





Proudly Operated by **Battelle** Since 1965

# 2018 Aboratory Agenda

### A Message from Steve and Roger



Pacific Northwest National Laboratory distinguishes itself in many ways, notably our commitment to deliver outstanding science & technology to our sponsors that makes a difference to the nation. We are guided by a sound strategy with a focus on advancing scientific discovery, improving energy resiliency, and enhancing national security. Underpinning our ability to deliver important outcomes in these areas are nationally recognized capabilities, including chemistry, earth sciences, and data analytics.

The challenges we tackle are complex and require close collaboration with academia, industry, and other key stakeholders. We will expand and strengthen these partnerships, with an emphasis on regional engagements in areas where the Northwest is uniquely suited to lead the nation. We will also build on our ties with industry to speed innovation.

Investments to grow our capabilities and modernize our campus are critical to meet the evolving priorities of our sponsors

and nation for decades to come. This year, we completed construction of the General Purpose Chemistry Laboratory and nearby Engineering and Analysis Building, and we broke ground on the long-anticipated collaboration center, Discovery Hall, to be completed in the spring of 2018. These facilities are part of our plan for a mission-ready campus that is modern, collaborative, flexible, and sustainable.

While we pride ourselves on excellence in science & technology, PNNL embraces Battelle's philosophy of simultaneous excellence, which also encompasses excellence in management and operations and in community service. Our ability to execute our programs safely, securely, and in an environmentally responsible manner is vital to achieving our mission. We are equally committed to serving as a good neighbor through Team Battelle projects, Battelle's philanthropic giving, and volunteer efforts that help make our community a better place to live.

At the heart of PNNL is you—our talented scientists, engineers, and support professionals. We thank you for the vital contributions you make to the Laboratory, our sponsors, the community, and the nation. It is through your hard work and exemplary dedication that PNNL is widely recognized for exceptional science & technology, strong operational performance, and a long history of serving as a good neighbor.

We are pleased to offer the 2018 Laboratory Agenda and invite you to read on to learn more about PNNL's strategy and the priorities we will focus on in the coming year and well beyond.

Steven Ashby, Director Pacific Northwest National Laboratory Roger Snyder, Manager DOE Pacific Northwest Site Office At PNNL our **MISSION** is to transform the world through courageous discovery and innovation.

It is our **VISION** that PNNL science & technology inspires and enables the world to live prosperously, safely, and securely.

It is no easy task, and with our Values of integrity, creativity, collaboration, impact, and courage, our staff delivers time and time again.







### **Simultaneous Excellence**

PNNL's strategy is founded on Battelle's principle of simultaneous excellence in science & technology, management & operations, and community engagement.

**Excellence in Science & Technology** begins with our scientific vision, to understand, predict, and control the behavior of complex, adaptive systems. Underpinning this vision are strategic investments for the achievement of specific long-term goals, PNNL's six Laboratory Objectives.

#### **Excellence in Management & Operations**

is vital to our achievement of science & technology goals. PNNL has an obligation to be a good steward of the resources with which our sponsors entrust us, and a responsibility to manage and carry out our programs safely, securely, and in an environmentally responsible way.

#### **Excellence in Community Engagement**

means ongoing engagement with our neighbors to improve lives, provide opportunities, and be an economic partner and resource for local industry. PNNL is deeply involved in our community, through individual efforts, Team Battelle projects, and Battelle corporate philanthropy.



Malin Young Deputy Director for Science & Technology

"All national labs have a special role to play by providing world-class science & technology to help the nation address its biggest problems. One attribute that sets PNNL apart is its ongoing attention to the Four Pillars. The effect that our actions and investments have on these factors is central to our strategic decision making."

## Four Pillars of Science & Technology Success

PNNL cultivates distinction in four areas that are critical to the Laboratory's successful execution of its mission.



PNNL is the nation's premier chemistry, environmental science, and data analytics Laboratory.



DOE recognizes 19 core capabilities at PNNL, spanning the chemical & materials sciences, mathematical & computational sciences, engineering, and earth & biological sciences.



PNNL's strategic partnerships include joint research institutes and joint appointments with U.S. universities, and long-term research collaborations with laboratories, academic institutions, and the private sector.



PNNL nurtures a culture of curiosity, innovation, and research excellence through programs and investments offering staff career growth opportunities that develop thought leadership.

PNNL delivers excellence in science and technology in three areas:

*Scientific Discovery* – PNNL is the nation's leading laboratory for research in chemistry, Earth sciences, and data analytics.

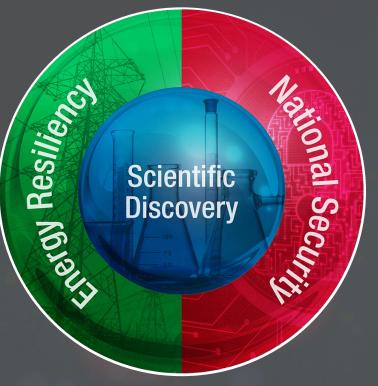
**Energy Resiliency** – PNNL's research focuses on the fundamental science and on technology development for the modernization of the U.S. electric power grid, and for advanced energy storage solutions.

**National Security** – PNNL is a leading source of innovation for the detection of illicit nuclear materials and nuclear non-proliferation, and for the development of cybersecurity technologies to protect critical U.S. infrastructure.

PNNL applies its strengths to address many of the largest scientific questions and technological challenges facing the nation and the world today. As a DOE national Laboratory, PNNL focuses on multidisciplinary and highconsequence "grand challenge" problems.

Mastering grand challenges requires deep expertise and leadership, world-class capabilities including state-of-the-art equipment and facilities, strong partnerships with other leading research institutions, and a culture of innovation. PNNL cultivates these Four Pillars of Science & Technology Success as the foundation for research excellence in each of its mission areas.

At the heart of PNNL's science & technology strategy are six Laboratory Objectives, longterm research commitments that build on the Four Pillars and draw together the Laboratory's



signature strengths. Laboratory Objectives focus on problems that are complex, urgent, and important to society—problems uniquely suited to the mission and resources of a national laboratory.

As the following pages show, each of PNNL's Laboratory Objectives embodies a vision of the world in 2025, addressing one central question: How would our success change the world for the better? Each Laboratory Objective applies PNNL's established and emerging science & technology leadership to transform the nation and the world in the next decade.

# Reinventing Chemical Catalysts and Catalytic Processes

**2025 Vision:** Once considered a waste product, carbon now is the foundation of a vibrant new U.S. energy industry. Strides in catalysis research allow U.S. firms to create high-quality fuels and advanced materials from abundant, domestic carbon feedstocks.

#### Goals

- Integrate and focus PNNL's world-leading capabilities in catalysis science for precise design and synthesis of hierarchical catalysts at atomic and molecular levels
- Develop bioinspired catalysts with faster reaction rates at lower temperatures and pressures to produce a cleaner, more resilient, more efficient, and costeffective energy infrastructure
- Create analytical methods for realtime monitoring of catalytic processes
- Craft theories describing complex reactions at interfaces and facilitating integration of chemistry and data science

### **Research Partners**













"DOE's investments at PNNL in the Institute for Integrated Catalysis and the Center for Molecular Electrocatalysis have helped us to achieve global leadership in the field. With DOE's support and our network of partners across Washington State, the United States, and the world, PNNL is leading in the discovery of new chemical pathways for the sustainable production and use of energy."



Lou Terminello Steward



Karl Mueller Science Lead

PNNL's Energy Sciences Capability, opening in 2020, will consolidate the Laboratory's world-class catalysis research and establish a global center for research collaboration in chemical and materials sciences.

## Understanding Multiscale Earth System Processes and Dynamics

**2025 Vision:** The Laboratory's advanced simulation tools now equip decision-makers to foresee and prepare for major environmental changes, and to avoid their worst impacts. PNNL researchers have achieved an integrated modeling framework capturing complex Earth systems as an integrated continuum, from molecular to global scales.

#### Goals

- Develop a holistic, integrated research framework to measure, test, and model ecosystem processes across the atmosphere-land-water continuum, with particular emphasis on terrestrial-aquatic interfaces
- Establish *The System for Terrestrial-Aquatic Research*, a distributed observation and analytics network with integrated computational tools, enabling validation of predictive Earth system models in real time
- Build a Coastal Observation & Research Partnership in collaboration with key research institutions, creating a testbed for technologies and data systems for measuring stresses and responses on terrestrial-aquatic ecosystems

### **Research Partners**



"As an established global leader in Earth system science, PNNL is now leading the community into the new frontier of terrestrial-aquatic ecosystems. Through our internal investments in initiatives like Predicting Ecosystem Resilience through Multiscale Integrative Science and with those of key sponsors in DOE's Office of Biological and Environmental Research, PNNL is pursuing an ambitious research program to unravel key mysteries of the Earth system, and include our research findings in highly sophisticated models leveraging the full potential of high-performance computers."

asset in research on the role of terrestrial-aquatic ecosystems in Earth system dynamics.

PNNL's Marine Sciences Laboratory,

located in Sequim, WA is a critical



Allison Campbell Steward



Charlette Geffen Science Lead

# Accelerating Scientific Discovery with Data Analytics and Simulation at Extreme Scales

**2025 Vision:** Data- and compute-intensive operations are coequal partners in research, promoting accelerated scientific discovery on extreme-scale computing platforms.

#### Goals

- Accelerate research and discovery integrating scalable data analytics and predictive modeling and simulation, addressing a key challenge in basic computer science and mathematics research with initial impacts in grid, cyber, climate, and chemistry domains
- Focus on advancing computing as an independent research field and on applying computing and data analytics to scientific discovery in multiple fields
- Develop and integrate software applications, tools, architectures, and methods to exploit the rapid and complex growth of data in scale, velocity, hetrogeneity, and dimensionality
- Lead machine learning for DOE missions and coupled human-machine discovery

### **Research Partner**

UNIVERSITY of WASHINGTON



Lou Terminello

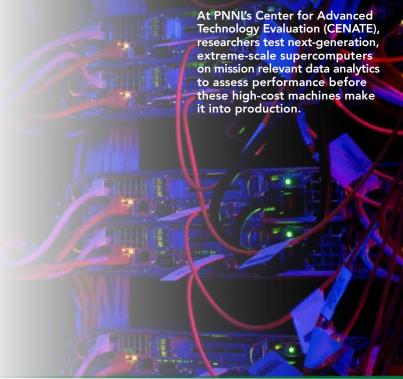
Steward



Nathan Baker Science Lead



Bill Pike Science Lead



"PNNL is a leader in the development of software applications for some of today's largest and fastest computing systems. With our sponsors in DOE's Office of Science and the Department of Defense, PNNL is successfully integrating data- and computingintensive architectures to unlock major advances in energy and materials sciences, human health, and national security."

# Mastering Phenomena Associated with Radioactive and Irradiated Materials

**2025 Vision:** A decade of rapid advances in understanding the behavior of radioactive materials has hastened the processing and safe storage of U.S. radioactive waste stockpiles, and deterred would-be proliferators by developing predictive identifiers of nuclear processing.

### Goals

- Direct and control chemical reactivity in radioactive materials and radiation environments
- Harness radiation-induced interfacial processes to create smart, sustainable new technologies
- Understand microstructural evolution in response to irradiation and radioactive environments

#### **Research Partners**

PNNL's Radiochemical Processing Laboratory is a vital resource for addressing Hanford tank waste, subsurface contamination, and other environmental challenges. A Hazard Category II Non-Reactor Nuclear Facility, RPL's capabilities are used to develop, test, and implement processes for environmental cleanup and other needs.

WASHINGTON STATE UNIVERSITY

University of Missouri











"With support from DOE's Office of Science, Office of Environmental Management, and the National Nuclear Security Administration, PNNL is moving the field from empirically driven approaches to scientifically driven development, dramatically expanding the range of solutions we can deploy to address the nation's environmental stewardship and non-proliferation challenges. With research centers like the Interfacial Dynamics in Radiation Environments and Materials, PNNL is in a strong position to lead this transition. In fact, if we do not, no one else will."



Tony Peurrung Steward



Sue Clark Science Lead

# Realizing a Secure, Flexible, and Resilient Electric Power System

**2025 Vision:** Innovations at PNNL have led the way to a renaissance of America's electric power system. The U.S. grid is now on the global leading edge, with technologies enabling the smooth integration of renewable energy sources, large-scale energy storage, and analytics for real-time, agile power management and secure data use.

#### Goals

- Develop exascale computing approaches to grid optimization
- Advance novel data analytic and computational approaches to drive threat-informed cybersecurity technology innovations
- Integrate innovations in materials science to realize safe, low-cost energy storage technologies

### **Research Partners**







Jud Virden Steward



Carl Imhoff Science Lead

PNNL's Electricity Infrastructure Operations Center (EIOC) features two full-function grid control rooms. Here, researchers design, test, and evaluate tools and concepts in a setting that mirrors current industry conditions. The EIOC is also a state-of-the-art training center for grid operations professionals.

"In collaboration with our long-term sponsors in DOE's Office of Electricity Delivery & Energy Reliability and Buildings Technology Office, PNNL aims to transform the 21st century grid by delivering key science & technology outcomes in three critical areas—grid flexibility and resiliency, cybersecurity, and energy storage. The PNNL campus will serve as a best-in-class testbed for coordinating building energy, while adding distributed energy resources that communicate with utilities and demonstrate energy savings, grid flexibility, and resiliency benefits."

### Protecting High-Consequence Cyber-Enabled Systems

**2025 Vision:** PNNL has reshaped the cyber landscape by revealing adversary strategies and tactics and developing situational analysis tools that are now the standard for the DOE and the nation's 17 critical infrastructures.

#### Goals

- Define and lead the "Science of Cyber" to discover secure design principles
- Drive developmental capability into operations across the DOE complex
- Provide a proving ground for technology transition into energy grid defense

### **Research Partners**









Tony Peurrung Steward



Dennis Nelson Science Lead

PNNL's state-of-the-art cyber training facility allows professionals to work with real-time data and control technologies to simulate a wide range of cybersecurity situations.

"Hardening U.S. cyber defenses is an urgent national security challenge. With our sponsors in the Departments of Energy, Defense, and Homeland Security, PNNL will deliver scientific and technological advances that fundamentally change the nature of the cyber landscape to mirror conventional conflict, where the defender has a distinct advantage."

### **Scientific User Facilities**

PNNL is home to two DOE Office of Biological and Environmental Research national scientific user facilities. These unique facilities are critical assets in the advancement of PNNL's sponsored research programs and LDRD-funded projects. Each year, they provide access to hundreds of academic, national laboratory, and industry scientists from across the nation.

The Environmental Molecular Sciences Laboratory (EMSL) pioneers molecular-level discoveries and equips the scientific community to generate new knowledge and predictive understanding of the Earth's atmosphere and subsurface, microbial communities, and cell functions.

The Atmospheric Radiation Measurement (ARM) Climate Research Facility is the world's premier observation system for climate change research. ARM is a global network of instrumented fixed, mobile, and aerial observatories for the measurement of clouds and aerosols, solar and thermal radiation, surface heat and moisture, and meteorological conditions.





Allison Campbell Associate Laboratory Director, Earth & Biological Sciences

"ARM and EMSL lie at the heart of our science & technology strategy. The combination of expertise and research instrumentation that these facilities house is not found anywhere else in the world. Our global reputation as a leader in climate and environmental science is directly linked to the research programs that ARM and EMSL make possible."

### **Excellence in Management & Operations**

Excellence in management & operations is vital to achieving our scientific vision. Our purpose is simple and clear: to make it easier for our scientists and engineers to become thought leaders and deliver world-class research for our sponsors and stakeholders. We strive to simplify the way we work, and to provide our staff members with the safest workplace, the most modern systems and tools, and the maximum time and resources to perform research. Our management & operations goals are:

- building greater workforce diversity
- driving innovation with new opportunities for collaboration internally and with external partners
- becoming a world leader in scientific data management
- leveraging our leadership in data analytics to derive new insights from operational and performance data streams to drive better decision-making
- improving the way we work by applying the scientific and technological advances we develop for our sponsors
- modernizing PNNL's campus



Mike Schlender Chief Operations Officer "Our 10-year campus strategy will transform PNNL and provide a state-of-the-art foundation of facilities, infrastructure, and instrumentation, allowing us to continue delivering world-class innovation solutions to our sponsors and the nation."

### **Excellence in Community Engagement**

Inspired by the belief that PNNL science & technology can strengthen the U.S. workforce and make the world a better place, we bring our expertise to bear on important local and regional outcomes, and help inform decisions that enhance the nation's future. Whether connecting decision-makers with trusted PNNL experts, facilitating community volunteerism and leadership, or furthering science, technology, engineering, and math (STEM) education, PNNL has built a strong and enduring foundation of external engagement and outreach.



PNNL provides career-focused learning experiences for students from middle school through postsecondary education.





Last year, PNNL staff members volunteered over 45,000 hours to Team Battelle projects.



Federal and state officials frequently turn to PNNL for technical advice.



Paula Linnen Executive Director, External Affairs

"PNNL is a proud and active member of the Tri-Cities community. The Laboratory has a wide range of outreach programs that allow us to engage in meaningful ways, and many individual PNNL staff members also serve in leadership roles in organizations across the region. Through all of these diverse engagements, we believe PNNL is an outstanding ambassador for science."



### **On the Cover**

#### The Mass Spectrometry of Nano-Gold

Environmental Molecular Sciences Laboratory (EMSL) material scientists are collaborating with physical chemistry scientists utilizing a single-particle mass spectrometer (SPLAT II) to push the frontiers of quantitative imaging of nanoparticles used in energy applications as well as those found in environment, like atmospheric aerosols. This work is in developing newer and more powerful characterization techniques that can image and quantify the dimension, density, and shape of nanoparticles, which exist in nature and can be artificially synthesized for a variety of applications. The image shows the scanning electron microscope image of an array of gold nanorods used as standards to calibrate the SPLAT II system in EMSL.

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#### www.pnnl.gov