of the year's LDRD projects is provided in the *Laboratory Directed Research and Development 2016 Annual Summary Report*.\*

\* Available online at [www.inl.gov/LDRDINL](http://www.inl.gov/LDRDINL).



# LDPRD Project Highlights

## Advancing Nuclear Energy

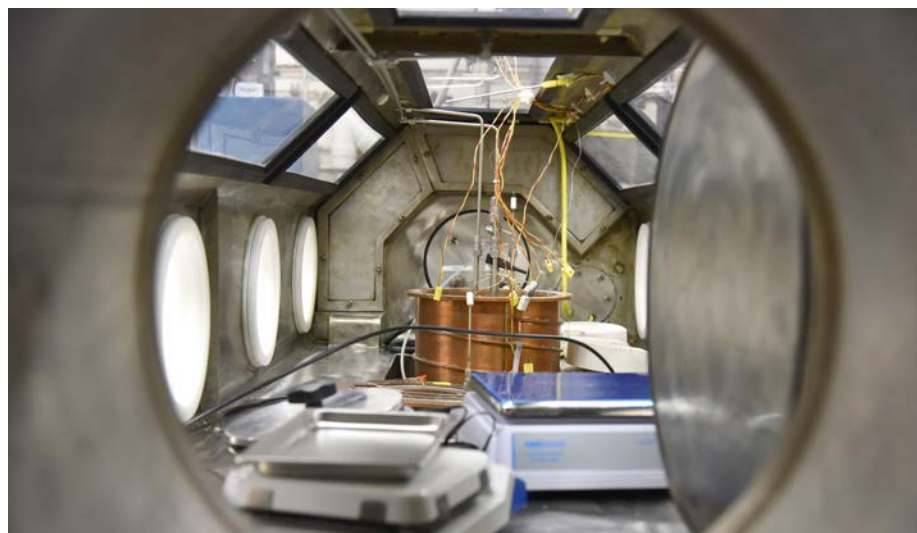
### SMALL MODULAR REACTOR

**Development of an INL Capability for High-Temperature Flow, Heat Transfer, and Thermal Energy Storage with Applications in Advanced Small Modular Reactors, High-Temperature Heat Exchangers, Hybrid Energy Systems, and Dynamic Grid Energy Storage Concepts (Project 14-009)**

James E. O'Brien,<sup>1</sup> Piyush Sabharwal,<sup>1</sup> and Su Jong Yoon<sup>1</sup>

#### SCIENTIFIC ACHIEVEMENT

A conceptual design was developed for a high-temperature, multifluid, multiloop test facility to support heat-transfer, flow, materials, and thermal-energy-storage research for nuclear and nuclear-hybrid applications. These heat-transport systems will require advanced high-temperature materials and working fluids such as molten salts. Molten salts have excellent high-temperature heat-transfer and chemical-stability characteristics. In its initial configuration, this facility will include a high-temperature helium loop, a liquid salt intermediate heat-transport loop, and a hot water/steam loop. The three loops will be thermally coupled through an intermediate heat exchanger and a secondary heat exchanger. Research includes the characterization and performance evaluation of candidate compact heat exchangers such as printed circuit heat exchangers (PCHEs) at prototypical operating conditions, resolution of flow and heat-transfer issues related to core thermal hydraulics in advanced helium- and salt-cooled reactors, and evaluation of corrosion behavior in new cladding materials and accident-tolerant fuels for light-water reactors at prototypical conditions. The research will also include detailed computational fluid dynamic evaluation of the heat-transfer and pressure-drop performance of PCHEs, including parametric studies to determine the effects of various geometric flow configurations available with PCHEs. Finally, a new experimental laboratory for small-scale



*INL conducts research in high-temperature flow, heat transfer, and thermal energy storage.*

preparation and purification of fluoride salt mixtures is being developed. The new laboratory facility has been named the Advanced Reactor Technology Integral System Test (ARTIST) facility.

#### SIGNIFICANCE

This project has laid the foundation for development of a new thermal-hydraulic experimental capability at INL. The high-pressure water loop will operate at pressurized-water reactor conditions to support research related to fuel cladding corrosion, accident-tolerant fuels, natural circulation studies, and hybrid energy systems. The small-scale molten salt preparation and purification facility will support development of the molten salt flow loop of the ARTIST facility, as well as basic

thermophysical property measurements and corrosion studies. The project supported a postdoc fellow who was later hired as a full-time INL employee. The project also supported three master's degree students and one Ph.D. student from The Ohio State University.

#### KEY PUBLICATIONS

- Sabharwal, P., J. O'Brien, S. J. Yoon, and X. Sun, 2015, "Experimental Facility for Development of High-Temperature Reactor Technology: Instrumentation Needs and Challenges," *European Physical Journal of Nuclear Science and Technology*, Vol. 1, No. 14, December 2015.

<sup>1</sup> Idaho National Laboratory

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## MODELING AND SIMULATION

### **Use of Linear Variable Differential Transformer (LVDT)-Based Methods to Detect Real-Time Geometry Changes during Irradiation Testing (LDRD 14-010)**

Kurt Davis,<sup>1</sup> Richard Skifton,<sup>1</sup> John Crepeau,<sup>2</sup> and Steinar Solstad<sup>3</sup>

#### SCIENTIFIC ACHIEVEMENT

New materials are always being considered for fuel, cladding, and structures in advanced and existing nuclear reactors. Such materials can undergo various dimensional changes during irradiation. Currently, in the United States, such changes are measured by the “cook and look” method (i.e., repeatedly irradiating a specimen for a specified period of time and then removing it from the reactor for evaluation). This approach is expensive because of the time and labor needed to remove irradiated samples from the reactor, examine them and return them to the reactor for each measurement. In addition, such techniques provide limited data, and handling may disturb the phenomena of interest. In-pile detection of changes in geometry will help overcome the constraints described above and will help us understand, in real-time, behavior during irradiation testing of fuels and materials in high-flux U.S. material and test reactors.

A linear variable differential transformer was modified and used to measure a simulated fuel rod with calibrated known dimensions to within  $\pm 3 \mu\text{m}$  of the calibrated diameter and within  $\pm 90 \mu\text{m}$  of the location of the diameter measurement. Under the design parameter that the pressure in the reactor’s test loop drive the sample/fuel rod, an innovative hydraulic piston

was designed to keep a seal on the loop fluid medium while still permitting axial motion of the apparatus.

#### SIGNIFICANCE

This LDRD provides benchmark studies on the way to real-time monitoring of dimensional changes in fuels (i.e., radially and axially) during irradiation testing in material test reactors — a capability that does not currently exist at such reactors in the United States. This LDRD also supports opportunities for the DOE Office of Naval Reactors (e.g., the Advanced Test Reactor); the DOE Office of Nuclear Energy (e.g., Nuclear Sciences User Facilities, Next Generation Nuclear Plant, Fuel Cycle Research and Development, Nuclear Energy Enabling Technology and Light Water Reactor Sustainability); and industry (e.g., Electric Power Research Institute, Westinghouse and General Electric). Additionally, this project provides research support for a Ph.D. candidate involved in work being done at INL’s High-Temperature Test Laboratory.

#### KEY PUBLICATIONS

- **Davis, K., D. L. Knudson, J. C. Crepeau, and S. Solstad**, 2015, “Measurement of Diameter Changes during Irradiation Testing,” *9th International Topical Meeting on Nuclear Plant Instrumentation, Control, and Human Machine Interface Technologies (NPIC&HMIT)*, Paper #12432.

- **Davis, K. L., D. L. Knudson, J. L. Rempe, J. C. Crepeau, and S. Solstad**, 2015, “Design and Laboratory Evaluation of Future Elongation and Diameter Measurements at the Advanced Test Reactor,” *Nuclear Technology*, Vol. 191, No. 1.
- **Rempe, J., D. Knudson, J. Daw, T. Unruh, B. Chase, K. Davis, R. Schley, J. Palmer, C. White, and K. Condie**, 2014, *Status Report on Efforts to Enhance Instrumentation to Support Advanced Test Reactor Irradiations*, INL/EXT-13-30427, Idaho National Laboratory.
- **Rempe, J. L., D. L. Knudson, J. E. Daw, T. C. Unruh, B. M. Chase, K. L. Davis, A. J. Palmer, and R. S. Schley**, 2014, “Advanced In-Pile Instrumentation for Materials Testing Reactors,” *IEEE Transactions on Nuclear Science*, Vol. 61, No. 4, pp. 1984–1994.

#### INVENTION DISCLOSURES

- It is anticipated that an invention disclosure request that was submitted from the work performed in this LDRD will be accepted.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> University of Idaho

<sup>3</sup> Halden Reactor Project, Institute for Energy Technology, Norway

# LDRD Project Highlights

## Advancing Nuclear Energy

### MODELING AND SIMULATION

#### **Multidimensional Multiphysics Modeling of Fuel Behavior During Accident Conditions (Project 14-031)**

Richard Williamson,<sup>1</sup> Giovanni Pastore,<sup>1</sup> Jason Hales,<sup>1</sup> Stephen Novascone,<sup>1</sup> and Wen Jiang<sup>1</sup>

#### **SCIENTIFIC ACHIEVEMENT**

Developing computational tools for reliably predicting thermo-mechanical behavior and the lifetime of nuclear fuel rods during abnormal reactor events is essential from both a safety and an economic standpoint. Fuel performance codes able to cope with accident analysis are needed for safety assessments and design purposes, as well as for development of accident-tolerant fuel concepts. This project achieved significant advances relative to state-of-the-art accident fuel analysis, building on INL's multi-dimensional, multi-physics, fully coupled fuel performance code, BISON. The outcome is a tool that is able to model integral fuel rod behavior during normal reactor operation and accident conditions beyond the limitations of traditional analysis and with improved accuracy. BISON was expanded with capabilities to reproduce all main phenomena involved in light-water reactor fuel during loss-of-coolant-accident (LOCA) conditions. Significant validation of the expanded BISON code was performed to both separate effects cladding tests and integral LOCA experiments. Results demonstrate good accuracy of BISON predictions.

#### **SIGNIFICANCE**

This project directly benefits the mission of the DOE Office of Nuclear Energy by addressing one of today's most critical nuclear energy concerns — design-basis accidents. Following the Fukushima

accident, and given the experimental evidence from programs such as the Halden Reactor Project, understanding LOCAs and reducing their likelihood are key concerns. This work advances the state of the art of fuel modeling by providing the ability to explore accident behavior in a novel and improved way. This LDRD project represents a strong addition to current nuclear fuel modeling efforts at INL and further demonstrates INL's developing excellence in modeling and simulation science. The project resulted in the hiring of a highly talented postdoc and supported multiple Ph.D. student interns. The project also led to the establishment of key international collaborations.

#### **KEY PUBLICATIONS**

- **Barani, T., E. Bruschi, D. Pizzocri, G. Pastore, P. Van Uffelen, R. L. Williamson, and L. Luzzi**, 2016, "Analysis of Transient Fission Gas Behaviour in Oxide Fuel Using BISON and TRANSURANUS," *Journal of Nuclear Materials*, in press.
- **Pastore, G., D. Pizzocri, J. D. Hales, S. R. Novascone, D. M. Perez, B. W. Spencer, R. L. Williamson, P. Van Uffelen (ITU), and L. Luzzi (POLIMI)**, 2014, "Modelling of Transient Fission Gas Behaviour in Oxide Fuel and Application to the BISON Code," *Proceedings of the Enlarged Halden Programme Group Meeting*, Røros, Norway, September 7 through 12, 2014.

- **Pastore, G., S. R. Novascone, R. L. Williamson, J. D. Hales, B. W. Spencer, and D. S. Stafford**, 2015, "Modeling of Fuel Behavior during Loss-of-Coolant Accidents using the BISON Code," *Proceedings of the Reactor Fuel Performance Meeting – Top Fuel 2015*, Zurich, Switzerland, September 13 through 17, 2015.
- **Pastore, G., R. L. Williamson, S. R. Novascone, B. W. Spencer, and J. D. Hales**, 2016, "Modelling of LOCA Tests with the BISON Fuel Performance Code," *Proceedings of the Enlarged Halden Programme Group Meeting*, Fornebu, Norway, May 8 through 13, 2016.
- **Pizzocri, D., C. Rabiti, L. Luzzi, T. Barani, P. Van Uffelen, and G. Pastore**, 2016, "PolyPole-1: An Accurate Numerical Algorithm for Intra-granular Fission Gas Release," *Journal of Nuclear Materials*, Vol. 478, pp. 333–342.
- **Williamson, R. L., G. Pastore, S. R. Novascone, J. D. Hales, B. W. Spencer, and D. M. Perez**, 2014, "Modeling LOCA Behavior with the BISON Fuel Performance Code," *20th QUENCH Workshop*, Karlsruhe, Germany, November 11 through 13, 2014.

<sup>1</sup> Idaho National Laboratory



# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## NUCLEAR NONPROLIFERATION

### *End-to-End Radiation Detector Enhancements for Improved Safety and Security in Safeguarded Facilities (Project 14-045)*

*Scott J. Thompson,<sup>1</sup> C. S. Sosa,<sup>1</sup> David L. Chichester,<sup>1</sup> D. Shy,<sup>1</sup> and Mara M. Grinder<sup>1</sup>*



*Principal investigators employ extensive knowledge to develop safeguards measurement and interrogation technologies.*

#### **SCIENTIFIC ACHIEVEMENT**

This project explored novel modeling, simulation and experimentation approaches with radiation detectors to identify improved component and system designs for safeguarding facilities. The project sought to enhance the nation's nuclear-nonproliferation and emergency-response-measurements capabilities through a focus on understanding how the shape and reflective-boundary conditions of organic scintillators can influence the light-collection process resulting

from radioactive decay. Any increase in light-collection efficiency will improve the energy resolution and sensitivity of the detector, thus increasing the acuity of measurements and potentially the ability to differentiate between incident neutron and photon radiation. Models were validated with benchmark laboratory measurements using custom-fabricated scintillator materials. Experimental results demonstrated that light collection is improved significantly by minimizing the number of photon reflections that occur

before collection. This discovery challenges the current systems' standard use of a right circular cylinder scintillator to match the shape of a photomultiplier tube, because this new configuration does not minimize the number of reflections.

#### **SIGNIFICANCE**

This research demonstrated that a significant increase in the fidelity of detector performance and sensitivity can be achieved through simple and inexpensive geometric optimization of currently deployed technologies. Examples of common implementations of these detectors include portal monitors, hand-held survey instrumentation, and vehicle-mounted search systems for screening individuals, vehicles and cargo for radiation sources. Not only do these findings support DOE's mission to enhance nuclear security through transformational technology solutions for nuclear-nonproliferation and international-safeguards efforts, they also have the potential to influence the fields of industrial manufacturing, medical physics and others. Three student internships were supported through this project, and the work will be the subject of a doctoral dissertation in nuclear engineering at the University of Michigan.

<sup>1</sup> *Idaho National Laboratory*

# LDRD Project Highlights

## Advancing Nuclear Energy

### MODELING AND SIMULATION

#### **Development of a Multiphysics Algorithm for Analyzing the Integrity of Nuclear Reactor Containment Vessels Subjected to Extreme Thermal and Overpressure-Loading Conditions (Project 14-104)**

*Richard C. Martineau,<sup>1</sup> Ben Spencer,<sup>1</sup> Ray Berry,<sup>1</sup> David Andrs,<sup>1</sup> Hongbin Zhang,<sup>1</sup> and Yidong Xia<sup>1</sup>*

#### **SCIENTIFIC ACHIEVEMENT**

The objective of this project is to develop a first-of-its-kind, multiscale, multiphysics algorithm for analyzing the integrity of nuclear reactor containment vessels subjected to extreme thermal and overpressure-loading conditions. The result combines the following into one cohesive, tightly coupled, multiphysics approach: radiative heat transfer in the MOOSE-based radiation transport application, Rattlesnake; improved multiphysics capabilities in the MOOSE framework; and shock capturing in the MOOSE-based computational fluid dynamics application, Bighorn.

#### **SIGNIFICANCE**

This work is directed at creating a new algorithm for thermal-mechanical, fluid-structure interaction to address structural integrity in the presence of thermal radiation, natural and forced convection, and strong hydrodynamic forces. While this effort is undertaken with nuclear safety for nuclear power plants in mind, applications for nuclear security are numerous. Successfully developing an advanced,



*An INL researcher simultaneously analyzes the many factors affecting the performance of a reactor containment vessel under extreme conditions.*

strongly coupled multiphysics thermal-mechanical and hydrodynamic algorithmic approach for extreme thermal and overpressure-loading conditions in containment vessels will further position INL at the forefront of nuclear plant safety and analysis.

#### **KEY PUBLICATIONS**

- **Xia, Y., D. Andrs, and R. C. Martineau**, 2016, *BIGHORN Computational Fluid Dynamics Theory, Methodology, and Code Verification & Validation Benchmark Problems*, INL/EXT-16-39214, Idaho National Laboratory, August 2016.

<sup>1</sup> Idaho National Laboratory

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## MODELING AND SIMULATION

### *Simulation-Based Analysis of Procedures and Accident Management Guidelines (Project 15-013)*

*Curtis Smith,<sup>1</sup> Tony Koonce,<sup>1</sup> Ronald Boring,<sup>1</sup> and Robert Youngblood<sup>1</sup>*



*Human factors researchers analyze procedures and accident management guidelines using the capabilities of the Human Systems Simulation Laboratory.*

#### **SCIENTIFIC ACHIEVEMENT**

The research behind this project will improve the state of the art of probabilistic risk analysis (PRA) by modeling plant logic, procedures and operator management guidelines in a unified way. This science will enable enhanced representation of human interactions within complex facilities such as nuclear power plants. The technical approach

uses simulation-driven representation of stochastic processes (such as specific human tasks) as a means of addressing uncertainty in the selection of actions by projecting the effect of those actions into the future. Using simulation of procedures, the project team will forecast decision-support options (for plant operators) from a large spectrum of potential simulation-based scenarios. The novel aspect of the

work is inclusion of a comprehensive set of procedures and accident-management guidelines in a simulation model of plant performance. This aspect is important because tasks such as operator actions still surprise observers (e.g., shutting off high-pressure injection at Three-Mile Island or shutting off systems at Fukushima).

#### **SIGNIFICANCE**

This project will advance the state of the art of PRA by providing insights into possible procedural actions that are and are not beneficial to plant stability or safety. This capability has the potential to improve modeling of humans in complex systems — such as those in research and test facilities at INL and elsewhere. INL will benefit from the latest PRA developments, which may also be applied at other DOE facilities. In addition, there is some potential for expanding this methodology beyond the nuclear industry and adapting it to other low-probability/high-consequence industries and infrastructure where humans interact with complex facilities or systems.

<sup>1</sup> Idaho National Laboratory

# LDRD Project Highlights

## Advancing Nuclear Energy

### MODELING AND SIMULATION

#### Development of Stochastic Three-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond-Design Basis Seismic Motions for Nuclear Facilities (Project 15-023)

Justin L. Coleman<sup>1</sup> and Swetha Veeraraghavan<sup>1</sup>

#### SCIENTIFIC ACHIEVEMENT

Soil properties at different nuclear and critical facility sites can vary widely. The stochastic nature of these properties is currently modeled in the industry using an indirect approach involving a statistically significant number of deterministic analyses. A more theoretically accurate approach is to perform stochastic site-response analyses, which will be used in this project after developing a stochastic elasto-plastic, finite-element formulation in the MOOSE-based application, MASTODON. Understanding the soil's response to seismicity at a particular site is significant, because the response of the soil during earthquakes has a direct effect on the energy transferred to a structure.



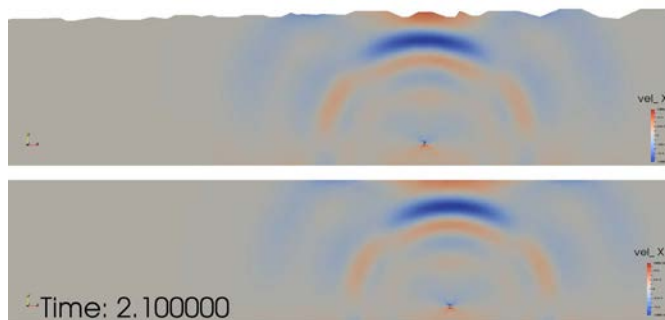
Justin Coleman, group lead for seismic R&D, analyzes the simulated effects of seismicity using MASTODON.

#### SIGNIFICANCE

Quantifying the uncertainty in soil properties that nuclear power plants and

critical facilities are founded on is critical to understanding the facility response to seismic motion. Implementation of this

capability will allow prudent decisions to be made in areas that include safety and economics when designing and siting nuclear power plants and critical infrastructure. This project has supported one postdoc.



Current linear seismic-analysis tools used to site nuclear power plants model surfaces as flat and assume vertically propagating seismic waves (bottom image), but MASTODON models nonlinear soil behavior, simulates three-dimensional seismic wave fields, and quantifies the effects of topography (top image).

#### KEY PUBLICATIONS

- Veeraraghavan, S., J. Bielak, and J. Coleman, 2017, "Effect of Inclined Waves on Deeply Embedded Nuclear Facilities," *SMiRT 24*, August 2017, in press.

<sup>1</sup> Idaho National Laboratory

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## I N · P I L E   S E N S O R

### **Acoustic Telemetry Infrastructure for In-Pile ATR and TREAT Monitoring (Project 15-040)**

Vivek Agarwal,<sup>1</sup> James A. Smith,<sup>1</sup> James Lee,<sup>1</sup> and James K. Jewell<sup>1</sup>

#### **SCIENTIFIC ACHIEVEMENT**

The internal environment of any nuclear reactor presents a particularly harsh environment (e.g., high temperatures and high radiation levels) for sensors and instrumentations. The reactor environment also imposes challenging constraints on signal transmission from inside the reactor to outside of the reactor vessel. In this research, an acoustic measurement infrastructure installed at INL's Advanced Test Reactor (ATR) is being further developed.

The existing acoustic receivers installed in the ATR are being used to collect data to provide a baseline for the development of acoustically telemetered sensors such as thermoacoustic and vibroacoustic technology. Intrinsic and cyclic acoustic signals generated by the operation of the primary coolant pumps are collected and processed. The intrinsic pump signals are surrogate signals for the acoustic telemetered signals. The intrinsic signals have the added benefit of being able to indicate the process state of the ATR (such as reactor startup, reactor criticality, reactor attaining maximum power and reactor shutdown) during operation. This research enabled wireless, non-intrusive, real-time monitoring of sensors and reactor characteristics utilizing acoustically telemetered signals.

#### **SIGNIFICANCE**

This research is critical in advancing DOE's nuclear energy mission by developing an advanced capability of in-pile temperature

and other measurements for materials irradiation in research and test reactors. This aligns with the Nuclear Science User Facilities mission in the area of advanced instrumentation for in-pile measurements. The research will enable direct technology and capability transfer opportunities to the nuclear industry to support current and next-generation reactor concepts. Successful completion of this research will significantly improve the quality and capability of INL to analyze in-pile data for materials and fuels and to carry out modeling and simulation R&D. This project has also allowed researchers to work closely with ATR personnel.

ATR turned to this project to supply vibration data to help understand a beryllium cracking issue near the hydraulic shuttle. The research augments the activities outlined in the INL Nuclear Science and Technology Directorate's "Gateway to Accelerated Innovation in Nuclear Initiative," because skills obtained through the project will be used to monitor a thermoacoustic sensor installed in the accident-tolerant fuel test train at ATR by INL and Westinghouse. This research led to the hire of a senior instrumentation-and-control scientist and support for two summer interns.

#### **KEY PUBLICATIONS**

- **Agarwal, V. and J. A. Smith,** 2017, "Real-Time In-Pile Acoustic Measurement Infrastructure at the Advanced Test Reactor," *ANS Nuclear Technology*, March 2017, in press.
- **Garrett, Steven L., James A. Smith, Robert W. Smith, Brenden J. Heidrich, and Michael D. Heibel,** 2016, "Fission-Powered In-Core Thermoacoustic Sensor," *Applied Physics Letters*, Vol. 108, No. 14, 144102 (doi: 10.1063/1.4944697).
- **Garrett, Steven L., James A. Smith, Robert W. Smith, Brenden J. Heidrich, and Michael D. Heibel,** 2016, "Using the Sound of Nuclear Energy," *Nuclear Technology*, Vol. 195, No. 3, pp. 353–362, September 2016.

#### **PATENTS**

- Provisional Patent BA-893 (filed), Tracking No. 4112, "Acoustic Measurement Infrastructure Method and System for Process Monitoring, Diagnostics and Prognostics."

<sup>1</sup> Idaho National Laboratory

# LDRD Project Highlights

## Advancing Nuclear Energy

### MODELING AND SIMULATION

#### Development of Efficient TREAT Modeling Capabilities with Graphite Data Improvement (Project 15-060)

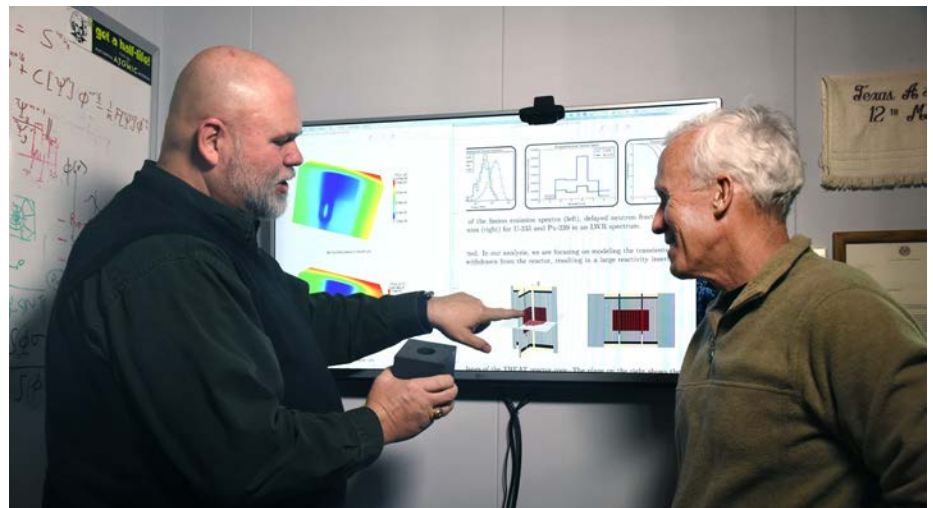
Mark DeHart,<sup>1</sup> Ayman Hawari,<sup>2</sup> Todd Palmer,<sup>3</sup> Edward Blandford,<sup>4</sup> and Benoit Forget<sup>5</sup>

#### SCIENTIFIC ACHIEVEMENT

This project focuses on improvements in multiphysics modeling and simulation capabilities in support of the INL Transient Test Reactor (TREAT). The research will in turn serve to improve graphite data, integrate Monte Carlo simulations of thermal neutron scattering within graphite for sensitivity studies and uncertainty analyses, and aid in development of closure relationships for the Reactor Excursion Leak Analysis Program (RELAP)-7 within MAMMOTH. The project validates the multiphysics reactor analysis package MAMMOTH, including Rattlesnake, and develops methods for calculating accurate diffusion coefficients in highly anisotropic regions. The project also measures surface properties for, and collects critical heat flux data on, accident-tolerant fuel cladding samples.

#### SIGNIFICANCE

This effort builds capabilities and data in support of modeling and simulation, experiment design, and operations analysis for TREAT. Benchmark specifications developed can be added to the International Reactor Physics Experiment Benchmark handbook. Improved characterization of reactor-grade graphite will broaden its applicability to other graphite reactor systems. The thermal-hydraulic measurements of proposed accident-tolerant fuel materials will provide closure relationships and improve modeling accuracy for the accident-tolerant fuel experiments. The results are also applicable in multi-



Researchers develop methods to model the TREAT reactor core in both steady-state and transient conditions by combining several of INL's industry-leading modeling platforms.

physics analysis in other systems, including light-water and graphite-moderated systems. University collaborations provide experience to graduate students and completion of graduate degrees for many.

#### KEY PUBLICATIONS

- DeHart, M., F. Gleicher, J. Ortensi, A. Alberti, and T. Palmer, "Multi-Physics Simulation of TREAT Kinetics using MAMMOTH (INL/CON-15-35771)," *Transactions of the American Nuclear Society*, November 2015.
- Ellis, M., D. Gaston, B. Forget, and K. Smith, 2016, "Continuous Temperature Representation in Coupled OpenMC/ MOOSE Simulations," *PHYSOR 2016*

– *Unifying Theory and Experiments in the 21st Century*, May 2016.

- Ellis, M., D. Gaston, B. Forget, and K. Smith, 2016, "Preliminary Coupling of the Monte Carlo Code OpenMC and the Multiphysics Object-Oriented Simulation Environment (MOOSE) for Analyzing Doppler Feedback in Monte Carlo Simulations (INL/CON-15-34625)," *Nuclear Science and Engineering – M&C 2015 Special Issue*, 2016.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> North Carolina State University

<sup>3</sup> Oregon State University

<sup>4</sup> University of New Mexico

<sup>5</sup> Massachusetts Institute of Technology

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## PROLIFERATION-RESISTANT DESIGN

### **Evaluation and Demonstration of the Integration of Safeguards, Safety, and Security by Design (3SBD) (Project 15-094)**

Jay Disser,<sup>1</sup> Janine Lambert,<sup>1</sup> Edward Blandford,<sup>2</sup> Edward Arthur,<sup>2</sup> Bobbi Merryman,<sup>2</sup> and Nicholas Osterhaus<sup>2</sup>

#### SCIENTIFIC ACHIEVEMENT

The Safeguards, Safety and Security by Design (3SBD) concept is designed to capture and potentially optimize inter-relationships between the safety, security and international safeguards of a nuclear facility. Because the pebble-bed fast-high-temperature reactor (PB-FHR) design process is in its beginning stages, it was chosen as a test case of the 3SBD approach. The project team modeled the PB-FHR in RELAP5-3D and analyzed the direct reactor auxiliary cooling system, which is a part of the reactor's decay heat removal system. RELAP5-3D is a reactor physics code to complete the thermohydraulic analysis of the PB-FHR. The Reactor Analysis and Virtual Control Environment (RAVEN) program was then chosen to couple with RELAP5-3D due to its ability to manipulate RELAP5-3D and its dynamic event tree functionality. To evaluate the safeguards significance of the PB-FHR, a nuclear material accountancy analysis was performed, and three facility misuse scenarios were examined. The conclusions of the work showed that the responses of the decay heat removal systems to partial blockages were fairly robust, requiring multiple high-percentage blockages to lead to large temperature excursions. Security insights can be inferred from this analysis to show which reactor systems are more sensitive to disruption from a physical-protection or cybersecurity point of view.

#### SIGNIFICANCE

China is actively developing and demonstrating two pebble-bed reactors. The Chinese PB-FHR is being developed by the Chinese Academy of Sciences, and construction is expected to begin in 2017. Critically thinking about using safety, security, and safeguards insights early in the design process can improve next-generation nuclear infrastructure. This project will place the United States in a stronger position when engaging other countries on 3SBD for critical nuclear infrastructure by providing a more objective method for 3SBD evaluation. One of the key outcomes of this work was the coupling of multiple reactor safety codes developed by INL for the analysis of nuclear security (including cybersecurity) features of a nuclear reactor. This project establishes the foundation to move 3SBD from a concept to practice. This project has supported two undergraduate students as well as one graduate intern who was hired as an INL staff member in November 2016.

#### KEY PUBLICATIONS

- **Arthur, E., E. Blandford, J. Disser,** et al., 2016, "Demonstration of the 3SBD Concept for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR)," *INMM Annual Meeting Proceedings*, July 2016.
- **Disser, J., E. Arthur, and J. Lambert,** 2016, "Preliminary Safeguards Assessment for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR) Concept," *Advances in Nuclear Nonproliferation Technology & Policy Conference Proceedings*, American Nuclear Society, September 2016.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> University of New Mexico

# LDRD Project Highlights

## Advancing Nuclear Energy

### SENSOR · IMAGE ANALYSIS

#### **Change Detection System for Nuclear Applications (Project 16-009)**

*Troy Unruh,<sup>1</sup> Greg Lancaster,<sup>1</sup> Michael Overton,<sup>1</sup> Walter Williams,<sup>1</sup> Jeff Brower,<sup>1</sup> and Ken Thomas<sup>1</sup>*

#### **SCIENTIFIC ACHIEVEMENT**

The focus of this effort is to conceptualize and design a set of systems for performing image analysis that will aid researchers and workers at nuclear facilities to identify, analyze, and track nuclear materials and anomalies. INL has developed an advanced image alignment capability called the Change Detection System (CDS). This innovative software has been widely used in applications related to national security and is globally considered to be the preeminent system for image change detection. CDS has been deployed to numerous government agencies in addition to receiving two patents and winning two R&D 100 Awards. When deployed for nuclear applications, CDS will transform the way work is accomplished by leveraging powerful computer vision techniques for the identification and analysis of objects/areas not currently available to the nuclear reactor community.

#### **SIGNIFICANCE**

The project team furthered nuclear-focused development activities of CDS.



*The Change Detection System can help operators quickly identify tiny changes in large, highly complex systems.*

Examples of the applications evaluated include blister formation during annealing in a hot cell, neutron radiographs, research reactor fuel element scratch identification, visual and thermal electronics assembly analysis, and nuclear facility control panel inspections. Other areas identified that would benefit from the inclusion of CDS

image analysis techniques include facility work flow operations, independent remote verifications, work zone inspections in contamination areas, normal versus abnormal status indications, damage analysis (water hammer, seismic, etc.), live electrical connections thermography, and fresh boron stain tracking.

<sup>1</sup> Idaho National Laboratory



# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## MODELING AND SIMULATION

### **Stress Corrosion Cracking Testing in Supercritical Carbon Dioxide (Project 16-050)**

Sebastien Teysseyre,<sup>1</sup> Piyush Sabharwall,<sup>1</sup> Joe Palmer,<sup>1</sup> Robert Fox,<sup>1</sup> and Julie Tucker<sup>2</sup>

#### **SCIENTIFIC ACHIEVEMENT**

This project included building a corrosion loop to generate corrosion data on Ni-based alloys and their joints at temperatures ranging from 300 to 750°C. In addition to analyzing the corrosion data, the project team is working on adapting an INL technology to test for stress-corrosion cracking in a nuclear reactor to the corrosion loop. This work will allow the team to perform the first in-line measurement of stress-corrosion crack growth in supercritical CO<sub>2</sub>.

The characterization of corrosion in supercritical CO<sub>2</sub> led to the following information:

- Temperatures at 750°C for 600 hours led to significant void density underneath the oxide layer and internal oxidation. The project team observed a high concentration of aluminum along the oxidized grain. The primary surface oxide was identified as Cr.
- At 650°C, oxide pegs or protrusions growing into the matrix were shown to have a greater depth and density with longer exposure times.
- At 650°C, there was noticeable evidence of precipitation at grain boundaries and intragranularly; underneath the scale, there was a precipitate-free zone that was also associated with a Cr depletion area and a layer of newly formed, possibly recrystallized, grains. The as-received sample has no recrystallized zone

compared to the cross-sectional results seen after 200 and 600 hours.

- At 650°C at various time intervals, a recrystallization zone underneath the oxide was observed.
- Mean thickness of scale increased with a function of temperature but stayed relatively similar as a function of time at 650°C. The precipitate-free zone grew slightly as a function of time.

#### **SIGNIFICANCE**

The S-CO<sub>2</sub> Brayton cycle is being considered for power conversion systems for a number of nuclear reactor concepts. To be able to deploy such technology, it is necessary to select suitable component materials for use in this environment. This project is developing the capability to test for stress-corrosion cracking to generate the first stress-corrosion cracking data in supercritical CO<sub>2</sub> and support corrosion experiments. This project supports one graduate student and one undergraduate student.

#### **KEY PUBLICATIONS**

- **Teeter, L., B. Adam, W. Marcum, J. Kruzic, M. Anderson, and J. D. Tucker**, 2015, “Corrosion of Energy System Materials in Supercritical Carbon Dioxide (SC-CO<sub>2</sub>),” *EPRI International Conference on Corrosion in Power Plants*, San Diego, California, October 13, 2015.

- **Teeter, L., B. Adam, W. Marcum, J. Kruzic, M. Anderson, and J. D. Tucker**, 2015, “OSU Supercritical Carbon-Dioxide System for Materials Corrosion Testing,” presentation at Idaho National Laboratory, April 20, 2015.
- **Teeter, L., F. Teng, W. Marcum, J. Kruzic, M. Anderson, and J. D. Tucker**, 2015, “Supercritical Carbon-Dioxide System for Materials Corrosion Testing,” *Oregon State University Engineering Research Expo*, March 4, 2015.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> Oregon State University

# LDPRD Project Highlights

## Advancing Nuclear Energy

### M A T E R I A L S I M A G I N G S E N S O R

#### **Evaluation of Advanced Digital Neutron Imaging Systems for PIE of Nuclear Fuel (Project 16-071)**

Aaron E. Craft,<sup>1</sup> Glen C. Papaioannou,<sup>1</sup> and Anton S. Tremsin<sup>2</sup>

#### **SCIENTIFIC ACHIEVEMENT**

The goal of this project is to test an advanced micro-channel plate (MCP) digital neutron-imaging system for its potential application for examination of irradiated nuclear fuel. The MCP system and supporting hardware were assembled in the North Radiography Station at INL, and real-time digital neutron radiographs were acquired from American Society for Testing and Materials (ASTM) image-quality indicators and a Siemens star line-pair phantom. This was the first time that an MCP system acquired neutron radiographs with a radial neutron beam with direct line of sight to the reactor core, which has significantly higher gamma radiation content compared to most neutron-imaging beams, measured to be 100 R/hour. The MCP system was able to produce neutron radiographs in this high-gamma radiation field without significant degradation, lending optimism to the prospect of using the MCP system to image irradiated fuel. Irradiated fuel produces a gamma dose rate of ~1,000 to 10,000 R/hour, which



*INL continues to expand the value of the Neutron Radiography Reactor by developing a capability for digital three-dimensional tomography.*

would be reduced to <100 R/hour with lead filtering (~2.5 cm). The detector response was tested with lead filters of varying thickness (0 to 5 cm) positioned in the neutron beam.

#### **SIGNIFICANCE**

These were the first fully digital neutron radiographs ever acquired at INL. From the initial evaluations and calculations,

it seems plausible that an MCP neutron-imaging system could be used to evaluate irradiated nuclear fuel, even in the high gamma fields from INL's Neutron Radiography Reactor neutron beams and in the presence of irradiated nuclear fuel. Upcoming efforts will seek to acquire digital neutron radiographs of an irradiated fuel pin using the same MCP system.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> University of California-Berkeley

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## NUCLEAR NONPROLIFERATION

### Production of Fluoroanion Targets for Accelerator Mass Spectrometry (Project 16-085)

Christopher Zarzana,<sup>1</sup> Gary Groenewold,<sup>1</sup> Michael Benson,<sup>1</sup> Kristyn Roscioli-Johnson,<sup>1</sup> Rika Hagiwara,<sup>2</sup> and Chien Wai<sup>3</sup>



*INL is leading a DOE initiative to ensure the timely, efficient and cost-effective integration of safeguards and security measures.*

#### SCIENTIFIC ACHIEVEMENT

Detection of actinide element nuclides is critical for verifying compliance of nuclear facilities with international nonproliferation treaties. Current analysis methods require time-consuming and expensive sample preparation to achieve results acceptable to decision-makers. Future analytical performance with markedly improved accuracy, precision, and sensitivity and faster sample throughput will be required to keep up with an increasingly complex nuclear-proliferation environment. The objective

of this project is to develop technology for rapid production of sample targets for actinide analysis using accelerator mass spectrometry. To accomplish this objective, the project team is investigating the interactions between ionic liquid anion and cation clusters in the gas-phase using infrared multi-photon dissociation techniques in collaboration with the FELIX Laboratory at Radboud University in the Netherlands. These studies revealed that the anions and cations bind in specific ways depending on their structure, which suggests the fluorination chemistry

can be controlled by varying the ionic liquid structure; this is one of the main hypotheses of this project. Additionally, these results have suggested further experiments that could provide new insight into the mesoscopic ordering of ionic liquids (an area that is challenging to study) and open it to further exploration.

#### SIGNIFICANCE

This project is developing novel methods for rapid actinide analysis that are urgently needed by DOE and other national security organizations. Rapid, inexpensive actinide analysis methods will greatly enhance the ability of the international community to ensure compliance with international treaties, increasing global security. Additionally, this project is exploring the fundamental actinide chemistry needed to develop these methods, furthering DOE's basic science mission.

#### KEY PUBLICATIONS

- Zarzana, C. A., G. S. Groenewold, M. Benson, K. Roscioli-Johnson, J. Martens, J. Oomens, R. Hagiwara, and T. Tsuda, 2016, "Spectroscopic and Mass Spectral Characterization of Uranium Fluoroanions Formed from an Ionic Liquid," *Plutonium Futures – The Science 2016*, Baden, Germany, September 18 through 22, 2016.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> Kyoto University, Japan

<sup>3</sup> University of Idaho

# LDPRD Project Highlights

## Advancing Nuclear Energy

### NUCLEAR POWER PLANT AUTOMATION

#### **Supporting Operator Performance and Situation Awareness in Highly Automated Nuclear Power Plants (Project 16-096)**

*Katya Le Blanc<sup>1</sup> and Johanna Oxstrand<sup>1</sup>*

#### **SCIENTIFIC ACHIEVEMENT**

Automation is being introduced or proposed in existing nuclear power plants through a wide variety of systems and technologies and will likely be part of advanced nuclear power plant designs. Advanced displays, computer-based procedures, advanced alarm systems and computerized operator support systems are part of advanced light-water reactor control rooms and may be implemented as part of upgrades to existing light-water reactors. Additionally, new reactor concepts, such as small modular reactors (SMRs), include increased automation and reduced staffing. With increased automation comes an increased challenge for the human operator. Research reveals a fundamental tradeoff between increased use of automation and human situation awareness. This project identifies how to design human/system interfaces to keep human operators engaged and aware in highly automated nuclear power plants and how to identify optimal human/automation interaction design to support human/system performance and human situation awareness.

#### **SIGNIFICANCE**

The results of this research will determine effective principles for



*Researchers analyze operator response and performance using the capabilities of the Human Systems Simulation Laboratory.*

human/automation interaction that can be applied to a variety of challenges facing industries designing and deploying advanced technologies with increased automation, including SMRs, advanced reactors, grid technologies, hybrid energy systems, and autonomous and semi-autonomous cars. This work will also enable the deployment of an SMR by overcoming one of the barriers to licensing a NuScale SMR (i.e., providing an empirical basis for an

exemption to the Nuclear Regulatory Commission staffing rule).

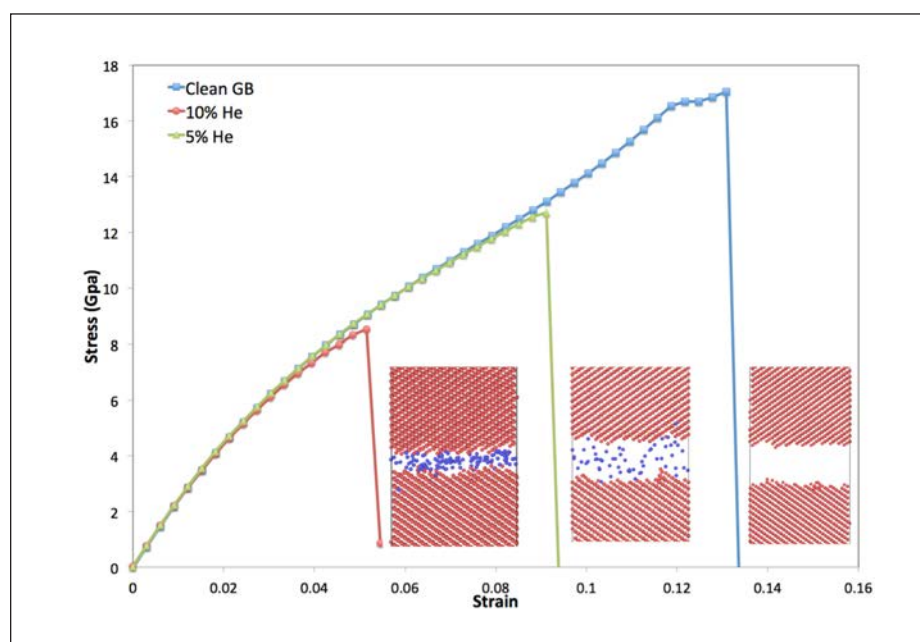
Finally, this work will advance the methodology used to assess human performance by allowing human operators to cope with a large amount and complexity of information to work effectively with automated systems. This project supported one postdoc and an intern.

<sup>1</sup> *Idaho National Laboratory*

## M A T E R I A L S   S E N S O R S

### Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys (Project 16-187)

Chao Jiang,<sup>1</sup> Wen Jiang,<sup>1</sup> Brian Jaques,<sup>2</sup> Indrajit Charit,<sup>3</sup> and Ray Fertig<sup>4</sup>



*Molecular-dynamics simulated stress-strain curves for  $\Sigma 3\langle 110 \rangle\{111\}$  grain boundary in body-centered cubic molybdenum with different helium loadings.*

#### SCIENTIFIC ACHIEVEMENT

Metallic alloys are widely used as structural and cladding materials in current fission nuclear reactors and are planned for use in future fusion nuclear reactors. During operations, the cohesion strength of grain boundaries (GBs) in an alloy may be drastically reduced due to interactions with irradiation-induced defects (e.g., vacancies and self-interstitials) and impurity elements (e.g., helium atoms

produced by nuclear transmutation reactions), leading to intergranular fracture and embrittlement. The objective of this project is to use transmission electron microscopic in situ cantilever testing and multi-scale modeling to quantify the effects of irradiation on GB cohesion. In FY 2016, efforts have been made to synthesize Fe-Cr alloys from their constituent powders using high-energy ball milling followed by spark plasma sintering and to develop

capabilities for measuring GB cohesion strength at the Center for Advanced Energy Studies. Furthermore, INL researchers have performed molecular dynamics simulations to predict the effects of helium loading on the GB cohesion strength in body-centered cubic metals such as molybdenum. On the continuum scale, research has been focused on improving the numerical stability of the cohesive zone method and its coupling with radiation damage.

#### SIGNIFICANCE

The radiation-induced degradation of material mechanical properties poses serious limitations to nuclear energy applications. The capabilities of transmission electron microscopic in situ mechanical testing and MOOSE-based fracture models developed for this work will help to understand and predict the performance of materials in reactors. In turn, it would enable safer and more economical nuclear energy in the future. Results from this project will contribute to the DOE's leading role on research of materials behavior and performance in radiation environments.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> Boise State University

<sup>3</sup> University of Idaho

<sup>4</sup> University of Wyoming

# LDRD Project Highlights

## Clean Energy Deployment

### M A T E R I A L S   F O R   E X T R E M E   E N V I R O N M E N T S

#### **Extended Stability Gamma-Gamma Prime Containing Nickel-Base Alloys (Project 14-078)**

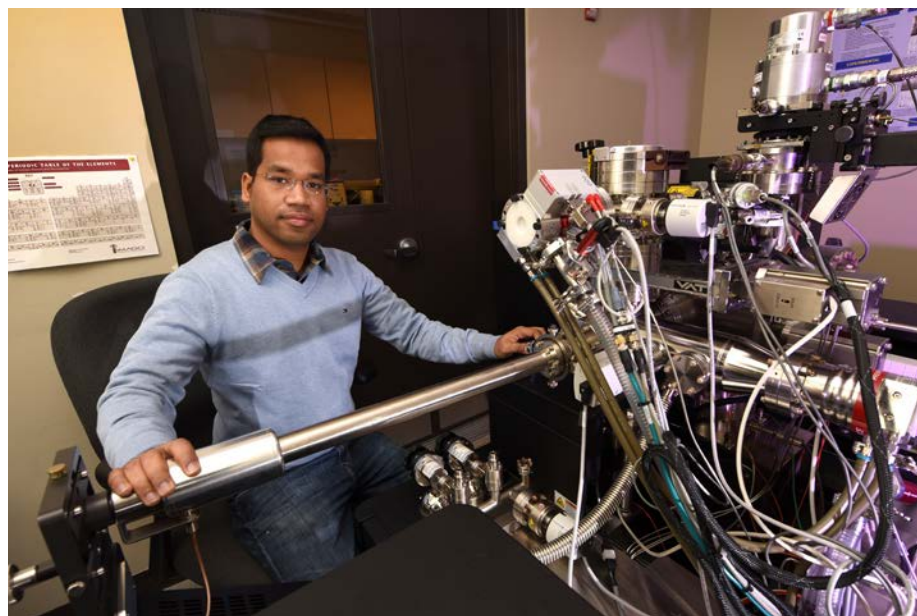
Subhashish Meher,<sup>1</sup> Larry K. Aagesen,<sup>1</sup> Laura J. Carroll,<sup>1</sup> Mark C. Carroll,<sup>1</sup> and Tresa M. Pollock<sup>2</sup>

#### **SCIENTIFIC ACHIEVEMENT**

Improving efficiencies for electricity and power generation by concentrating solar, nuclear and fossil energy continues to place increasing demands on materials because of higher operating temperatures and longer service durations. These demands require performance characteristics and stable strength values that exceed the properties of state-of-the-art materials currently available. This project addressed the scientific challenge of achieving materials with extended stability by developing microstructural strategies for high-temperature  $\gamma$ - $\gamma'$  alloys through a combination of experimental and modeling techniques. Targeted materials design through chemistry and processing followed by microstructural characterization and analysis at the nanometer scale of three classes of superalloys — Ni-base, NiCr-base and CoNi-base — provided critical inputs integrated into computational kinetic modeling to simulate the microstructure during long-term, high-temperature exposures.

#### **SIGNIFICANCE**

The investigated  $\gamma$ - $\gamma'$  alloy design strategies achieved materials with hierarchical  $\gamma$ - $\gamma'$  microstructures and low interfacial  $\gamma$ - $\gamma'$  energies, both of which offer promise for high-temperature, extended-service durations by retaining a larger fraction of their initial strength even when exposed to extreme environments. The



*Subhashish Meher studies superalloys using the local electron atom probe (LEAP) at the Center for Advanced Energy Studies.*

new phase transformation pathways investigated introduce the potential for inherent long-term stability by achieving coarsening resistance for the strengthening  $\gamma'$  precipitate structure, thus providing fundamental strategies for future high-temperature alloy development for energy applications. This project also resulted in the hiring of a postdoc candidate with extensive expertise in atom probe tomography.

#### **KEY PUBLICATIONS**

- Meher, S., L. J. Carroll, T. M. Pollock, and M. C. Carroll, 2016, "Solute

partitioning in multi-component  $\gamma/\gamma'$  Co Ni-base superalloys with near-zero lattice misfit," *Scripta Materialia*, Vol. 113, pp. 185–189.

- Meher, S., L. K. Aagesen, L. J. Carroll, M. C. Carroll, and T. M. Pollock, 2016, "Understanding of Inverse Coarsening of  $\gamma'$  Precipitates in Ni-base Superalloys," *Microscopy and Microanalysis*, Vol. 22, No. S3, pp. 1258–1259.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> University of California-Santa Barbara

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## M A T E R I A L S   M E A S U R E M E N T   T E C H N O L O G Y

### *In Situ Measurement of Electrolyte Chemistry in Battery Cells during Operation (Project 14-095)*

*Gary S. Groenewold,<sup>1</sup> David Jamison,<sup>1</sup> Cathy Rae,<sup>1</sup> Kristyn Roscioli-Johnson,<sup>1</sup> Chris A. Zarzana,<sup>1</sup> and Kevin Gering<sup>1</sup>*



*Salene Rowe, as part of DOE's Science Undergraduate Laboratory Internships program, was one of three interns who supported LDRD Project 14-095.*

#### SCIENTIFIC ACHIEVEMENT

Monitoring changes in lithium-ion batteries is a subject of acute interest because of the risk of fire and explosion subsequent to repetitive charge/discharge cycling. Measuring the chemistry in these systems is challenging because of the small volumes and inaccessibility of the lithium-ion battery systems. INL researchers have developed nano-fluidic approaches that are capable of analyzing microscopic volumes for changes in electrolyte composition. The volume of sample required is on the order of  $3 \times 10^{-8}$  L and is formed as a

droplet on the end of a non-conducting capillary. Application of a surface charge “launches” the droplet from the capillary into the aperture of a fast-scanning mass spectrometer. This enables quantitative measurement of changes in electrolyte composition and fire-retardant additives without perturbing the function of the cell under investigation.

#### SIGNIFICANCE

Lithium-ion batteries have excellent capacity, power-density, lifetime and recharge attributes, and they are

ubiquitous in modern life. However, they can undergo spontaneous ignition and occasionally explosion, which affects air transportation and consumer safety. These detrimental performance characteristics have made lithium-ion battery safety a matter of high significance to the United States, and to its governmental entities, and have motivated extensive efforts to mitigate safety risks. The approach taken here is to initiate development of advanced diagnostic tools that will have the ability to provide data that can be used to forecast failure events.

#### KEY PUBLICATIONS

- Sauter III, A. D., D. Sauter, K. Roscioli-Johnson, C. Zarzana, G. S. Groenewold, R. Ross, and P. Limbach, 2016, “Droplets for IBF Mass Spectroscopy and Analytical Chemistry,” *64th American Society for Mass Spectrometry Conference*, San Antonio, Texas, June 5 through 9, 2016.

<sup>1</sup> Idaho National Laboratory

# LDRD Project Highlights

## Clean Energy Deployment

### HYBRID ENERGY SYSTEM

#### **Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment (Project 15-039)**

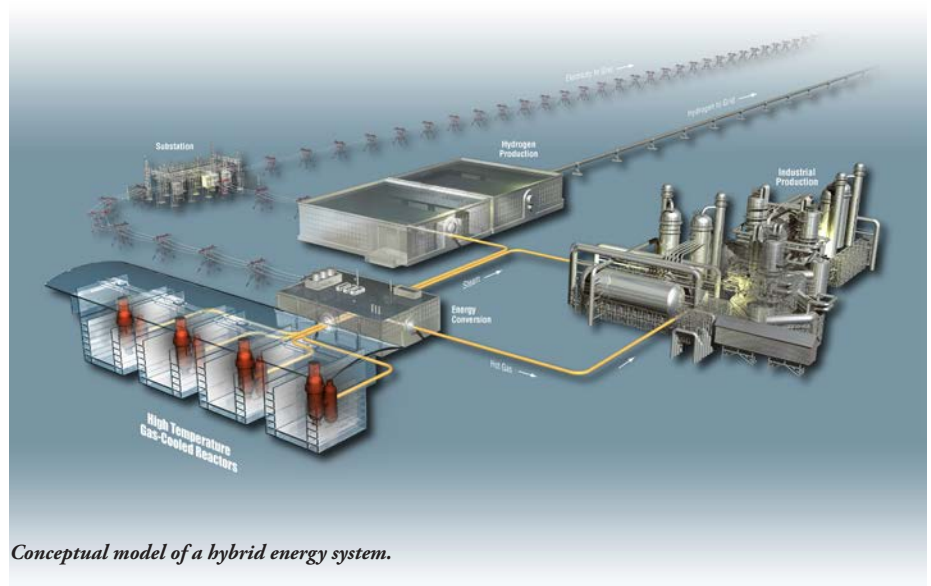
Shannon M. Bragg-Sitton,<sup>1</sup> J. Michael Doster,<sup>2</sup> Stephen D. Terry,<sup>2</sup> Carol Smidts,<sup>3</sup> Qiao Wu,<sup>4</sup> Andrew Klein,<sup>4</sup> Charles Forsberg,<sup>5</sup> and Patrick McDaniel<sup>6</sup>

#### SCIENTIFIC ACHIEVEMENT

Validated modeling tools are required to adequately characterize the responses of energy systems when coupled with each other (e.g., nuclear, renewables, and energy storage in the electricity, industrial, and transportation sectors) and in combination with operational strategies, control algorithms to optimize for transient maneuvers, and potential impacts of degrading component health. For example, diversion of steam in a nuclear hybrid energy system to thermal storage or other applications will initiate a reactor transient in a tightly coupled system. This project advances dynamic modeling of energy storage for non-emitting energy systems integrated with nuclear systems, modeling anticipated transient behavior/response of subsystems, conducting limited experiments and mining of existing data to validate these models, and assessing the impact of aging and degradation of key components (e.g., valves) on system operation. Data collected for preliminary model validation will further enhance the dynamic system modeling capability, and new methods that are developed will be used to evaluate the probability of control system stability for complex integrated energy systems.

#### SIGNIFICANCE

This modeling system could play a major role in future U.S. energy planning and development to achieve extensive decarbonization goals established in the 2015 Paris Accord (COP21 meeting). Additionally, the testing conducted through



Conceptual model of a hybrid energy system.

a distributed test facility will provide a basis for multilaboratory, integrated testing of simulation models and hardware to further advance nuclear hybrid energy system concepts. The modeling and hardware development will enable more rapid adoption of the proposed hybrid energy system technology by industry. The partnerships between INL and universities under this project have supported numerous students. This project has led to one undergraduate honors thesis, three master's theses, and one doctorate dissertation.

#### KEY PUBLICATIONS

- Misenheimer, C. and S. D. Terry, 2017, "Modeling Hybrid Nuclear Systems with

Chilled-Water Storage," *Journal of Energy Resources and Technology*, Vol. 139, No. 1, pp. 012002-1–012002-9, January 2017 (doi: 10.1115/1.4033858).

#### PATENTS

- Application Reference Number T2016-220, "Distributed Test Facility for Digital Instrumentation and Control Systems."

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> North Carolina State University

<sup>3</sup> The Ohio State University

<sup>4</sup> Oregon State University

<sup>5</sup> Massachusetts Institute of Technology

<sup>6</sup> University of New Mexico



# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## MODELING AND SIMULATION

### **Microstructural Evolution and Mesoscale Coupled Flow-Reaction-Fracturing Processes in Organic-Rich Nanoporous Shales (Project 15-128)**

Hai Huang,<sup>1</sup> Earl Mattson,<sup>1</sup> Travis McLing,<sup>1</sup> Darryl Butt,<sup>2</sup> and Paul Leonard<sup>3</sup>

#### SCIENTIFIC ACHIEVEMENT

This project integrates experimental, observational, and computational techniques to fill fundamental knowledge gaps in understanding the following: dynamics of fluids confined in organic-rich nanoporous shale; how microstructure changes in response to variations in stress, fluid pressure, and fluid chemical compositions; and the effects of microstructure changes on larger-scale transport and mechanical properties. The project coordinates an array of state-of-the-art characterization and imaging tools to characterize and image the pore structure in detail and at the highest possible resolution. The computational component aims to develop multiscale multiphysics models to provide physics-based predictions of fluid dynamics and microstructural changes of organic-rich nanoporous shale.

Critical experimental and modeling capabilities and impactful research results include:

1. Focused-ion beam scanning-electron/transmission-electron microscopy imaging and characterization helped systematically characterize and image the nanostructured shale samples.
2. A reactive force field molecular dynamics model was used to build realistic three-dimensional, cross-linked, polymeric kerogen molecule models, which revealed a great amount of subnanometer porosities that could

potentially transform our perception of in-place resource estimates and the fundamental understanding of transport mechanisms in shales.

3. A grain-scale discrete element model helped predict the deformation and microfracturing of shale matrix induced by the swelling stress of kerogen and clay due to adsorption and/or water imbibition.

#### SIGNIFICANCE

The objective of this project is to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies. Research into areas such as microstructural changes of nanostructured organic-rich shales—coupled with fluid flow and volume-changing/stress-generating processes such as chemical transformations, swelling/shrinking, sorption/desorption, and thermal expansion/contraction—has important implications for sustainable and environmentally friendly recovery of shale gas and oil, geological storage of CO<sub>2</sub> in depleted shales, and underground storage of nuclear and other hazardous wastes.

#### KEY PUBLICATIONS

- **Huang, H., P. Meakin, and A. Malthe-Sorensen**, 2016, “Physics-based Simulation of Multiple Interacting Crack Growth in Brittle Rocks Driven by Thermal Cooling,” *International Journal for Numerical and Analytical Methods in Geomechanics* (doi: 10.1002/nag.2523).
- **Zhou, J., H. Huang, and M. Deo**, 2016, “Numerical Study on the Critical Role of Rock Heterogeneity in Fracture Generation,” *50th US Rock Mechanics/Geomechanics Symposium*, Houston, Texas, June 26 through 29, 2016.
- **Zhou, J., H. Huang, and M. Deo**, 2016, “Simulation of Hydraulic and Natural Fracture Interaction Using a Coupled DFN-DEM Model,” *50th US Rock Mechanics/Geomechanics Symposium*, Houston, Texas, June 26 through 29, 2016.
- **Zhou, J., H. Huang, J. McLennan, P. Meakin, and M. Deo**, 2016, “A Dual Lattice Discrete Element Model to Understand Hydraulic Fracturing in a Naturally Fractured System,” *Hydraulic Fracturing Journal*, accepted.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> Boise State University

<sup>3</sup> Pioneer Natural Resources, Texas

# LDRD Project Highlights

## Clean Energy Deployment

### ELECTRIC GRID

#### *Dynamic Simulations for Large-Scale Electric Power Networks in Real-Time Environment Using Multiple RTDS (Project 15-135)*

*Manish U. Mohanpurkar,<sup>1</sup> Rob Hovsopian,<sup>1</sup> and Siddharth Suryanarayanan<sup>2</sup>*

#### SCIENTIFIC ACHIEVEMENT

This project aims to test and evaluate necessary components for geographically distributed real-time simulation using real-time simulators and interconnectivity between different locations. This connectivity will be used to conduct dynamic and transient tests to analyze large-scale power and energy systems. Another objective of this project is to address the existing gaps in modeling and simulation of newer devices such as power converters operating in timescales of microseconds to minutes. This will enable characterization of the devices under real-world operating conditions. In FY 2016, the project team developed analytical techniques for mitigating data latency for distributed real-time simulations based on linear prediction methods and time-frequency representation of interface quantities. The research activities address the challenge of mitigating data latency in geographically distributed real-time simulations involving hardware in the loop (HIL) by providing a theoretical framework for evaluating stability and accuracy in geographically distributed real-time simulation. The results indicate critical issues of latency effect and serve as a basis to further improve latency

mitigation techniques. Better techniques will enable higher-fidelity simulations by reducing the effects of data latency. This will help in leveraging specialized hardware resources across multiple geographic locations. The connectivity between real-time simulators at INL and the National Renewable Energy Laboratory enabled first-of-its-kind distributed power HIL experimentation.

#### SIGNIFICANCE

Challenges in predicting transients (microseconds to seconds) under increasing penetration of hybrid energy systems consisting of distributed and renewable sources at the regional and national levels will also be addressed through this research. Large-scale, real-time simulations with HIL are important in understanding the close-to-real-world response of electric power systems with integration of newer technologies and renewable energy sources. The project enables de-risked, large-scale deployment of renewable energy and smart grid technologies pertinent to national and regional power grids of the future. This helps address the existing gaps in the design and operational tools for modeling and simulation of the dynamics of power electronics operating in timescales of microseconds to milliseconds. As part of the project research collaborations, three Ph.D. student interns and one summer intern were supported.

#### KEY PUBLICATIONS

- **Liu, R., M. Mohanpurkar, M. Panwar, R. Hovsopian, and A. Srivastava,** 2017, “Geographically Distributed Real-time Digital Simulations Using Linear Prediction,” *International Journal of Electrical Power and Energy Systems*, Vol. 84, pp. 1–9.
- **Luo, Y., M. Panwar, M. Mohanpurkar, and R. Hovsopian,** 2016, “Real Time Optimal Control of Supercapacitor Operation for Frequency Response,” *2016 IEEE Power and Energy Society General Meeting (PESGM)*, Boston, Massachusetts, pp. 1–5 (doi: 10.1109/PESGM.2016.7742036).
- **Mohanpurkar, M., M. Panwar, S. Chanda, M. Stevic, R. Hovsopian, V. Gevorgian, S. Suryanarayanan, and A. Monti,** 2016, “Distributed Real-time Simulations for Electric Power Engineering,” in *Cyber-physical Social Systems and Constructs in Electric Power Engineering*, The Institution of Engineering and Technology, London, United Kingdom, November 2016.
- **Stevic, M., A. Monti, and R. Hovsopian,** “A Theoretical Framework for Interface Design for Geographically Distributed Real-time Simulation of Power Systems,” *IEEE Transactions on Power Systems*, submitted.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> Colorado State University

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## CATALYTIC CONVERSION

### *Tailoring the Kinetic Function of a Surface through the Electronic Effects of Nanoscale Architecture (Project 15-146)*

Rebecca Fushimi<sup>1</sup>



Research scientist Rebecca Fushimi oversees the Temporal Analysis of Products (TAP) reactor in the Center for Advanced Energy Studies.

#### SCIENTIFIC ACHIEVEMENT

The surface of a solid catalyst orchestrates the making and breaking of chemical bonds. While there are endless varieties of catalytic architectures one can create, there are only a few chemical bonds one needs to break/form in catalytic chemical synthesis: C-H, C-C, C-O, O-H, etc. Specifically, this project is focused on the selective dehydrogenation of light alkanes—for example, conversion of ethane to ethylene. This work utilizes a unique, low-pressure transient kinetic

technique known as TAP (Temporal Analysis of Products) to understand how nanoscale bimetallic architectures, namely core-shell configurations of different precious metals (Pt, Pd, Re, Au) and base metals (Co, Ni, Sn), can be used to direct the activation of light alkanes.

#### SIGNIFICANCE

Energy supply plays a key role in our national security. At present, our abundant domestic shale gas resources are mainly used for heat and power generation, with

a large quantity sold to foreign markets. With new catalytic technology, the United States can upgrade its shale gas resources to more valuable chemical building blocks to replace the conventional production of fuels and chemicals that are currently based on breaking down petroleum. This research contributes to the fundamental understanding of how catalytic materials can be improved to control a desired sequence of chemical reactions, starting from simple molecules and leading to more efficient generation of valuable products such as ethylene and propylene, which are the cornerstone on which consumer goods such as polymers, fibers, paints, plastics, and pharmaceuticals are built. This work supports two postdoc researchers.

#### KEY PUBLICATIONS:

- Fushimi, R., J. Gleaves, and G. Yablonsky, 2015, “Experimental Methods for the Determination of Parameters,” in Z. I. Onsan and A. K. Avci (Eds.), *Multiphase Catalytic Reactors: Theory, Design, Manufacturing, and Applications*, John Wiley & Sons.
- Wang, L. C., C. Friend, R. Fushimi, and R. J. Madix, 2016, “Active Site Densities, Oxygen Activation and Adsorbed Reactive Oxygen in Alcohol Activation on npAu Catalysts,” *Faraday Discussions*, Vol. 188, pp. 57–67.

<sup>1</sup> Idaho National Laboratory

# LDRD Project Highlights

## Clean Energy Deployment

### B I O M A S S   C O N V E R S I O N

#### Advanced Carbon Feedstock Processing Using Ionic Liquids (Project 16-002)

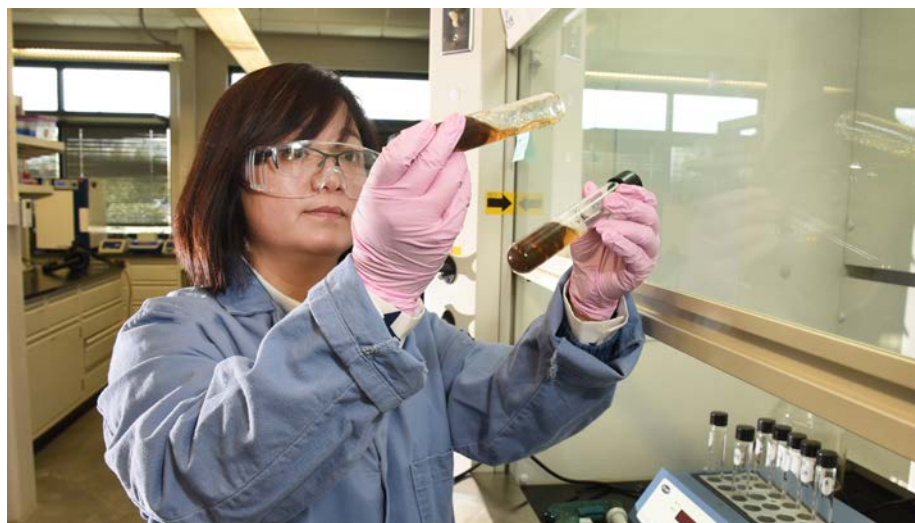
Chenlin Li,<sup>1</sup> Luke Williams,<sup>1</sup> Hongqiang Hu,<sup>1</sup> and Katie Li<sup>2</sup>

#### SCIENTIFIC ACHIEVEMENT

This project focuses on developing efficient coal and biomass conversion technologies by developing and demonstrating laboratory R&D efforts pertaining to ionic liquid (IL)-based carbon conversion processes targeting low-rank Wyoming coal and lignocellulosic biomass feedstocks. Coal and lignocellulosic biomass are the two major carbon-based domestic energy sources receiving intensified interest for efficient conversion into fuels and chemicals. Developing environmentally benign and low-energy conversion technologies is necessary to address the concerns of energy security and process economics. Both coal and biomass have macromolecular networks and cross-link structures and also contain valuable rare-earth elements, as well as inhibitory ash and minerals, requiring efficient depolymerization, extraction, and demineralization to be transformed into clean fuels, chemicals, and high-value materials. ILs are utilized for carbon feedstock depolymerization and upgrading.

#### SIGNIFICANCE

This research enables a fundamentally novel approach to carbon engineering and biomass/coal refining. The research aims to establish capabilities pertaining to an efficient, low-energy, and environmentally benign IL-mediated process for the production of clean fuels and high-value materials. This work supports the mission of the DOE Office of Energy Efficiency & Renewable Energy (Bioenergy Technologies



Principal Investigator Chenlin Li is studying new ways to break molecular linkages in biomass such as corn stover.

Office) to transform biomass into fuels and chemicals. This work also supports the mission of the DOE Office of Fossil Energy to ensure the continued use of traditional resources for clean, secure, and affordable energy. This project supported an intern, graduate students, and a postdoc.

#### KEY PUBLICATIONS

- Li, C., et al., 2010, "Comparison of dilute acid and ionic liquid pretreatment of switchgrass: Biomass recalcitrance, delignification and enzymatic saccharification," *Bioresource Technology*, Vol. 101, No. 13, pp. 4900–4906.
- Li, C., et al., 2013, "Comparing the Recalcitrance of Eucalyptus, Pine, and Switchgrass Using Ionic Liquid and Dilute

Acid Pretreatments," *BioEnergy Research*, Vol. 6, No. 1, pp. 14–23.

- Li, C., "Towards the Application of Biomass Ionic Liquid Pretreatment for Biofuels Production – A Technical Review," invited paper for the special issue "Ionic Liquids and Deep Eutectic Solvents for Synthesis," *Materials and Energy of Molecules*, in preparation.
- Li, C., C. L. Williams, J. Allen, B. Thomas, and H. Hu, "Sub-bituminous Coal Dissolution and Dispersion Behavior in Various Ionic Liquids," *Applied Energy*, in preparation.

<sup>1</sup> Idaho National Laboratory

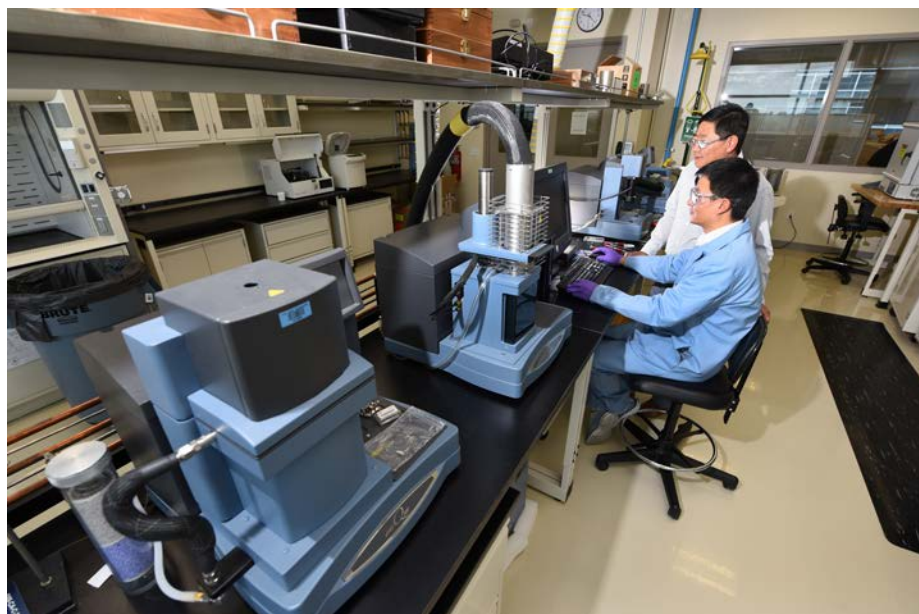
<sup>2</sup> University of Wyoming

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## DIRECT-CARBON FUEL CELL

### Development of Direct-Carbon Fuel Cells (Project 16-176)

Ting He<sup>1</sup> and Maohong Fan<sup>2</sup>



*Directorate Fellow Ting He (left) and Research Scientist Dong Ding use an instrument for measuring thermal properties of bioderived carbon to determine its potential for use as fuel in direct-carbon fuel cells.*

#### SCIENTIFIC ACHIEVEMENT

This project aims to develop robust, reduced-temperature, direct-carbon fuel cells (DCFC). The DCFC technology will offer a new paradigm to the coal industry and achieve a close-to-zero (operating) carbon footprint without employing expensive carbon capture technologies. This project aims to fundamentally

change the coal industry paradigm from “combustion” to “electrochemical oxidation” so that carbon derived from coal (or biomass or eventually biowaste) can be used as a clean energy source. The success of this project will impact not only the regional, national, and global coal industry but also the way we think of energy and our energy future.

#### SIGNIFICANCE

Energy security, economic vitality, and climate change are challenges facing our nation. The DCFC technology developed during this project will play key roles across the board for high energy efficiency and productivity. The project will also help address the nation’s transformation to sustainable and renewable energy self-reliance. The technology will help the regional, national, and global coal and power industries to dramatically reduce their carbon footprint, meet the Environmental Protection Agency’s Clean Power Plan target, and reduce environmental impacts from coal.

An early career engineer who brings knowledge and skills in electrochemical clean energy carbon conversion and upgrade was hired as a result of this project.

<sup>1</sup> Idaho National Laboratory

<sup>2</sup> University of Wyoming

# LDPRD Project Highlights

## Critical Infrastructure Protection

### CYBERSECURITY

#### Remote Vulnerability Analysis of CAN Bus Networks (Project 14-032)

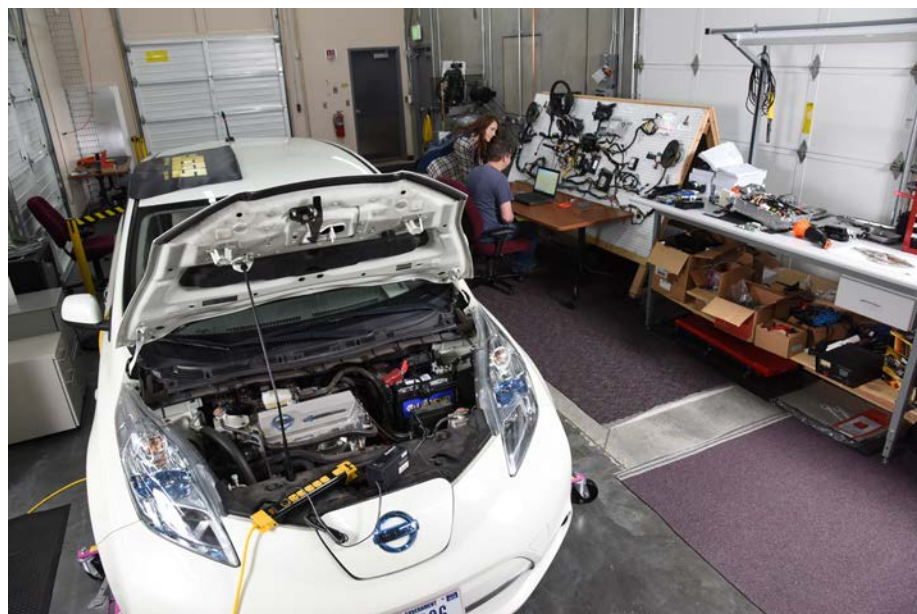
Jonathan Chugg<sup>1</sup> and Kenneth Rohde<sup>1</sup>

#### SCIENTIFIC ACHIEVEMENT

With the further development of “connected vehicles,” the use of outdated and vulnerable Controller Area Network (CAN) communications protocol, and the integration of these vehicles into various sectors of our nation’s infrastructure, additional vigilance is needed to ensure that cybersecurity is a priority in the development life cycle. The CAN protocol also supports many different protocols that are used in a wide variety of areas, including automobiles, road transportation, rail transportation, industrial automation, power generation, maritime transportation, military vehicles, aviation, and medical devices. This research enabled the discovery of new technologies capable of enhancing the cybersecurity of the CAN Bus networks that are used within a typical passenger vehicle, with applications that can also address transportation systems related to aerospace, rail, and maritime.

#### SIGNIFICANCE

The research being performed has already enhanced cybersecurity for sectors of the nation’s critical infrastructure that utilize CAN Bus networks, including transportation, law enforcement, energy, and nuclear security. This research initially focused on a typical passenger vehicle and is intended to result in deployed cybersecurity innovations that are used in all CAN Bus networks. A final goal of the research is to identify the security flaws of an electric vehicle, charging station, and the electric grid and interconnects between all three systems. This project provided the opportunity to develop the research and



*The CAN Bus lab illustrates the interconnection between the physical and mechanical parts with the computerized and automated functions.*

refine INL researcher skills and expertise necessary to advance state-of-the-art research into communications in and around the transportation sector. Ongoing and potential follow-on funding as a result of this research includes: four operational multiyear and multimillion dollar projects, two multiyear projects that are near a working agreement, and four projects that are in the initial stages of development.

#### KEY PUBLICATIONS

- **Chugg, J. and K. Rohde**, 2015, “Vehicle (In)Security,” *International Atomic*

*Energy Agency International Conference on Computer Security in a Nuclear World*, June 2015.

#### INVENTION DISCLOSURES AND PATENTS

- IDR BA-814, “CAN Bus Network Safety and Security System.”
- IDR BA-858, “Instrumentation to Monitor the Physical Properties of Serial Network.”

<sup>1</sup> Idaho National Laboratory

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## CRITICAL INFRASTRUCTURE DEPENDENCY

### All Hazards Critical Infrastructure Knowledge Framework (Project 14-093)

Ryan Hruska<sup>1</sup> and Cherrie Black<sup>1</sup>



*Advanced mapping and visualization help to clarify both the complex interaction of our nation's integrated infrastructure, and the complexity of systems that make up critical infrastructure across a region, state, or municipality.*

#### SCIENTIFIC ACHIEVEMENT

This project provided the preliminary proof-of-concept demonstration of innovative knowledge-discovery and decision-support methodologies that enable emergency planners and threat analysts to understand the complex, dependent relationships of critical infrastructure systems. The resulting All Hazards Knowledge Framework uses machine learning and advanced database methodologies to improve our ability to

collect, integrate, and leverage disparate information sources so we can fully understand the security and resilience posture of critical infrastructure.

#### SIGNIFICANCE

The knowledge gained and capabilities developed through this project have substantially enhanced the capacity of DOE and the Department of Homeland Security to effectively prepare for, protect against, and recover from a wide

variety of individual and combined hazards. The capability to conduct better dependency analyses addresses national objectives outlined in PPD-21, "Critical Infrastructure Security and Resilience"; NIPP 2013, "Partnering for Critical Infrastructure Security and Resilience"; and EO 13636, "Cybersecurity." This project provides a foundational level of understanding of critical infrastructure and its dependencies, enabling better risk and prioritization decisions.

#### KEY PUBLICATIONS

- **Amarasinghe, K., M. Manic, and R. Hruska**, 2015, "Optimal Stop Word Selection for Text Mining in Critical Infrastructure Domain," *IEEE Resilience Week*, Philadelphia, Pennsylvania, August 2015.

<sup>1</sup> Idaho National Laboratory

# LDRD Project Highlights

## Critical Infrastructure Protection

### CRITICAL INFORMATION VISUALIZATION

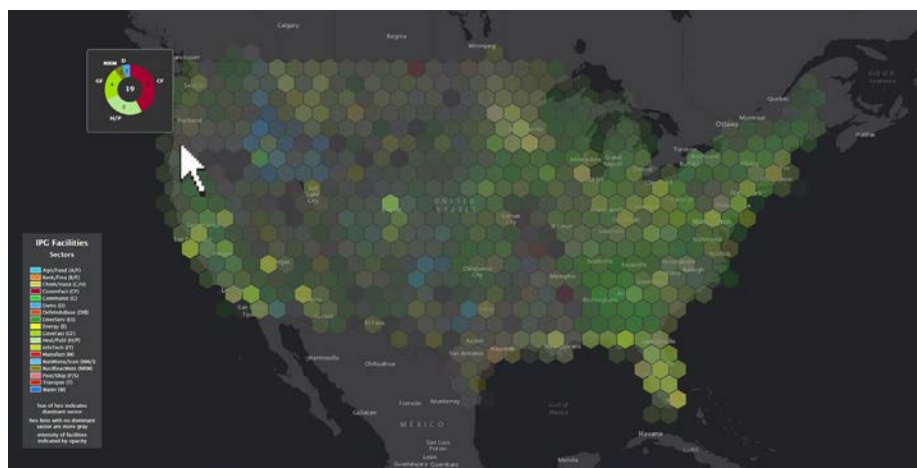
#### Visualizing Highly Dense Geospatial Data (Project 15-083)

Shane Cherry<sup>1</sup> and Robert Edsall<sup>1</sup>

#### SCIENTIFIC ACHIEVEMENTS

Analysts, responders, and decision-makers who consider the nation's critical infrastructure are faced with constantly changing and massive streams of data from disparate sources. These data streams are dense in time, space, and dimension—frequently updating for hundreds of thousands of critical infrastructure locations across the country, with dozens of variables about each location being logged with every record. Turning these raw data streams into actionable information, and in turn knowledge and insight, is extremely important for the protection of the nation's critical infrastructure and was the focus of this project.

Researchers designed and developed geovisual analytical tools for the examination of, in particular, the spatial character of critical infrastructure assets across the United States. Prior to this research, maps of critical infrastructure assets were either too cluttered to be useful or too simplified to reveal useful patterns. This LDRD resulted in two novel techniques to simultaneously provide a user both focus and context at multiple spatial scales of the dense, irregular, and multivariate data sets of critical infrastructure facilities. First, a generalization and aggregation technique called hexagonal binning was employed, providing statistical summaries of characteristics of the critical infrastructure facilities contained within a simulated standard-sized hexagon, one of thousands of hexagons in a simulated mesh overlaid across the nation. Additionally, a novel mapping tool called a Spyglass was introduced that



*Resilience centers on the notion of a complex system being able to recover and continue operating through disruptive, man-made, or natural events. INL has led in this area by spearheading groundbreaking technologies designed to incorporate and evaluate big data.*

allows the user to select a scale within an inset-map window—similar to a magnifying glass with custom magnification levels—and to examine local variation among assets while maintaining the context shown on the larger map. Both of these techniques were developed as dynamic and interactive, updating and recalculating in real time as the user pans and zooms the underlying map, and allowing flexible exploration of the data sets, revealing local detail while maintaining wider-scale context.

#### SIGNIFICANCE

With these new tools, time-critical analysis is facilitated in order to enhance the resilience of the nation's critical infrastructure. This project has been the subject of three national

presentations, a manuscript in preparation, a refereed book chapter to appear in 2017, and adoption for use by the Department of Homeland Security. The project supported the summer internship of a graduate student whose accomplishments and contributions in the project led to his subsequent hire as a full-time geospatial R&D scientist at INL.

#### KEY PUBLICATIONS

- Edsall, R., "Interface Modalities," in *International Encyclopedia of Geography*, Hoboken: John Wiley & Sons, in press late 2016.

<sup>1</sup> Idaho National Laboratory

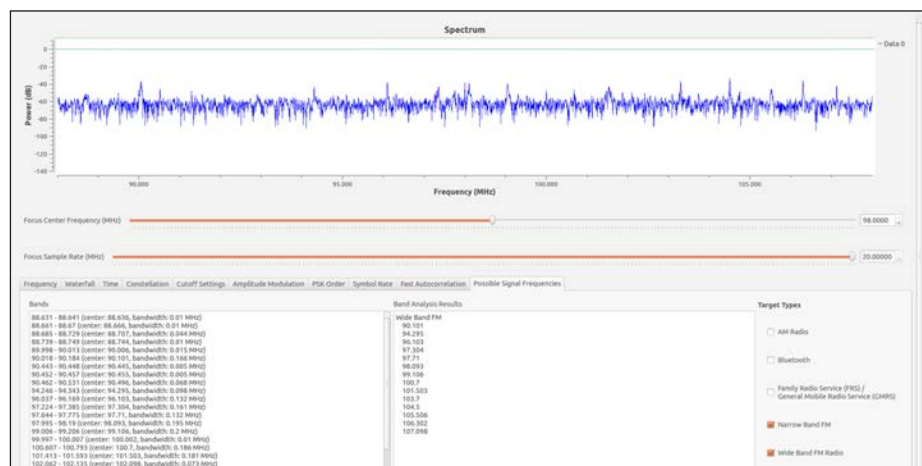


# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## SECURE WIRELESS COMMUNICATION

### Wireless Radiofrequency Signal Identification and Protocol Reverse Engineering (Project 16-152)

Kurt Derr<sup>1</sup> and Samuel Ramirez<sup>1</sup>



INL researchers work on cutting-edge ideas to increase network efficiency, improve security, and use available bandwidth more effectively.

### SCIENTIFIC ACHIEVEMENT

Most organizations have no idea of the breadth and depth of wireless communications in their surroundings or of the wireless signals emanating from mobile devices that may be used to attempt to perform malicious acts—or even just listen in—on their systems. The Wireless Radio Frequency Signal Identification and Protocol Reverse Engineering (WiFIRE) project is developing wireless classification algorithms to rapidly identify both known (such as WiFi, Bluetooth, and ZigBee) and unknown radio frequency signals. Machine learning, software-defined radio, and protocol reverse engineering techniques are being

utilized to create a tool that may identify malicious or unintentional wireless signals that could be interfering or tampering with legitimate communications.

### SIGNIFICANCE

Wireless communications devices are widely used in the areas of public safety, emergency response, nuclear power plants, and critical infrastructure applications. The WiFIRE capability will enable INL and others to determine the network protocols in use by a wireless black box device that may pose a threat to the U.S. Government and INL customers. WiFIRE will also enable the potential discovery of exploitable vulnerabilities of the black box device; uncovering these vulnerabilities

may lead to control of the device and mitigation of any malicious actions.

Two Ph.D. interns and one professor from the University of Utah are collaborating with INL personnel on this research. One visiting faculty member and an undergraduate intern from Weber State University provided technical support in the summer of 2016.

### KEY PUBLICATIONS

- **Becker, C., A. Baset, S. K. Kasera, T. Denning, K. Derr, and S. Ramirez**, “Real-time Wireless Signal Classification Combining Energy Detection and Cyclostationary Techniques,” *ACM MobiCom 2017, 23rd International Conference on Mobile Computing and Networking*, to be submitted March 2017.
- **Hearn, C., A. Kuznicki, C. Becker, K. Derr, and S. Ramirez**, 2016, “Data Acquisition in Wireless Router Link Testbed using GNU Radio Companion,” *GNU Radio Conference Proceedings*, Boulder, Colorado, September 2016.

<sup>1</sup> Idaho National Laboratory

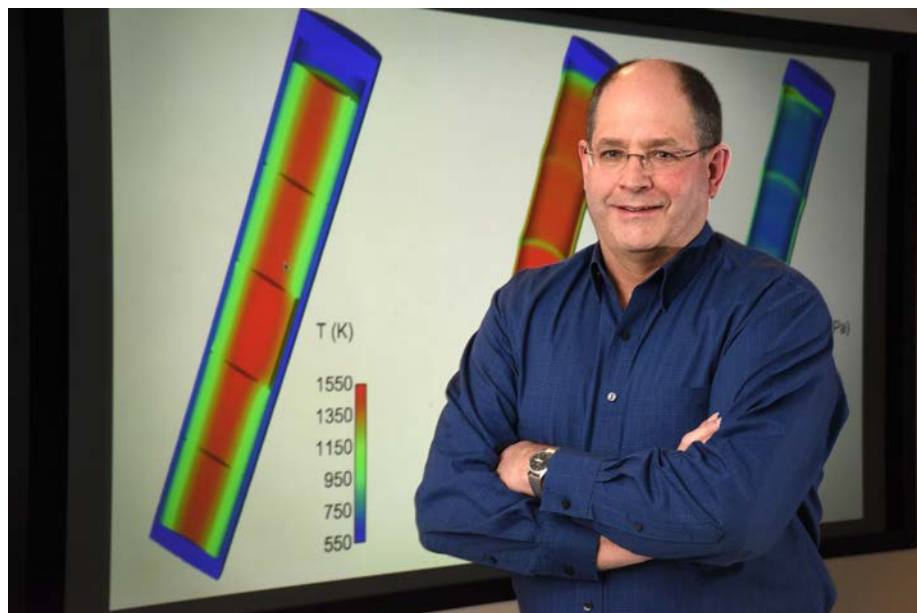
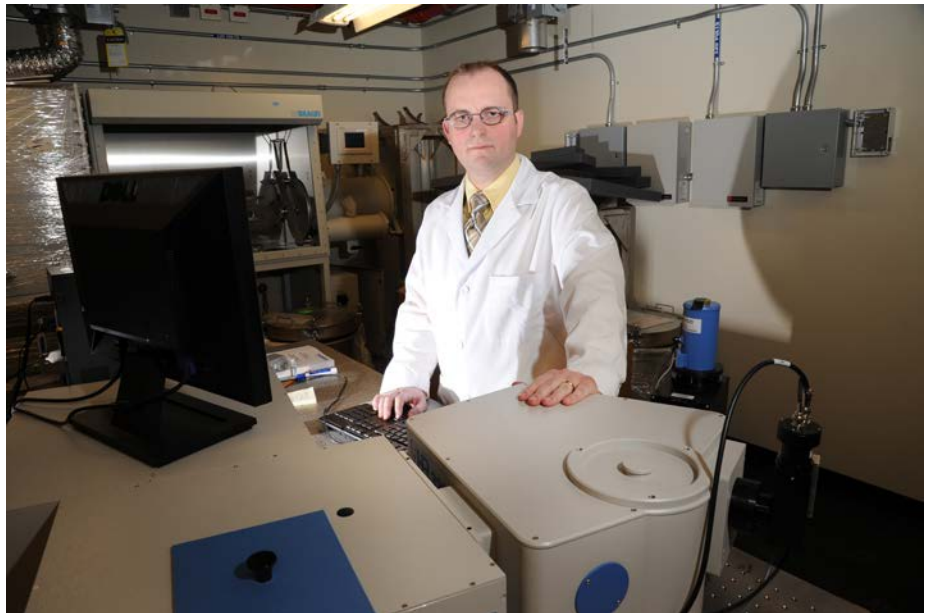
# Awards, Publications, Patents

## AWARDS AND RECOGNITION

### **Leigh Martin**

*Award: Early Career Fellow of the Industrial & Engineering Chemistry Division of the American Chemical Society*

Leigh Martin was named an Early Career Fellow by the Industrial & Engineering Chemistry Division of the American Chemical Society. This award recognizes innovative contributions to and publications on applied chemistry or engineering from early career (under 40 years of age) members of academic, industrial, or government laboratories. Martin received the award based on his extensive and frequently cited work in nuclear fuel cycle chemistry, including aqueous separations and actinide/lanthanide separations processing (Project 13-933).



### **Richard Williamson**

*Award: 2015 American Nuclear Society Materials Science & Technology Division Special Achievement Award*

INL's Richard Williamson, in collaboration with Michael Tonks, an assistant professor of mechanical and nuclear engineering at Penn State University, received this award for developing the BISON-MARMOT fuel performance codes, which are used to predict how reactor fuel behaves throughout its time in a reactor. The goal of the codes is to understand how heat is conducted through the reactor, understand how the reactor mechanically deforms to prevent adverse effects from happening, and ensure that the reactor is efficient. The codes use modern computer architectures effectively, can run on large supercomputers, and are flexible in the type of geometry they can model (Project 14-031).

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## PUBLICATIONS AND PATENTS

Publications are focused within three initiatives: advancing nuclear engineering, clean energy deployment, and critical infrastructure protection. The number and quality of publications related to the INL

LDRD Program are increasing (see table below). More than 50% of INL's LDRD project-related publications are developed with external collaborators, including

personnel from universities, national laboratories, and industry. A small portion of LDRD-related publications is developed with international collaborators.

### FY 2015 and 2016 Publications Comparison

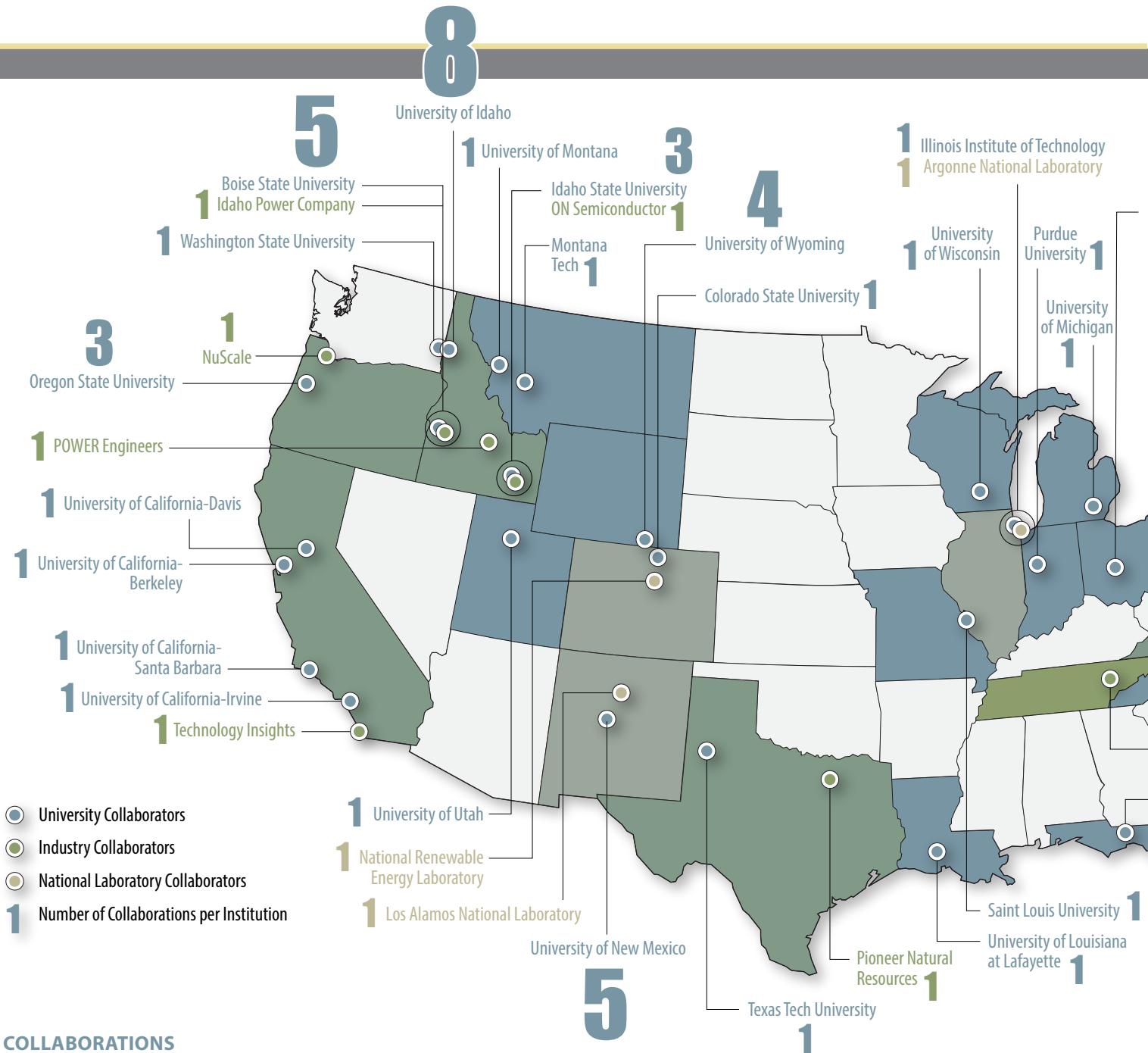
Publication Measures	FY 2015	FY 2016
Total	32	44
Advancing Nuclear Engineering (% of total)	15 (47%)	21 (48%)
Clean Energy Deployment (% of total)	11 (34%)	22 (50%)
Critical Infrastructure Protection (% of total)	6 (19%)	1 (2%)
Average Journal Impact Factor <sup>a</sup>	2.94	3.6
Lowest Impact Factor	0.936	0.59
Highest Impact Factor	9.22	31.083
Publications with External Collaborators	25 (76%)	22 (50%)
Number of External Collaborators	38	30
Number of Publications with International Collaborators	6	1

### 2016 LDRD Program Patents

Title and Patent Number	Inventors
Dry Recycle of Spent Nuclear Fuel—Separation of the Rare-Earth Fission Project Poisons (9,428,401)	James W. Sterbentz, Jerry D. Christian Project: 99-292
Alteration of Enzyme Stability and Activity via Covalent Modification (9,234,228)	David N. Thompson, William A. Apel, Vicki S. Thompson, David William Reed, Jeffrey A. Lacey Project: GB103
Self-Generating Fault-Tolerant Encryption Key (9,215,587)	Hussein Moradi, Behrouz Farhang, Rangam Subramanian Project: 13-093
Thermolytic Draw Solute for Osmotically Driven Membrane Processes (9,399,194)	Aaron D. Wilson, Christopher J. Orme Project: 14-079
Methods and Apparatuses Using Filter Banks for Multi-carrier Spread Spectrum Signals (9,369,866)	Hussein Moradi, Behrouz Farhang, Carl A. Kutsche Project: 10-075

a. The impact factor of an academic journal is a measure reflecting the average number of citations to recent articles published in that journal. The impact factor is frequently used as a proxy for the relative importance of a journal within its field; journals with higher impact factors are deemed to be more important than those with lower ones.

# Collaborations



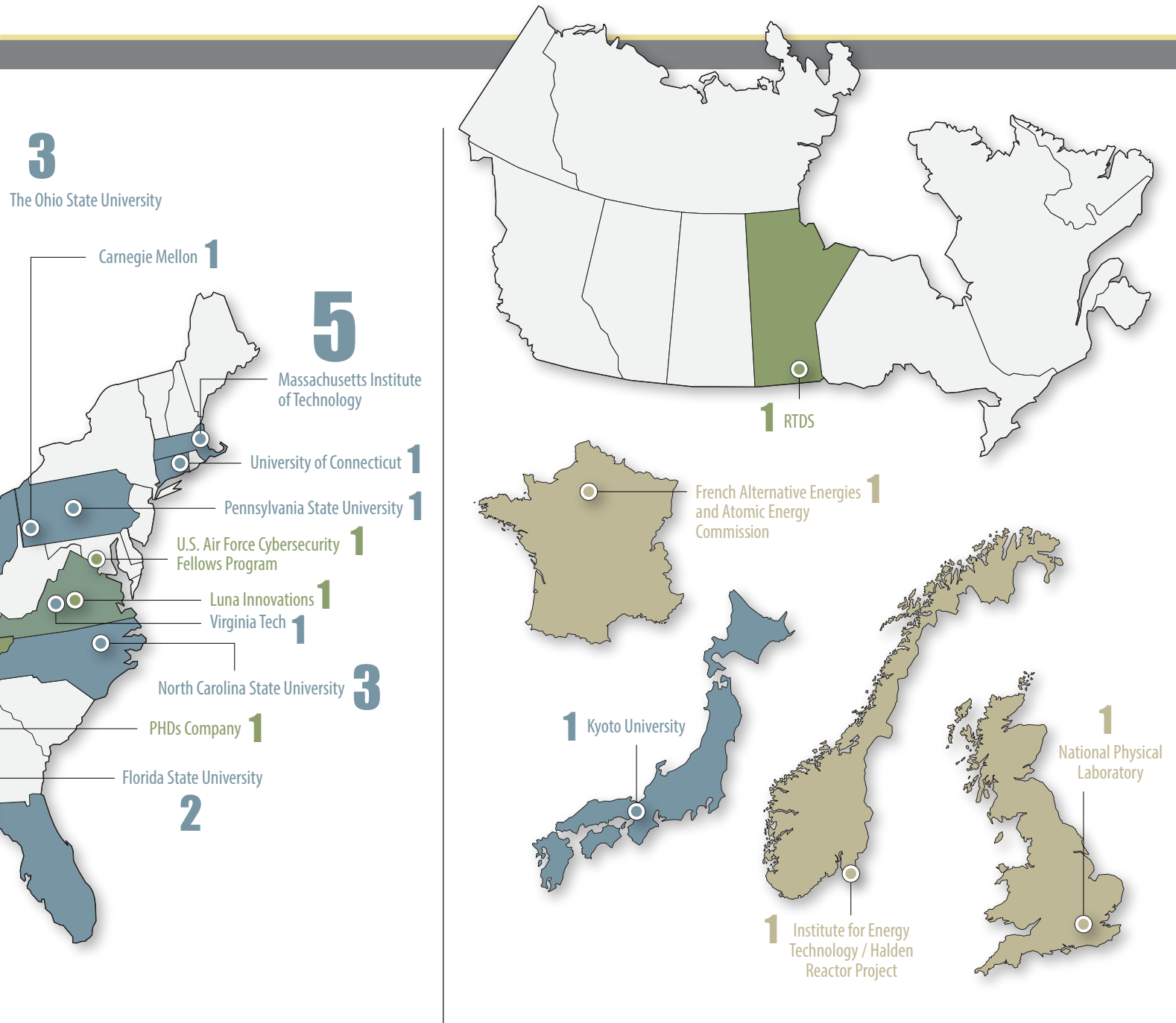
## COLLABORATIONS

The LDRD Program's collaborations with university researchers, national laboratory researchers, and industry (both nationally and internationally) help build a pipeline of competent researchers, create multidisciplinary

teams with complementary capabilities, foster creativity, and create opportunities to find and accelerate innovations to address science and technology challenges and advance DOE mission objectives. Of the 71 LDRD projects funded in

FY 2016, more than half (59% or 42 projects) involved at least one type of collaboration with universities, industry, and/or national laboratories and included one international collaboration. University collaborations dominate

# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016



the collaborations list, constituting 38 of the 42 (more than 90%) projects. INL LDRD projects had 60 university collaborations, 10 industry partners, and six national laboratory collaborations. Five LDRD projects included nine

industry partners. Five LDRD projects included collaborations with six national laboratories. Collaborations spanned R&D topics that will advance nuclear energy, accelerate clean energy deployment, and enhance critical infrastructure protection.

Collaborations with institutions such as universities addressed multiple research areas. The graphic above summarizes FY 2016 efforts in leveraging LDRD projects to advance INL's collaborations.

# Doctoral Research

## SUPPORTING INL DOCTORAL RESEARCH

LDRD investments help build a pipeline of science and technology personnel at INL by supporting doctoral and postdoc research being conducted by INL staff and through graduate and undergraduate R&D internships. INL's 71 LDRD projects in FY 2016 supported 105 student interns, including 39 doctoral candidates and 40 master's degree and 26 undergraduate research interns. The tables below summarize FY 2016 efforts in developing INL's science and technology pipeline.

### Staff Pursuing a Ph.D.

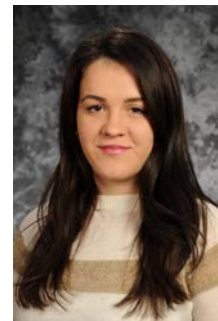
Staff Member	University Affiliation
Paul W. Talbot	University of New Mexico
Ryan Hruska	Idaho State University
Tony Koonce	Idaho State University
Justin Coleman	University of Buffalo, New York
Marija Stevic	RWTH Aachen University, Germany
Mayank Panwar	Colorado State University
Mathew Snow	Washington State University
Timothy Klett	University of Idaho



*Ryan Hruska (right)*



*Mayank Panwar*



*Marija Stevic*



*Paul Talbot*



*Justin Coleman (left)*

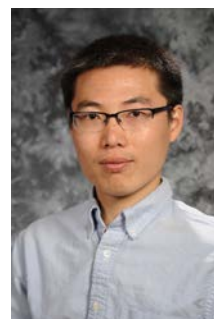
# Laboratory Directed Research and Development SNAPSHOT – FISCAL YEAR 2016

## Postdoctoral Fellows

Postdoc Name	Graduating University
Abir, Muhammad	Missouri University of Science and Technology
Adhikari, Birendra	University of Colorado
Antonio, Daniel J.	University of Nevada
Baroi, Chinmoy	University of Saskatchewan
Calderoni, Patrick	University of California
Diao, Weijian	University of South Carolina
Diaz Aldana, Luis A.	Ohio University
Fullerton, Michele	University of Florida
Heathman, Colt R.	Washington State University
Jiang, Wen	Duke University
LaBrier, Daniel	University of New Mexico
Liu, Maolong	University of New Mexico
Luo, Yusheng	Florida State University
Lwin, Soe	Lehigh University
McNally, Josh	Boston University
Meher, Subhashish	University of North Texas-Denton
Pawar, Gorakh M.	University of Utah
Price, Patrick	Boise State University
Rai, Durgesh	Massachusetts Institute of Technology
Redekop, Evgeniy	University of Oslo, Norway
Shi, Shanbin	The Ohio State University
Short, Michael	Massachusetts Institute of Technology
Shrestha, Keshav	University of Houston
Skifton, Richard	University of Idaho
Veeraraghavan, Swetha	California Institute of Technology
Wang, Congjian	Purdue University
Weaver, Gabriel	University of Illinois, Urbana-Champaign
Yadav, Vaibhav	University of Iowa
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## POSTDOCTORAL FELLOWS

Thirty-one postdocs were supported fully or partially through INL's FY 2016 LDRD projects.



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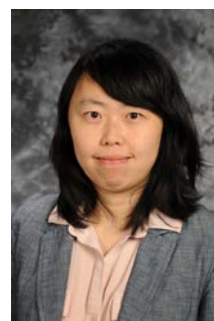
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