Argonne NATIONAL LABORATORY

THE POWER OF ONE

ENERGY & GLOBAL SECURITY ANNUAL REPORT 2014

THE POWER OF ONE

We are collaborators, integrators and conveners. Our deeply held belief is that a cross-disciplinary approach—spanning computing to life sciences, physics to engineering—enables us to make the most revolutionary scientific and technological breakthroughs imaginable. Our world-class researchers collaborate and work alongside experts from industry, academia and other government laboratories to address national challenges in clean energy, the environment, technology and national security. As ONE team united by a common goal, we are able to uncover new and inspired answers that alone we could never achieve.

Message from Mark Peters

Associate Laboratory Director, Energy and Global Security

This past year has been a transformational period for the Energy and Global Security (EGS) Directorate, with many positive changes that will set the stage for continued success in the coming years.

My colleagues in EGS performed groundbreaking research throughout 2014 even as the directorate underwent numerous changes, from a new name to new leadership and the addition of several departments that will better align our directorate to Argonne's strategic mission.

When I assumed leadership of EGS—then known as Energy Engineering and Systems Analysis—in June, the directorate was already known as the home of applied science and engineering at Argonne, tasked with discovering practical solutions to challenges in areas of great importance to our country and to the world. To better reflect these areas of emphasis, we changed the name of the directorate to demonstrate our focus on Energy and Global Security. At the same time, the Decision and Information Sciences division changed its name to reflect its enhanced focus on Global Security Sciences.

We are now envisioning our future with the creation of a detailed strategic plan that lays out the roadmap EGS will follow as we strive to break new ground as modern-day pioneers and set milestones for progress and development worldwide. The plan identifies three key areas of immediate focus: Safe, Secure and Sustainable Nuclear Energy Systems; Building Resilient Communities; and Computationally Enhanced Mobility. The strategic plan also identifies four emerging trends that will become focus areas in their own right over the coming years. We can say with confidence that our pursuit of these new areas of research will yield exciting results and impact our nation, and the world, for years to come.

As part of this pursuit of innovation, EGS is committed to driving Argonne's ongoing effort to create teams that cut across divisions and directorates and partners with industry and academia to answer the big, ambitious scientific questions and help to ensure the future prosperity of the United States. Our goal is to lead the way at Argonne in creating true team dynamics that leverage the unique knowledge, skills and facilities that can only be found at a national lab.

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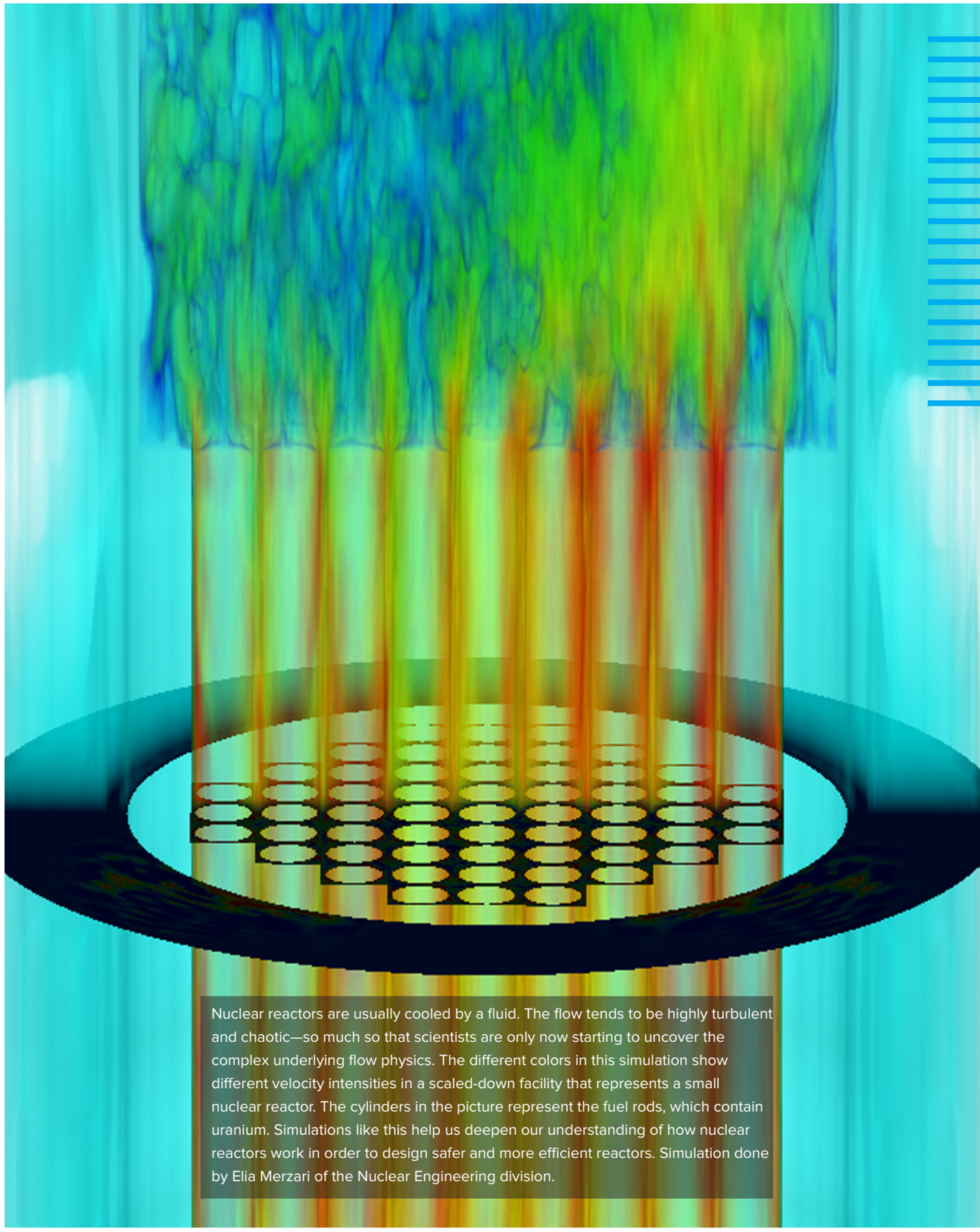


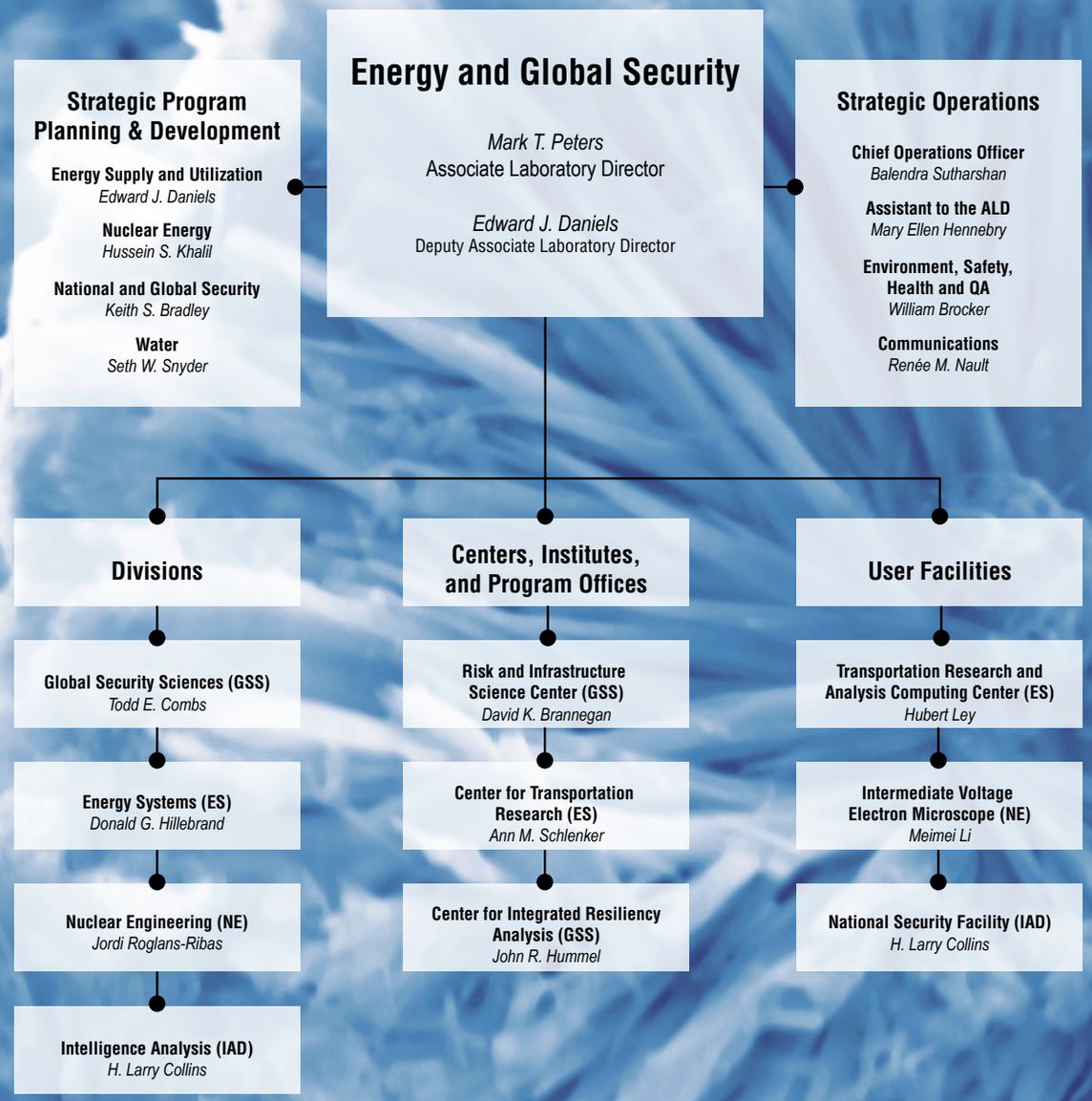
Nuclear reactors are usually cooled by a fluid. The flow tends to be highly turbulent and chaotic—so much so that scientists are only now starting to uncover the complex underlying flow physics. The different colors in this simulation show different velocity intensities in a scaled-down facility that represents a small nuclear reactor. The cylinders in the picture represent the fuel rods, which contain uranium. Simulations like this help us deepen our understanding of how nuclear reactors work in order to design safer and more efficient reactors. Simulation done by Elia Merzari of the Nuclear Engineering division.

WHO WE ARE

From our early beginnings as the nation's first national laboratory, Argonne has been at the forefront of thought leadership.

Today, Argonne National Laboratory's applied Energy and Global Security (EGS) Directorate continues with that tradition. EGS is pursuing unprecedented challenges and opportunities in domestic and global sustainable energy and security. We're not afraid to ask the biggest, most compelling questions to find solutions that will provide our nation with affordable, environmentally clean energy and limit the risk from diverse threats to national and global security. Based on our foundation of values, expertise and experience, EGS is geared for success and growth.

EGS comprises four divisions—Nuclear Engineering, Energy Systems, Global Security Sciences and Intelligence Analysis; three centers—Center for Transportation Research, Risk and Infrastructure Science Center and Center for Integrated Resiliency Analysis; and three user facilities—the Transportation Research and Analysis Computing Center, Intermediate Voltage Electron Microscope and National Security Facility.



When activated using a special technique called atomic layer deposition, yttrium oxide crystals become luminescent (glowing). Luminescent materials are crucial for energy-efficient lighting. Each crystal is smaller than the diameter of a single strand of spider silk. Image taken by Angel Yanguas-Gil, Jeffrey W. Elam and John N. Hryn of the Energy Systems division.

OUTSTANDING SAFETY PERFORMANCE

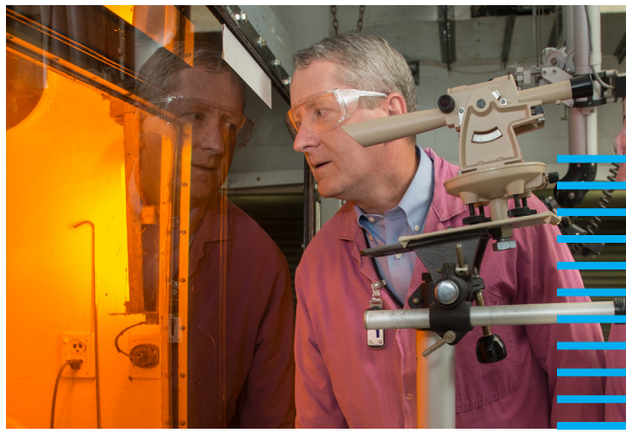
2014 James B. Porter, Jr. Team Award for Outstanding Safety Performance

The EGS Safety Team received the 2014 James B. Porter, Jr., Team Award for Outstanding Safety Performance from the UChicago Argonne LLC Board of Governors. The team comprises ESH coordinators from EGS and its four divisions: (from left, top) John Woodford, Will Brocker, Brian Wozny and Terry Aylesworth; (from left, bottom) Ryne Willig, Linda Pierce, Amy Harris, Marsha Mehaffey and Jeff Overby. The team promotes a strong safety culture using a collaborative approach. Team members are valued contributors to research project planning and performance, working closely with EGS research staff to ensure that Integrated Safety Management functions and principles are implemented.

Safety is built into all we do.

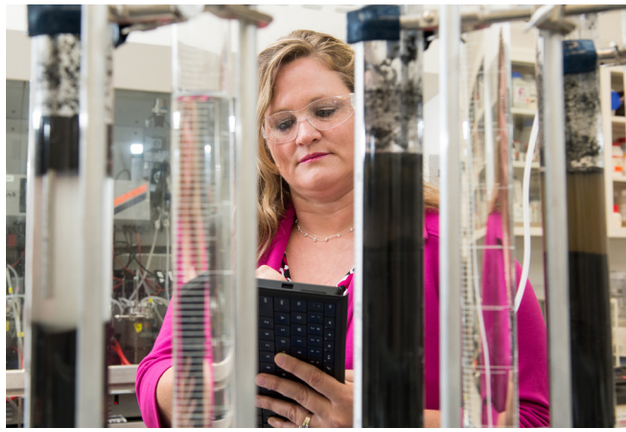
Statistics say a lot about the EGS culture of safety. We've swept Argonne's safety leadership awards two years in a row. As a group, EGS and its four divisions have received the prestigious National Safety Council Million Work Hours Award for operating 3,000,000 or more employee hours without occupational injury or illness involving days away from work. EGS has worked 5,000,000 hours without serious injury or illness involving days away from work since April 2010, when the EGS directorate was formed.

EGS actively embraces the principles and functions of Integrated Safety Management to drive our performance. Effective leadership and employee engagement enables us to conduct our research safely and promote a culture that learns from others and values debate. Quite simply, we look out for each other. And, we're never quite satisfied with our performance, always looking for improvements to be made.



2014 Director's Award for Outstanding Safety Leadership

Chris Grandy (above) leads some of the most hazardous research at Argonne in the Nuclear Engineering division's facilities. Amy Harris (below) ensures that work is done safely in the Energy Systems division's wide spectrum of applied engineering facilities and laboratories. Chris and Amy are co-recipients of the 2014 Director's Award for Outstanding Safety Leadership from the UChicago Argonne LLC Board of Governors.



At the December 2014 all-hands meeting, EGS Associate Laboratory Director Mark Peters (left) greeted employees with a reminder on the importance of safety during wintery conditions. He handed out bags of ice melt for employee use in parking lots and on sidewalks.

OUR IMPACT
ON THE WORLD

These are just a few of the innovations spawned by the ideas and know-how of EGS researchers and realized through the strength of our collaborations. It's this strength that enables us to break new ground as modern-day pioneers and set milestones for progress and development worldwide.

Securing the Nation's Critical Infrastructure System

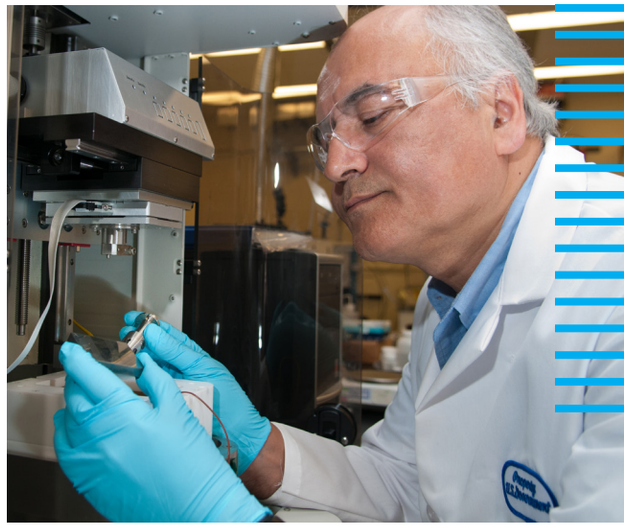
The Global Security Sciences (GSS) division has developed numerous resilience assessment tools through its years as the technical leader of the Department of Homeland Security's Regional Resiliency Assessment Program. GSS published a summary of its resilience work, "Resilience Assessment Tools for Critical Infrastructure Systems," in The CIP Report produced by George Mason University's School of Law.

Argonne Launches the Virtual Engine Research Institute and Fuels Initiative (VERIFI)

VERIFI is the first and only source in the world for high-fidelity, three-dimensional, end-to-end combustion engine simulation/visualization and simultaneous powertrain and fuel simulation, with uncertainty analysis. Led by the Energy Systems division, an unequaled multidisciplinary team of experts in high-performance computing, fuel chemistry, combustion science and engine performance employs some of the world's fastest supercomputers, most diverse engine labs and world's brightest X-ray beams to answer complex engine questions. The ultimate result of their work will shrink engine development timescales, accelerate time to market and reduce development costs, while ensuring the timely achievement of energy security and emissions targets and enhancing U.S. industrial competitiveness.

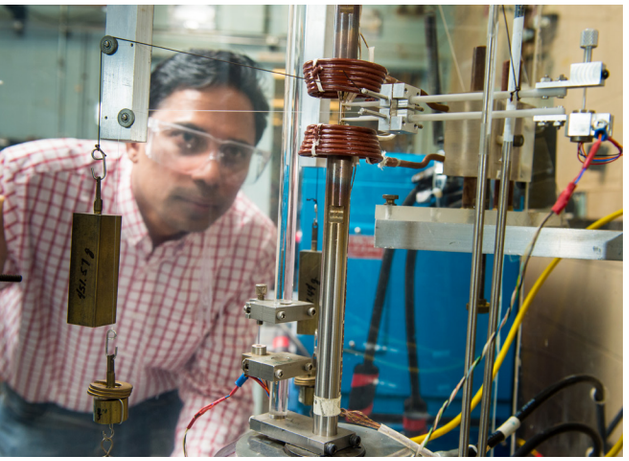
Researchers Fight Friction and Wear with One-Atom-Thick Graphene

When designing a mechanical system to last as long as possible, scientists and engineers must find ways of overcoming friction. Argonne researchers have identified the properties of a new, exceptionally wear-resistant substance that works in a broad range of environments. Nanoscientist Anirudha Sumant of the Center for Nanoscale Materials and Argonne Distinguished Fellow Ali Erdemir (seen here) of the Energy Systems division found that a one-atom-thick layer of graphene lasted for more than 6,500 "wear cycles," a dramatic improvement over conventional lubricants like graphite or molybdenum disulfide. For comparison, conventional lubricants would need about 1,000 layers to last for 1,000 wear cycles.



New Tool Predicts Economic Impacts of Natural Gas Stations

Systems analyst Marianne Mintz of the Energy Systems division has developed a new tool called JOBS NG for analyzing the economic impacts of building new compressed natural gas fueling stations. The tool is freely available to the public and is designed to help states and local governments evaluate possible economic benefits related to natural gas stations when they are setting new policies.



Predicting Remaining Life of Light Water Reactor Components

Environmental-assisted fatigue and aging issues are among the major concerns for long-term survivability of nuclear power plants in the U.S., most of which were built before 1970. The potential exists to extend the licenses beyond 60 to perhaps 80 years, enabling existing plants to continue providing safe, clean and economic electricity without significant greenhouse gas emissions. Mechanical engineer Subhasish Mohanty (seen here) of the Nuclear Engineering division is developing a remaining-life-prediction framework that will be used by the U.S. Nuclear Regulatory Commission for assessing the long-term structural integrity of light water reactor components. This framework will also apply to advanced liquid metal and gas-cooled reactor components.

25 Years of Advanced Vehicle Technology Competitions (AVTCs) Give Students Hands-on Experience

In its 25-year history, more than 16,500 students from 91 educational institutions in North America have participated in the U.S. Department of Energy-sponsored AVTCs, held in partnership with the North American automotive industry. Managed by Argonne's Energy Systems division, the AVTCs represent a unique coalition of government, industry and academic partners who join forces to provide a real-world training ground for future engineers and automotive leaders. The EcoCAR 3 competition is challenging students to rebuild the Chevrolet Camaro for even greater efficiency and reduced emissions, all while keeping muscle car fanatics satisfied.

New Tool Analyzes Water Footprint of Biofuels

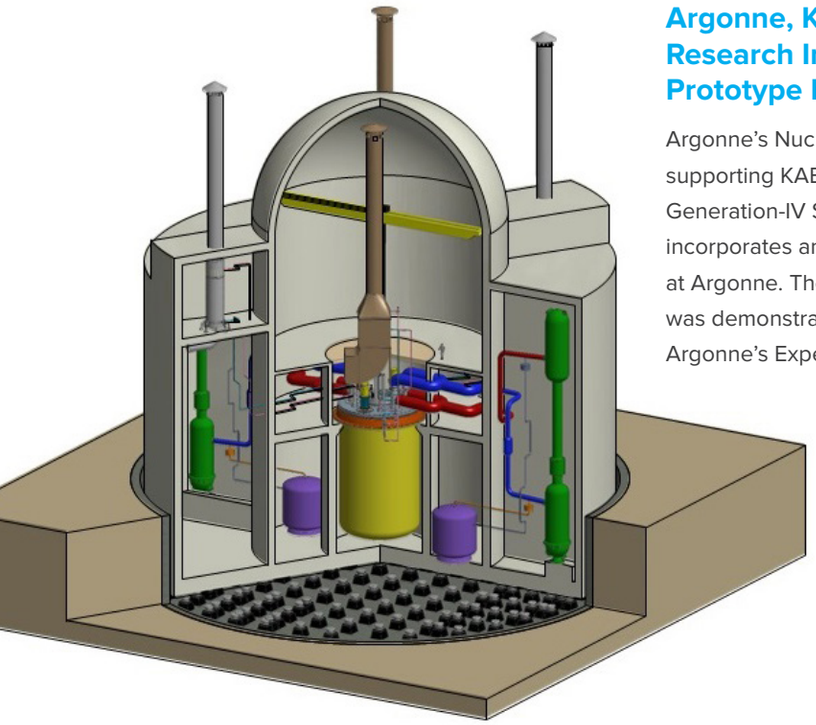
A new version of the Water Assessment for Transportation Energy Resources (WATER), created by Energy Systems division researchers, allows biofuels manufacturers to analyze the water consumption associated with use of cellulosic feedstocks, such as residue left from lumber production and other wood-based resources. The new tool provides analysis for the first time down to the county level in the U.S., assisting stakeholders and developers as they consider water sustainability in proposed projects. It also can help state and local governments estimate possible water consumption and impacts on water quality.

Argonne Studying Chicago River Microbe Population

The Energy Systems division initiated a five-year study with the Metropolitan Water Reclamation District of Greater Chicago to determine the potential sources of microbial contamination in the Chicago Area Waterways System (CAWS) as a $1.9 million Strategic Partnership Project. Argonne will conduct metagenomic analysis of water, soil and sediment samples collected at pre-defined locations in the CAWS and develop a predictive model framework. This new project is an element of Argonne's development of "Urban Science."

Argonne Leads SAE Effort on Uniform Practices for Specifying Powertrain Effective Horsepower Rating

The powertrain configurations of hybrid electric vehicles are highly varied and combine traditional internal combustion engines with one or multiple electric motors. The individual component ratings are misleading since they are typically reported by adding their peak power outputs together. The SAE Hybrid-EV Committee has appointed principal mechanical engineer Mike Duoba (right) of the Energy Systems division as the chair of its J2908 Subcommittee, which is tasked with formulating some key metrics for evaluating real world measures of hybrid drivetrain power output. Duoba is seen here with U.S. Secretary of Energy Ernest Moniz during his visit to Argonne in June.

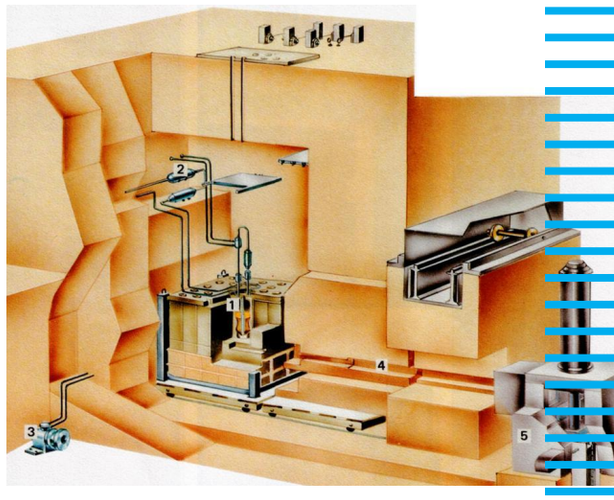


Argonne, Korean Atomic Energy Research Institute (KAERI) Developing Prototype Nuclear Reactor

Argonne's Nuclear Engineering division is supporting KAERI's development of a Prototype Generation-IV Sodium-cooled Fast Reactor that incorporates an innovative metal fuel developed at Argonne. The fuel's inherent safety potential was demonstrated in landmark tests conducted on Argonne's Experimental Breeder Reactor-II.

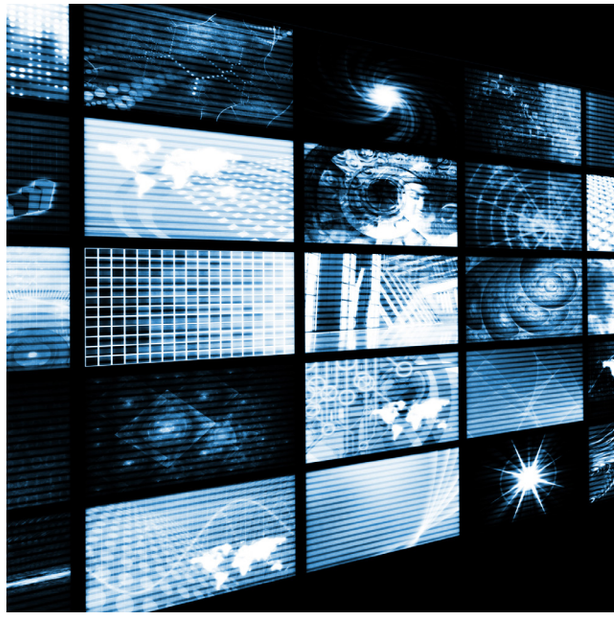
First Russian Research Reactor Converts to Low-enriched Uranium (LEU)

The Russian Federation's National Research Centre (NRC)-Kurchatov Institute announced that its ARGUS reactor had been converted to operation with LEU fuel during July 2014 as part of United States National Nuclear Security Administration's Global Threat Reduction Initiative program. ARGUS is one of six Russian research reactors that will be converted to LEU. Argonne's Nuclear Engineering division and NRC-Kurchatov Institute staff jointly performed conversion feasibility studies and reactor safety analyses with LEU fuel.

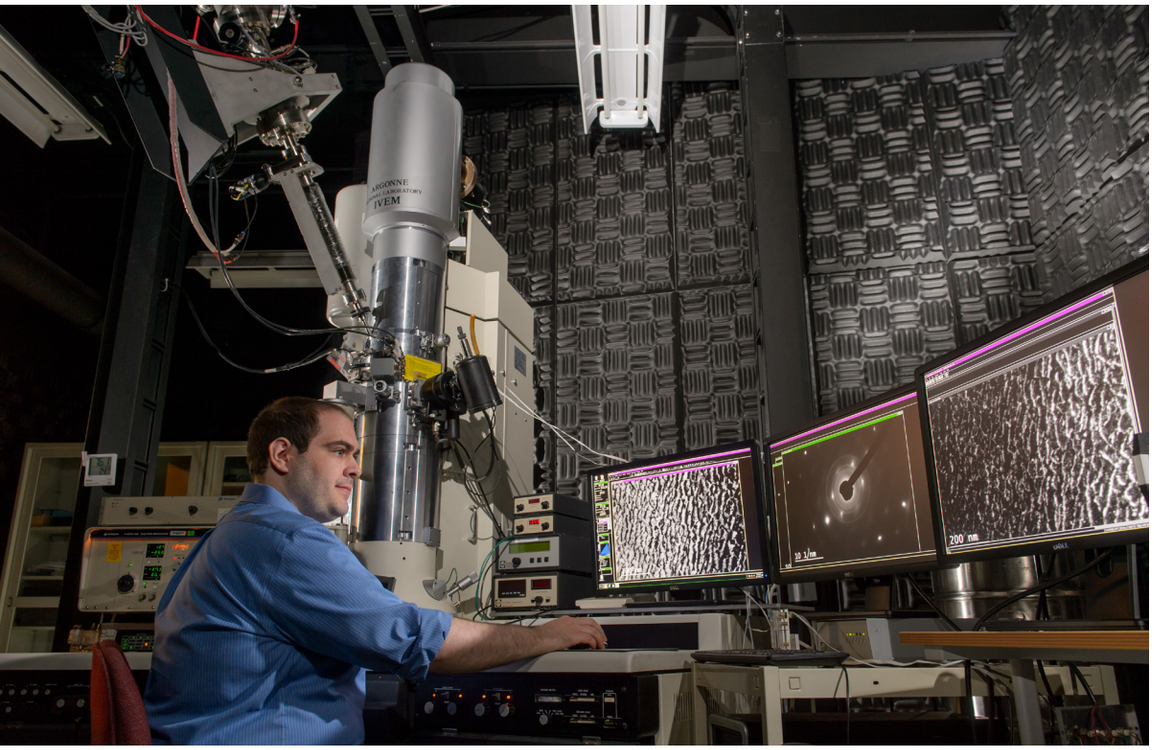


National Security Facility Experiences Significant Growth

The Intelligence Analysis division's Field Intelligence Element (FIE)—called the National Security Facility—provides tools and resources to enable and strengthen connections between government sponsors and the broad set of scientific and engineering capabilities and facilities at the Laboratory, with the overall goal of improving the national security of the United States. In 2014, FIE use by Argonne researchers increased by almost 50%. This enabled the lab to publish 31 Technical Reports for the intelligence community. It also facilitated delivery of quick-turnaround, specialized technology applications, and operational support based on Argonne's technological expertise, to the U.S. Department of Energy and the intelligence, law enforcement and special operations communities.



UNMATCHED
SCIENTIFIC FACILITIES

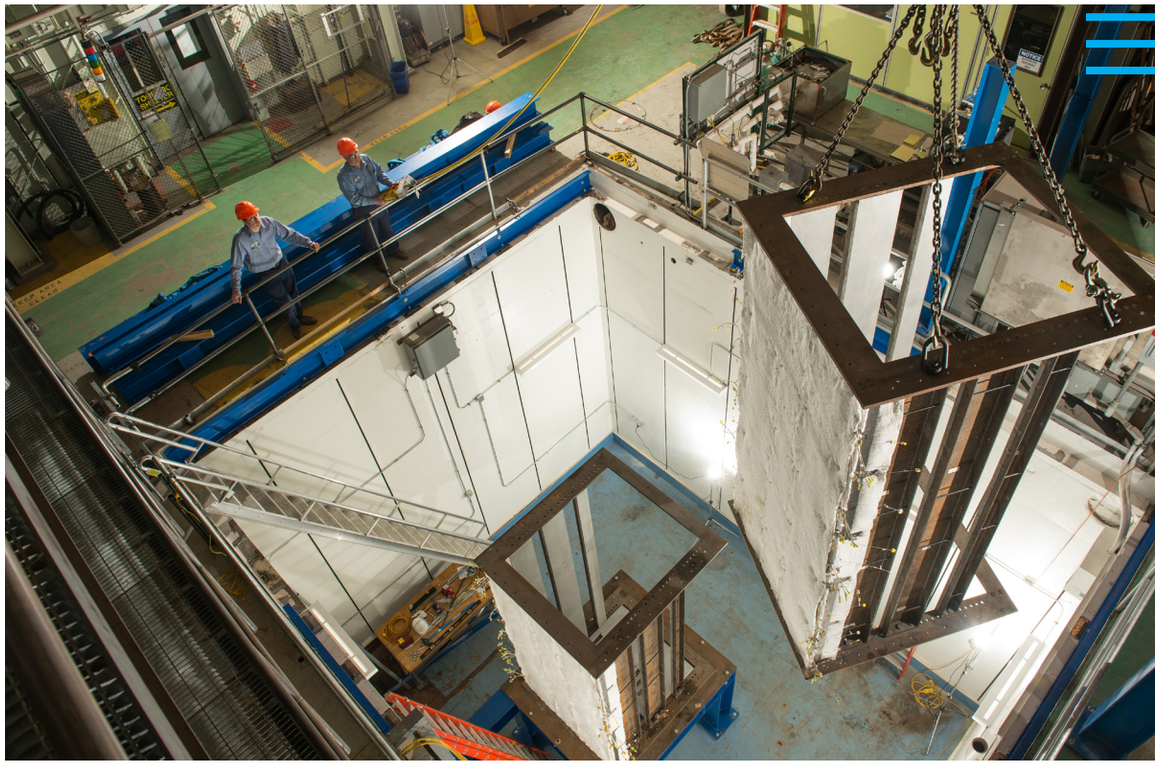


Intermediate Voltage Electron Microscope (IVEM) Facility

The IVEM-Tandem user facility is unique to the U.S. and one of only five in the world. It images the changes in atomic structure and defect formation during irradiation at high magnification. IVEM resumed operation this year within the Nuclear Engineering division.

Argonne offers its researchers a rich scientific environment, including an extraordinary range of cutting-edge facilities, scientific tools and six national users facilities to support in-depth research, drive technological breakthroughs and improve our nation's competitiveness and quality of life. The Energy and Global Sciences directorate is committed to maintaining and expanding the world-class experimental facilities that are essential to meeting our mission.

This year, two new facilities were brought online in EGS.



Natural Convection Shutdown Heat Removal Test Facility (NSTF)

Undergoing experimental operations in 2014 following renovations, the NSTF is one of the world's largest test facilities for ex-vessel passive decay heat removal in advanced nuclear reactors. The air-cooled NSTF is a state-of-the-art, large-scale facility for evaluating the performance capabilities of containment cooling systems while also providing reactor designers with data to validate computer simulations.

OUR **INTELLECTUAL PROPERTY**

Ultra-thin Coatings Maintain High Catalyst Activity and Stability

Catalysts are vitally important substances that enable the production of everything from gasoline to fertilizer. However, a number of common chemical and physical catalyst deactivation processes can lead to chemical reactor shutdowns and cause costly manufacturing plant interruptions. To overcome this, Energy Systems scientists are applying ultra-thin protective layers to the catalyst using atomic layer deposition; this reduces sintering and maintains high catalyst activity in high-temperature applications. Postdoctoral researcher Christian Canlas (seen here) weighs a catalyst sample in preparation for testing.

Energy and Global Security researchers and their collaborators are making revolutionary discoveries and finding solutions that translate into a real difference for this world. Our intellectual property is broad and diverse. The 2014 EGS patents are listed here.

1. "Lid Actuation System for Shielded Cask," Donald Preuss, James Morgan, Daniel Nestor, Facilities Management and Services division, Nuclear Engineering division, and Technical Services division, Pat. No. 8,550,283, issued October 8, 2013.

2. "Bioprocess Utilizing Carbon Dioxide and Electrodeionization," Edward St. Martin and YuPo Lin, Energy Systems division, Pat. No. 8,580,096, issued November 12, 2013.

3. "Low-Cost Method for Fabricating Palladium and Palladium-Alloy Thin Films on Porous Supports," Yunxiang Lu, Stephen Dorris, Uthamalingam Balachandran, Tae Lee, Chan Young Park, Energy Systems division, Pat. No. 8,585,807, issued November 19, 2013.

4. "Bus Bar Electrical Feedthrough for Electrorefiner System," Laurel Barnes, Mark Williamson, Robert Blaskovitz, Stanley Wiedmeyer, James Willit, Chemical Sciences and Engineering division and Nuclear Engineering division, Pat. No. 8,598,473, issued December 3, 2013.

5. "Resistive Spacers for Large Area Photodetectors," Jeffrey Elam, Henry Frisch, Anil Mane, Richard Northrup, Energy Systems division, Pat. No. 8,604,440, issued December 10, 2013.

6. "Ultrastable Substrates for Surface-Enhanced Raman Spectroscopy: A12O3 Overlayers Fabricated by Atomic Layer Deposition Yield Improved Anthrax Biomarker Detection," Jing Zhao, Xiaoyu Zhang, Richard Van Duyne, Jeffrey Elam, Alyson Whitney, Energy Systems division, Pat. No. 8,628,727, issued January 14, 2014.

7. "Anode-Cathode Power Distribution Systems and Methods of Using the Same for Electrochemical Reduction" Mark Williamson, Stanley Wiedmeyer, Eugene Koehl, Laurel Barnes, James Willit, Chemical Sciences and Engineering division and Nuclear Engineering division, Pat. No. 8,636,892, issued January 28, 2014.

8. "Method for Fabrication of Crack-Free Ceramic Dielectric Film," Uthamalingam Balachandran, Beihai Ma, Manoj Narayanan, Sheng Chao, Shanshan Liu, Energy Systems division, Pat. No. 8,647,737, issued February 11, 2014.

9. "Materials as Additives for Advanced Lubrication," Kuleep Mistry, Michael Thackeray, Ali Erdemir, Pol Vilas, Chemical Sciences and Engineering division and Energy Systems division, Pat. No. 8,648,019, issued February 11, 2014.

10. "Methane Production using Resin-Wafer Electrodeionization," Seth Snyder, Meltem Urgun-Demirtas, YuPo Lin, Energy Systems division, Pat. No. 8,679,314, issued March 25, 2014.

11. "Millimeter Wave Sensor for Far-Field Standoff Vibrometry," Apostolos Raptis, Nachappa Gopalsami, Sasan Bakhtiari, Thomas Elmer, Nuclear Engineering division, Pat. No. 8,686,362, issued April 1, 2014.

12. "Atomic Layer Deposition of Quaternary Chalcogenides," Michael Pellin, Jeffrey Elam, Alex Martinson, Shannon Riha, Elijah Thimsen, Materials Science division and Energy Systems division, Pat. No. 8,741,386, issued June 3, 2014.

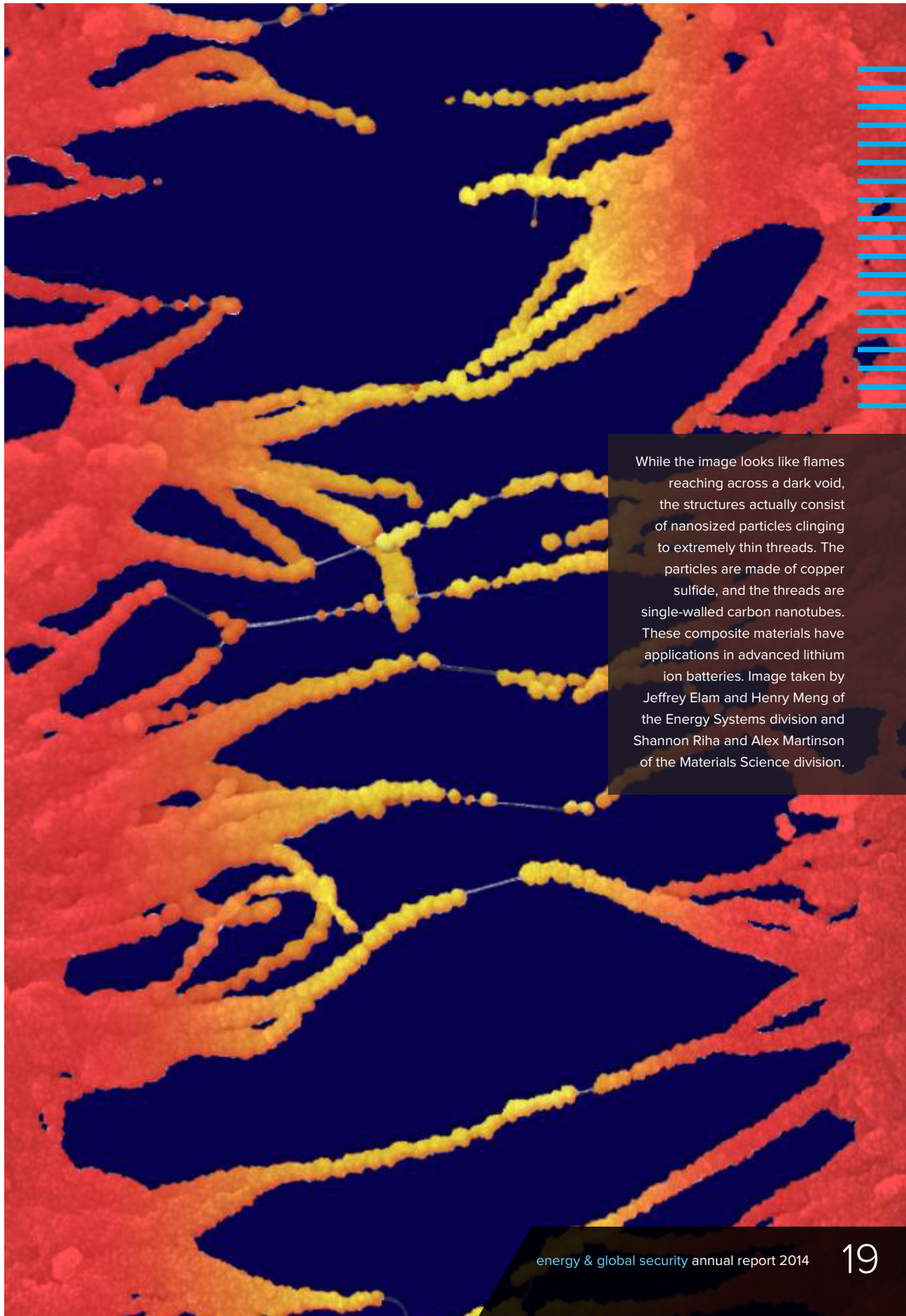
13. "Hydrothermal Performance of Catalyst Supports," Yomaira Pagan-Torres, Christopher Marshall, Joseph Libera, James Dumesic, Jeffrey Elam, Energy Systems division and Chemical Sciences and Engineering division, Pat. No. 8,741,800, issued June 3, 2014.

14. "Aluminum Phosphate Ceramics for Waste Storage," Arun Wagh, M. David Maloney, Energy Systems division, Pat. No. 8,742,195, issued June 3, 2014.

15. "Continuous Recovery System for Electrorefiner System," Stanley Wiedmeyer, Laurel Barnes, James Willit, Mark Williamson, Robert Blaskovitz, Chemical Sciences and Engineering division and Nuclear Engineering division, Pat. No. 8,746,440, issued June 10, 2014.

16. "Anode Shroud for Oxygen Off-Gas Capture and Removal from an Electrolytic Oxide Reduction System," James Bailey, Stanley Wiedmeyer, Mark Williamson, Laurel Barnes, James Willit, Chemical Sciences and Engineering division and Nuclear Engineering division, Pat. No. 8,771,482, issued July 8, 2014.

17. "Frequency Based Electric Vehicle Charge Controller System and Method for Implementing Demand Response and Regulation Services to Power Grid using Frequency Detection," Vladimir Koritarov, Global Security Sciences division, Pat. No. 8,786,249, issued July 22, 2014.



While the image looks like flames reaching across a dark void, the structures actually consist of nanosized particles clinging to extremely thin threads. The particles are made of copper sulfide, and the threads are single-walled carbon nanotubes. These composite materials have applications in advanced lithium ion batteries. Image taken by Jeffrey Elam and Henry Meng of the Energy Systems division and Shannon Riha and Alex Martinson of the Materials Science division.

AWARDS AND ACCOLADES

Throughout 2014, EGS's world-renowned researchers and EGS-led research teams were honored with awards and recognition for their distinguished performance and leadership; for their pioneering contributions to engineering and science; and for their dedication to educating and mentoring students in science, technology, engineering and mathematics.

The awards and accolades we receive are a testament to our success in resolving key technical challenges in energy access, environmental quality and international security. We're honored by the recognition, but know that each and every day will present new challenges and ambitious new goals. We believe that tomorrow will be another day in which to excel!

American Nuclear Society's Landis Young Member Award

In recognition of his pacesetting contributions to simulation of complex turbulent flows and multi-scale/multi-physics simulations of nuclear reactor designs, nuclear engineer Elia Merzari of the Nuclear Engineering division was recently chosen by the American Nuclear Society to receive its 2014 Landis Young Member Engineering Achievement Award. The Landis Award recognizes an individual who has made significant technical contributions, with an emphasis placed on achievement that demonstrates a high degree of technical merit and ingenuity.

Argonne Distinguished Fellows

Two EGS researchers were named as Argonne Distinguished Fellows—Balu Balachandran of Energy Systems (left) and Yousry Gohar of Nuclear Engineering. Distinguished Fellow is the highest scientific/engineering rank at the laboratory, and this distinction is held by only a small fraction—approximately 3 percent—of the research staff.

R&D 100 Award Winners

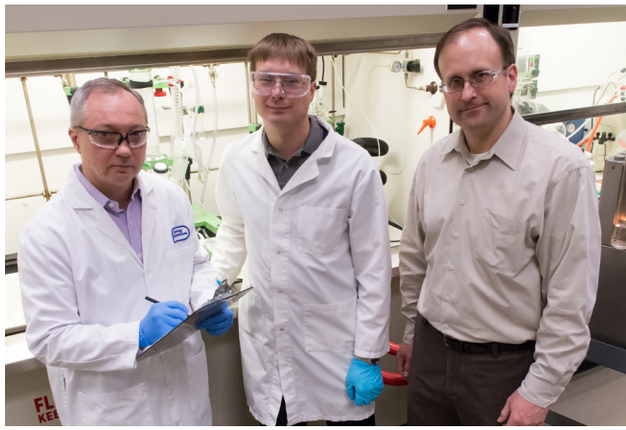
The ingenuity of several EGS scientists and engineers has been recognized by their receipt of 2014 R&D 100 awards, which highlight the most innovative and significant new technologies as they enter the marketplace.

Sequential Infiltration Synthesis (SIS) Lithography

Chemist Jeff Elam (left) and materials science engineer Anile Mane of Energy Systems, along with collaborators scientist Seth Darling and physicist Leonidas Ocola from the Nanoscience and Technology division, received an R&D 100 Award for their research on SIS. This new method of creating nanoscale patterns for microelectronics manufacturing will reduce cost and enable increased product performance.

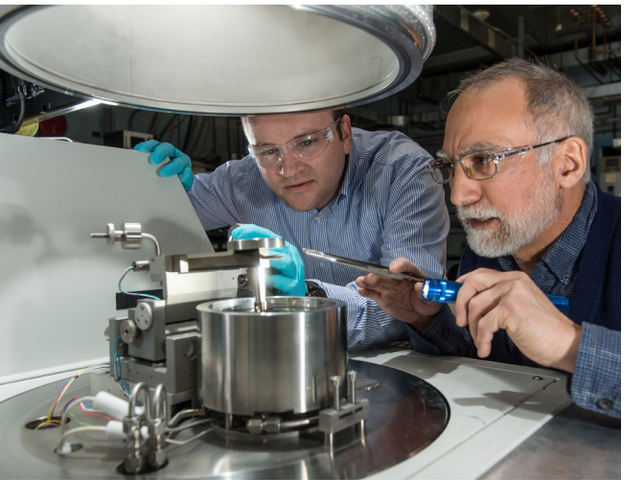
Advanced Redox Shuttle Additive

Chemist John Zhang of the Chemical Science and Engineering division invented a chemical solution to the problem of overcharging in lithium ion batteries used in electric vehicles. He turned to systems engineer Greg Krumdick (right) and process chemists Trevor Dzwiniel (center) and Kris Pupek of the Energy Systems division to scale up the materials from the gram-level to the kilogram-level, making them attractive candidates for commercializing and winning the collaborative team an R&D 100 Award.



Distinguished Performance Award

Considered to be the world-leading expert in the field of light water reactor severe-accident behavior, nuclear engineer Mitchell Farmer's expertise was central to U.S. efforts to aid Japan in its response and follow-up to the disastrous Fukushima accident in 2011. Throughout his career at Argonne, Farmer has demonstrated exceptional capability and breadth as an experimenter, analyst, and leader of large research efforts, including the experimental investigation and demonstration of key "passive safety" features of advanced reactors that employ coolants other than water. In 2014, he was recognized with the UChicago Argonne LLC Board of Governors' Distinguished Performance Award.

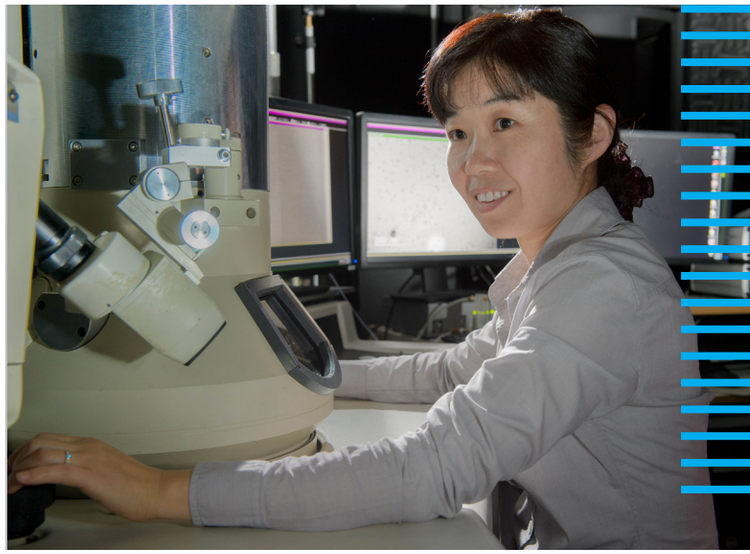


Pinnacle of Education Award

Postdoctoral students in the Energy Systems division know metallurgist Robert Erck (right) as a tireless advocate, mentor, educator and friend. In 2014, he received the UChicago Argonne LLC Board of Governors' Pinnacle of Education Award for his dedication. Erck provides a pathway towards STEM careers for students from all walks of life and does so with a supreme amount of awareness, knowledge and personal involvement. One of his students said of him, "The greatest scientist is one who learns for the sake of learning by working diligently and honorably, contributes to the field of interest by doing so, and imparts that passion to the next generation of scholars along the way."

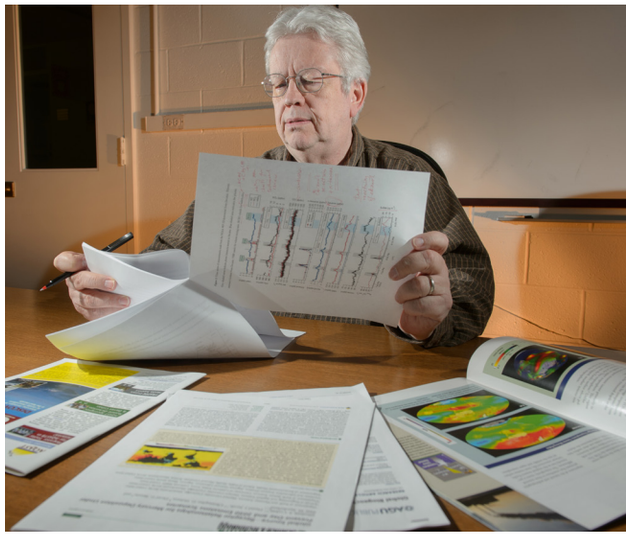
Presidential Early Career Award

Argonne nuclear engineer Meimei Li received a Presidential Early Career Award for Scientist and Engineers, the highest honor bestowed by the United States Government on science and engineering professionals in the early stages of their independent research careers. Li received the award for her contributions to the understanding of nuclear reactor materials, and was honored by President Obama during a White House ceremony.



Streets Recognized for His Influence

Environmental scientist David Streets of the Global Security Sciences division has been recognized as being in the top one percent of the most highly cited researchers in the world, according to a survey by Thomson Reuters. From 2002 to 2012, Streets authored or co-authored 250 peer-reviewed journal articles and book chapters. His research principally involves the effect of human activity on the atmosphere. Since 2000, he has participated in five NASA air quality missions to give scientists a comprehensive understanding of Asian air pollution and pollution transport to North America.



2014 WIST Diversity Award

Principal agronomist M. Cristina Negri has been selected as the recipient of Argonne's 2014 Women in Science and Technology (WIST) Diversity Award. Negri is a member of the Laboratory Director's Diversity and Inclusion Advisory Council, served as WIST Program Initiator from 2007 to 2010 and is a member of the WIST Steering Committee. Negri chaired three Science Careers in Search of Women (SCSW) event planning committees and has actively mentored young women at a multitude of SCSW and Introduce a Girl to Engineering Day events. She continues to mentor students, postdoctoral fellows and early-career scientists to help them successfully navigate their desired career paths.

VERIFI Researchers Win HPC Innovation Excellence Award

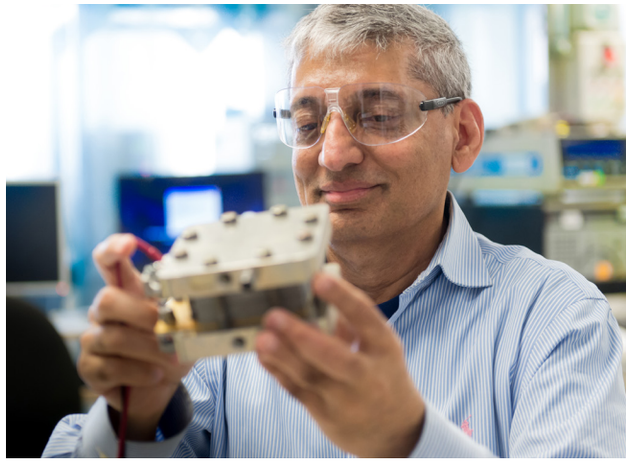
International Data Corporation announced in June that researchers from Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI) won a 2014 High Performance Computing (HPC) Innovation Excellence Award. The award recognized principal engineer Sibendu Som (left) from the Energy Systems division and senior computational scientist Ray Bair from the Computing, Environment and Life Sciences directorate, for their work with a major heavy-duty engine manufacturer and Convergent Science, Inc., to conduct one of the largest internal combustion engine simulations ever. The research has allowed the manufacturer to shrink its development timescales, resulting in significant cost savings.

NNSA Commends Peter Heine for Role in Strategic Trade Control

The National Nuclear Security Administration's Office of Nonproliferation and International Security commended nuclear engineer Peter Heine (right, back) of the Global Security Sciences division for his leadership and dedication on the World Customs Organization (WCO) Strategic Trade Control Enforcement (STCE) project. Heine sought and followed guidance from U.S. interagency leadership and their global partnerships and achieved consensus within the WCO 179 member states for the report. NNSA called the publication of this year's STCE Implementation Guide "a remarkable feat." The letter to Heine further stated, "Your sustained efforts in this field have had a profound impact on the export control paradigm...."

Ahluwalia Receives Hydrogen and Fuel Cells Program Award

DOE's Hydrogen and Fuel Cells Office recognized mechanical engineer Rajesh Ahluwalia of the Nuclear Engineering division with a Hydrogen and Fuel Cells Program Award for his accomplishments beyond a single area. With a career spanning more than two decades, Ahluwalia has provided "outstanding" technical insight and guidance on fuel cells, hydrogen storage and hydrogen production systems analysis. He is the co-developer of the Argonne General Computational Toolkit, or GCTool, a software package that helps design, analyze and optimize automotive and stationary distributed fuel cell power generation systems and other power-plant configurations.

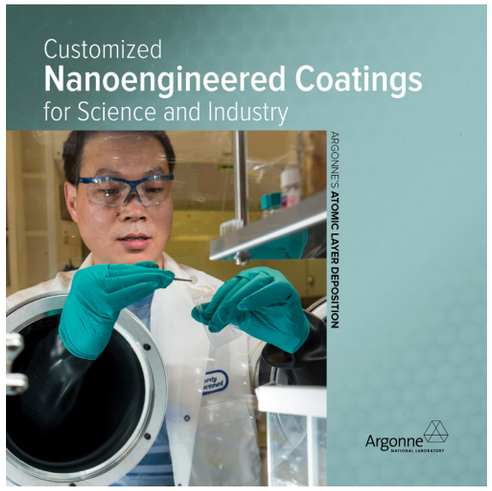


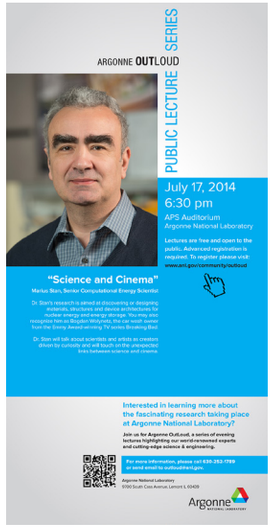
DEMONSTRATING OUR **THOUGHT LEADERSHIP**

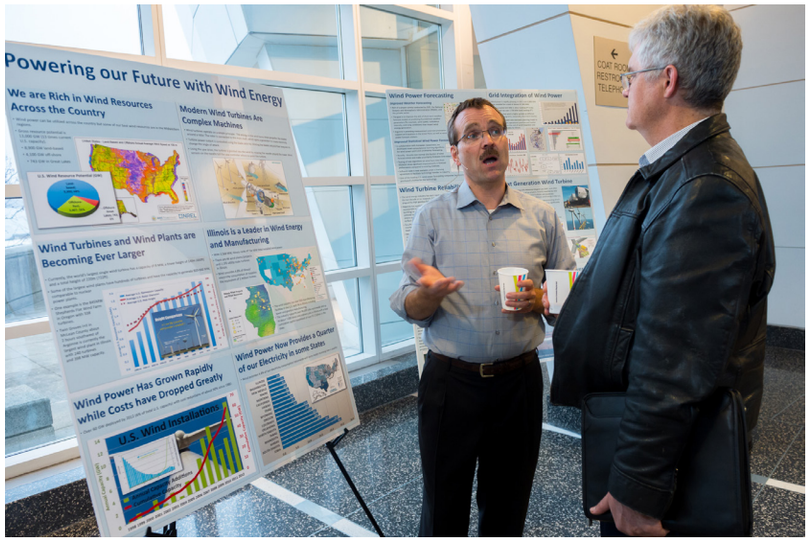
What we do matters.

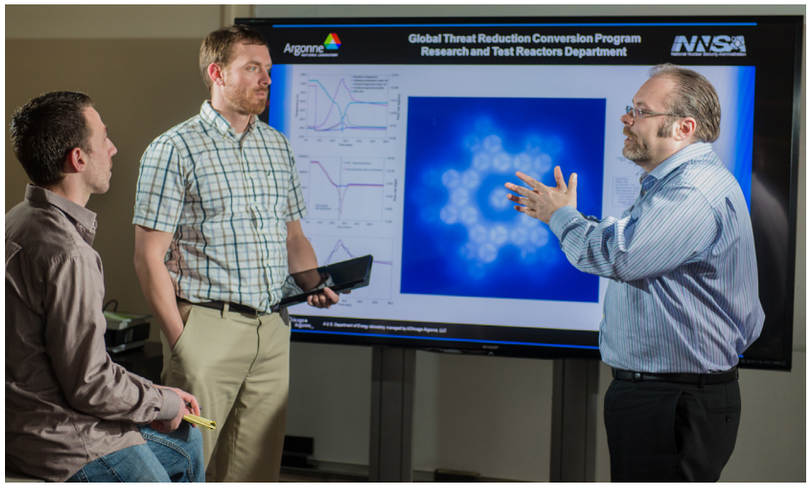
To remain at the forefront in their areas of expertise, EGS researchers demonstrate thought leadership by communicating their findings, hypotheses, theories, lines of reasoning and evidence. Our communications with multiple audiences is critical to the progress of science and engineering, as well as to our success in achieving the EGS mission and carrying out our strategic plan. Additionally, communication enables collaboration, helping us bring together the best thinkers of our time in pursuit of big, ambitious ideas.

EGS researchers distribute information about their ideas and research in many ways: informal communication with colleagues, through laboratory publications, by making presentations at conferences and by preparing peer-reviewed journal articles. Listed on the following pages by division are several key publications and presentations for 2014.









KEY **PUBLICATIONS AND PRESENTATIONS**

Energy Systems Division – FY2014

1. "Meeting World's Most Stringent Hg Criterion: A Pilot-Study for the Treatment of Oil Refinery Wastewater using an Ultrafiltration Membrane Process," M. Urgun-Demirtas, M. Cristina Negri, P.S. Gillenwater, A.G. Agwu Nnanna, J. Yu, *Journal of Environmental Management* 117C:65–75, March 15, 2013, doi: 10.1016/j.jenvman.2012.12.011.

2. "Temperature-Dependent Dielectric Nonlinearity of Relaxor Ferroelectric $Pb_{0.92}La_{0.08}Zr_{0.52}Ti_{0.48}O_3$ Thin Films," B. Ma, Z. Hu, S. Liu, S. Tong, M. Narayanan, R.E. Koritala, U. Balachandran, *Applied Physics Letters* 102:202901, May 2013, doi: 10.1063/1.4807665.

3. "Development of a Computational Approach to Detect Instability and Incipient Motion of Large Riprap Rocks," C. Bojanowski and S. Lottes, *2014 Transportation Research Board 93rd Annual Meeting Compendium of Papers*, January 14, 2014, Paper Number: 14-3035.

4. "A Markov Chain Approach to Simulate Atomic Layer Deposition Chemistry and Transport inside Nanostructured Substrates," A. Yanguas-Gil and J.W. Elam, *Theoretical Chemistry Accounts* 133:1465, February 26, 2014, doi: 10.1007/s00214-014-1465-x.

5. "Synchrotron X-Ray Techniques for Fluid Dynamics," A.L. Kastengren and C.F. Powell, *Experiments in Fluids* 55:1686, February 26, 2014, doi: 0.1007/s00348-014-1686-8.

6. "Examination of Nanoparticles from Gasoline Direct-injection (GDI) Engines using Transmission Electron Microscopy (TEM)," H. Seong, S. Choi, K. Lee, *International Journal of Automotive Technology* 15(2):175–181, March 5, 2014, doi: 10.1007/s12239−014−0019−5.

7. "Analysis of Cyclic Variability and the Effect of Dilute Combustion in a Gasoline Direct Injection Engine," N. Matthias, T. Wallner, R. Scarcelli, *SAE International Journal of Engines* 7(2):633–641, April 1, 2014, doi: 10.4271/2014-01-1238.

8. "Impact of Cetane Number on Combustion of a Gasoline-Diesel Dual-Fuel Heavy-Duty Multi-Cylinder Engine," A. Ickes, T. Wallner, Y. Zhang, W. De Ojeda, *SAE International Journal of Engines* 7(2):860–872, April 1, 2014, doi: 10.4271/2014-01-1309.

9. "Energy Efficiency and Greenhouse Gas Emission Intensity of Petroleum Products at U.S. Refineries," A. Elgowainy, J. Han, H. Cai, M. Wang, G.S. Forman, V.B. DiVita, *Environmental Science and Technology*, May 28, 2014, doi: 10.1021/es5010347.

10. "Phase Change Material with Graphite Foam for Applications in High-Temperature Latent Heat Storage Systems of Concentrated Solar Power Plants," W. Zhao, D.M. France, W. Yu, T. Kim, D. Singh, *Renewable Energy* 69:134–146, September 2014, doi: 10.1016/j.renene.2014.03.031.

Nuclear Engineering Division – FY2014

1. "A Breakthrough for Step Forward – Nano-particle Fueled Fluid Fast Reactor," T.K. Kim, U.S. Nuclear Infrastructure Council Special Technical Symposium on Technology and Process Innovation in Advanced Reactor Economics, Argonne, Illinois, January 2014.

2. "GTRI/LEU Conversion Program," J. Roglans-Ribas, presentation to Dr. Pete Lyons, DOE Assistant Secretary for Nuclear Energy, Argonne, Illinois, February 2014.

3. "IVEM and Proposed XMAT Beam Line for In Situ Studies of Radiation Damage to NE Fuels and Materials," M. Li and M. Pellin, presentation to Dr. Pete Lyons, DOE Assistant Secretary for Nuclear Energy, Argonne, Illinois, February 2014.

4. "Advanced Multi-Physics Modeling and Simulation Efforts for Fast Reactors," J. Thomas, E. Merzari, E. Shemon, A. Obabko, R. Jain, V. Mahadevan, T. Tautges, T. Solberg, R. Ferencz, R. Whitesides, Technical Meeting on Priorities in Modeling and Simulation for Fast Neutron Systems, Vienna, Austria, April 2014.

5. "Simulation of the Impact of 3-D Porosity Distribution in Metallic Uon in Fuels," D. Yun, A.M. Yacout, M. Stan, T.H. Bauer, A.E. Wright, *Journal of Nuclear Materials* 448, 129–138, May 2014, doi: 10.1016/j.jnucmat.2014.02.002.

6. "Design and Scaling of the Natural Convection Shutdown Heat Removal Test Facility," D. Lisowski, C. Gerardi, N. Bremer, M. Farmer, International Topical Meeting on Advances in Thermal Hydraulics (ATH'14), Reno, Nevada, June 2014.

7. "Overview of Recent U.S. Evaluation and Screening of Nuclear Fuel Cycle Options," T.A. Taiwo, Technical Meeting of the IAEA INPRO Collaborative Project Nuclear Fuel and Fuel Cycle Analysis for Future Nuclear Energy Systems (FANES), IAEA Headquarters, Vienna, Austria, June 2014.

8. "Neutron Channels Shield Design Analysis of KIPT Neutron Source Facility," Z. Zhong and Y. Gohar, PHYSOR 2014 International Conference, Kyoto, Japan, September 2014.

9. "Assessment of a Closed Fuel Cycle using Unattractive Material in a Small Modular Fast Reactor," N. Stauff, T.K. Kim, T.A. Taiwo, R.A. Wigeland, American Nuclear Society Winter Meeting, Anaheim, California, November 2014.

10. "The Australia Group Common Control List Handbook: Volume I: Chemical Weapons-Related Common Control Lists. Volume II: Biological Weapons-Related Common Control Lists," J.A. Carerra, A.J. Castiglioni, E.S. Rosenblum, U.S. Department of State, Washington, D.C., 2014. Available at http://www.australiagroup.net/en/controllisthandbooks.html.

Global Security Sciences Division – FY2014

1. "Using Integrated Process Teams for Interagency Coordination," K. Lerner, J. Zadra, P. Hewett, *The Public Manager*, December 15, 2013. Available at https://www.td.org/Publications/Magazines/The-Public-Manager/Archives/2013/Winter/Using-Integrated-Process-Teams.

2. "Very Short-Term Wind Power Forecasting: State-of-the-Art," J. Mendes, J. Sumaili, R. Bessa, H. Keko, V. Miranda, A. Botterud, Z. Zhou, ANL/DIS-14/6, December 2013. Available at http://www.ipd.anl.gov/anlpubs/2014/10/107926.pdf.

3. "China's International Trade and Air Pollution in the United States," J. Lin, D. Pan, S. Davis, Q. Zhang, K. He, C. Wang, D. Streets, D. Wuebbles, D. Guan, *Proceedings of the National Academy of Sciences of the United States of America*, 111(5):1736–1741, February 4, 2014, doi: 10.1073/pnas.1312860111.

4. "A Theoretical Formalism for Analyzing Agent-based Models," M. North, *Complex Adaptive Systems Modeling*, 2:3, May 7, 2014, doi: 10.1186/2194-3206-2-3.

5. "Modeling the Transmission of Community-Associated Methicillin-Resistant *Staphylococcus aureus*: A Dynamic Agent-Based Simulation," C. Macal, M. North, N. Collier, V. Dukic, D. Wegener, M. David, R. Daum, P. Schumm, J. Evans, J. Wilder, L. Miller, S. Eells, D. Lauderdale, *Journal of Translational Medicine*, 12(124), 12 pp., May 12, 2014, doi: 10.1186/1479-5876-12-124.

6. "Water Relationships in the U.S. Southwest: Characterizing Water Management Networks Using Natural Language Processing," J. Murphy, J. Ozik, N. Collier, M. Altaweel, R. Lammers, A. Kliskey, L. Alessa, D. Cason, P. Williams, *Water* 6(6):1601–1641, June 3, 2014, doi:10.3390/w6061601.

7. "Global Emission Projections for the Transportation Sector Using Dynamic Technology Modeling," F. Yan, E. Winijkul, D. Streets, Z. Lu, T. Bond, Y. Zhang, *Atmospheric Chemistry and Physics*, 14:5709–5733, June 10, 2014, doi: 10.5194/acp-14-5709-2014.

8. "Adaptive Simulation with Repast Simphony and Swift," J. Ozik, M. Wilde, N. Collier, C. Macal, Euro-Par 2014: Parallel Processing Workshops, 2nd Workshop on Parallel and Distributed Agent-Based Simulations (PADABS) Porto, Portugal, August 25–29, 2014. Available at http://link.springer.com/chapter/10.1007%2F978-3-319-14325-5_36.

9. "Using Decision Analysis to Construct Risk Performance Indicators," J. Phillips, F. Petit, D. Bessette, *The CIP Report*, 13(2):12–15, September 2014. Available at http://cip.gmu.edu/wp-content/uploads/2013/06/September-2014_Risk.pdf.

10. "Chance-Constrained Transmission Switching with Guaranteed Wind Power Utilization," F. Qiu and J. Wang, *IEEE Transactions on Power Systems*, 9 pp., 2014, doi: 10.1109/TPWRS.2014.2346987.

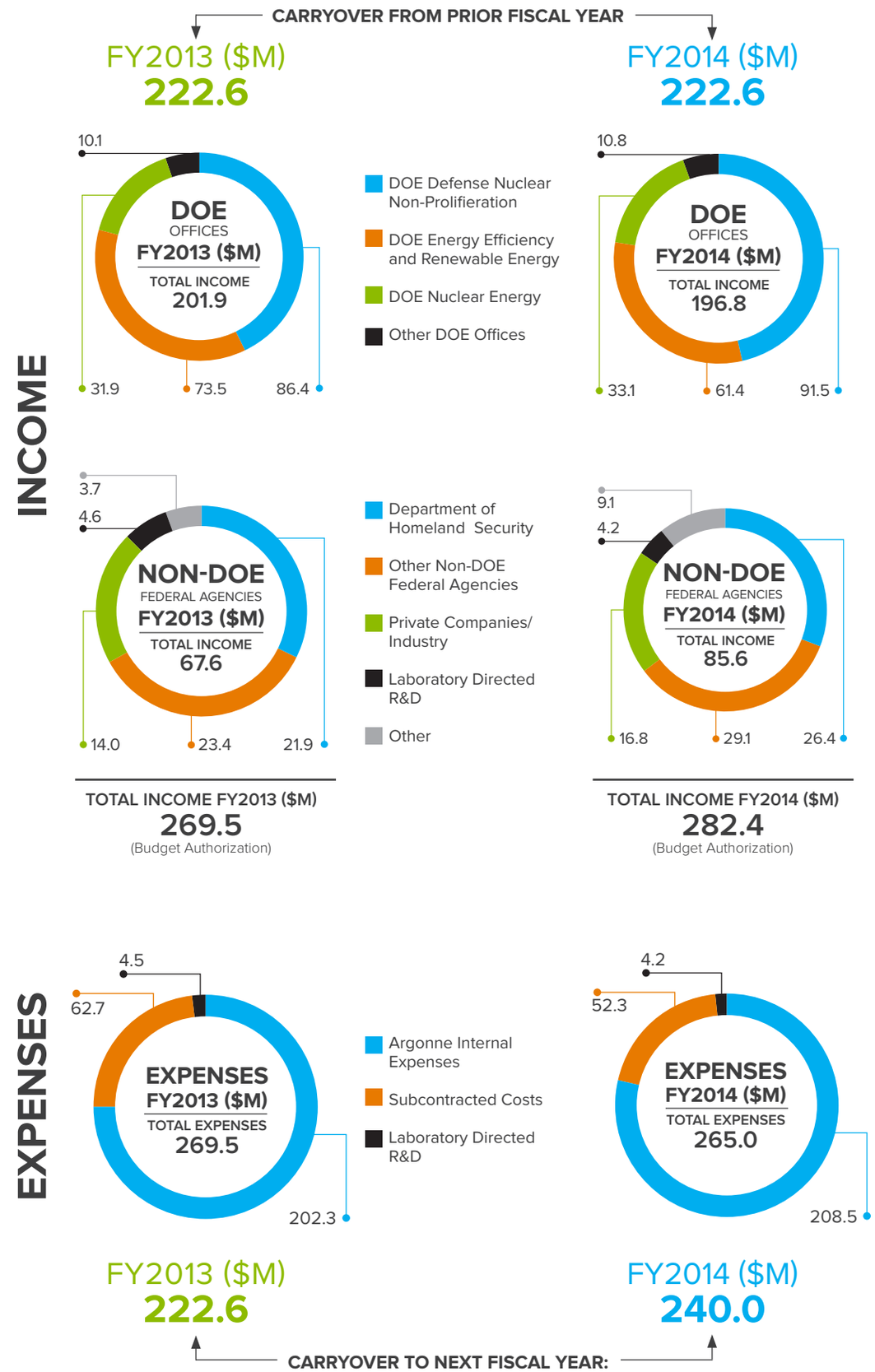
LakeSim is an Argonne-developed tool that merges urban design with scientific analysis to aid in the design of 21 century cities. LakeSim began with the need to answer practical questions about urban design and planning, requiring a better understanding about the long-term impact of design decisions on energy and transportation demand for a 600-acre development project on Chicago's South Side—the Chicago Lakeside Development project. To provide planners with better energy demand forecasts throughout the life of the development, LakeSim employs the Energy Performance Standard Calculation Toolkit (EECalc) developed by Argonne's Global Security Sciences division and the Georgia Institute of Technology. EECalc generates monthly estimates of a building's, or block's, thermal energy demand and consumption for heating and cooling. As each structure has unique architectural features, they also have unique demands on energy. Based on a number of end-user factors, including ventilation, lighting and heating and cooling, EECalc can assess the energy efficiency of an architectural design.

CONTINUING **OUR MOMENTUM**

The directorate is financially healthy; our new budget authorization (income) for fiscal year 2014 was $282.4 million tax. This is a modest increase relative to fiscal year 2013 income of $269.6 million but continues our upward momentum.

EGS receives funding from a diverse set of sponsors including 14 DOE program offices and 15 other federal agencies. In addition, approximately 5% of our funding comes from non-federal work-for-other sponsors. Four sponsors account for about 80% of the directorate's funding. These are DOE-National Nuclear Security Administration (32% of EGS funding), DOE-Energy Efficiency and Renewable Energy (22%), Department of Homeland Security (10%) and DOE Office of Nuclear Energy (12%).

The success we achieved in 2014 is a direct result of the long-term strategy and investments we began several years ago, serving as a sign of more to come. As we look to accelerate innovation, entrepreneurship, technology commercialization and transfer of ideas, we expect to capture funding opportunities that further our strategic goals.



Building a “Smart” Water Grid

Argonne researchers are working to create a “smart” water grid that would help us predict when trouble—like contamination, security threat or shortage—might occur so we can plan accordingly. Computer software engineer Tom Taxon of the Global Security Sciences division is developing a system for real-time software modeling of water distribution in concert with the U.S. Environmental Protection Agency’s National Homeland Security Research Center and the University of Cincinatti. The real-time system allows utilities to join their data with models that will help them improve day-to-day operations and enhance security in a more sustainable and productive manner. It will also help utilities lower the cost of water delivery and meet federal water quality regulations.

The Energy and Global Security Directorate is committed to bettering the human condition by pushing the boundaries of what seems possible. We bring scientists and engineers together as ONE team with a clear sense of purpose to find solutions and make discoveries that provide enduring value to our nation and to the future of the American scientific enterprise.

THE POWER OF ONE

GLOBAL SECURITY SCIENCES

ENERGY SYSTEMS

NUCLEAR ENGINEERING

INTELLIGENCE ANALYSIS

engineering
climate
energy
nanoscience
batteries
grid
machines
intelligence
resilience
water
intellect
nuclear
revolutionary
security
nonproliferation
synthesis
engines
science
systems
design
analysis
preparedness
testing
x-rays
leadership
growth
frontier
fuels
transportation
sustainable
cities
vehicles
network
connected
cybersecurity
computational
data
grid
virtual
lubricants
transformations
scalability
materials
modeling
simulation
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collaboration
industry
market
bonds
dynamics
quality
impact
safety
competitiveness
innovation
groundbreaking

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