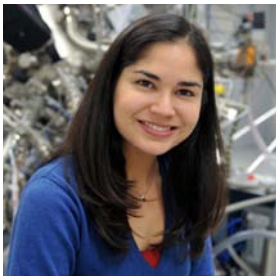

2010-2015

STRATEGIC PLAN

THE U.S. DEPARTMENT OF ENERGY'S

ARGONNE NATIONAL LABORATORY

Argonne NATIONAL LABORATORY

ARGONNE NATIONAL LABORATORY

2010-2015

STRATEGIC PLAN

Argonne's major research initiatives support U.S. needs for sustainable energy, national security, a clean environment, and a stable global climate.

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MESSAGE FROM THE DIRECTOR

This is an exciting time to be a member of the Argonne community. Argonne National Laboratory stands at the brink of a major opportunity to help achieve the vision set by President Barack Obama and Energy Secretary Steven Chu: an economy based on renewable energy, free of dependence on foreign oil and with a greatly reduced carbon footprint. The path to achieving this vision is through a strong linkage between basic research and applied research and engineering — all areas where Argonne excels.

Most known sustainable energy technologies, including solar, wind, nuclear, and energy storage, require fundamental breakthroughs in the physical sciences, particularly in materials and chemical processes. Translating fundamental breakthroughs into deployable, safe, reliable, and economically competitive technologies relies on world-class applied research and engineering. And collaboration — both internal and external — will be critical to success, because no single organization has the resources to overcome the major challenges alone.

Our challenge at Argonne is to think big. I have no doubt that future Nobel Prizes will come from mission-driven science aimed at solving energy problems. By combining Argonne's world-class science and engineering with new predictive theoretical and computational capabilities, the world will move toward a new era in which Argonne researchers can design new materials and chemistries with atomic precision, predict climate change on a regional level, and design future generation reactors — to name a few of the limitless possibilities. Argonne will be instrumental in creating this era. I invite you to use this Strategic Plan as a guide and inspiration as you embrace the vision and pursue the dream.

Eric D. Isaacs
Director

STRATEGIC PLAN OVERVIEW

This *Strategic Plan* presents a framework for Argonne National Laboratory's advancement of national priorities in grand challenge science and technology and a clean energy revolution. It is Argonne's goal to ignite an innovation ecology that strengthens research partnerships among universities, laboratories, and industry. In the past, these collaborations have created some of the great inventions of our time, such as the transistor, laser, charge-coupled device, and Internet, and fired national economies to create millions of high-quality jobs, raising quality of life around the world.

Specifically, Argonne is pursuing major advances in basic scientific discovery and innovation, with an eye towards technologies that support energy security, environmental sustainability, and a secure nation. Argonne is home to some of the world's top scientists and engineers and steward to unique and world-leading scientific facilities — many of which are open to and fully subscribed to the scientific user community. Argonne's complex network of research interactions enables the development and translation of new knowledge to both the scientific literature and marketplace. Such collaborations are critical to support long-term visionary thinking and to turn ideas into reality.

To achieve the goals presented here, Argonne has articulated a series of major initiatives, which are enabled by the Laboratory's core capabilities and support the national scientific agenda with four of the practical challenges it promotes.

Scientific Discovery and Innovation

Central to Argonne's research philosophy is a commitment to the high impact of the Laboratory's fundamental science. Argonne's researchers continually advance the core of the Laboratory's capabilities in the physical and biological sciences, and work to translate this research into revolutionary breakthroughs in energy-, environment-, health-, and security-driven challenges. Argonne endeavors to attract the very best and brightest scientists and engineers to strengthen this foundation and achieve the great discovery and technological innovation required by the nation and scientific community at large. Through rich educational and outreach programs, Argonne also strives to cultivate a new generation of skilled, educated, and science-savvy Americans.

Energy Security

Having reliable, clean, and affordable energy sources is a matter of urgent national importance. Argonne is committed to major advancement of the basic energy sciences, with focused research and development on a broad portfolio of sustainable and clean energy technologies. The national goal of doubling the generation of renewable energy in the next three years will require next-generation technologies and efficiencies with real innovations in materials, chemistry and engineering. Innovations in vehicular and grid-scale energy storage technologies and alternative energy sources, such as solar, biofuels and nuclear, are all required to achieve this goal. The successful transfer of new energy technologies to both small businesses and established industrial partners will be the ultimate measure of return on the national research investment.

Environmental Sustainability

Closely linked to requirements for energy security is an understanding of the impact energy production and use has on the world around us. Creating a mitigation strategy for the effects and causes of a changing climate and environment requires a clear understanding of interactions at the regional level. Argonne's biological and environmental research is focused on understanding the physical impact of climate change throughout the ecological continuum from soil to sky and assessing the regional economic, health, and social consequences of these changes.

A Secure Nation

Enhancing our national and homeland security requires substantial technological advancements ranging from clearly identified needs in sensor and detector development, nuclear forensics, infrastructure assurance, risk and vulnerability assessments, and even cyber security. Argonne pursues innovation in national security technologies with novel application of research, development, and engineering expertise to specific security and defense requirements — particularly in the verification of arms control and nonproliferation agreements.

Argonne's Core Capabilities

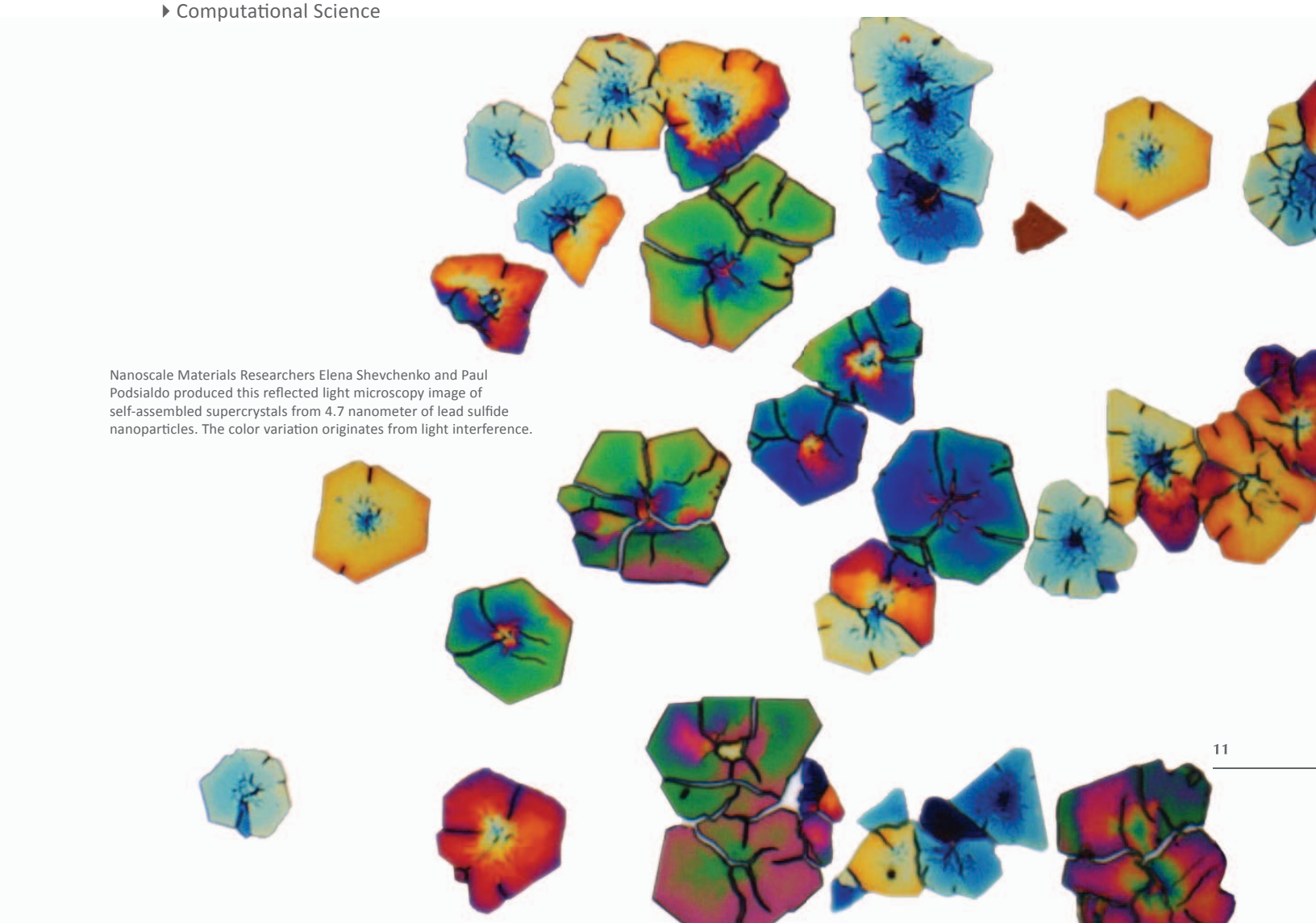
Argonne's research, development, and engineering expertise reside within a series of core capabilities encompassing a substantial combination of scientists, engineers, facilities and equipment — all having a very unique or world-leading component. Included here are the Laboratory's world-class user facilities which are open for use to the entire research community. Crosscutting research among these activities promotes an open innovation model; the entire research and development effort is open to many researchers at all stages of the innovation cycle from idea creation to deployable technology. The following core capabilities serve as building blocks for all of Argonne's research activities:

Fundamental Sciences

- Nuclear Physics
- Particle Physics
- Accelerator Science and Technology
- Condensed Matter Physics and Materials Science
- Chemical and Molecular Science
- Advanced Computer Science, Visualization, and Data
- Applied Mathematics
- Biosciences
- Computational Science

Applied Sciences and Engineering

- Applied Materials Science and Engineering
- Chemical Engineering
- Applied Nuclear Science and Technology
- Systems Engineering and Integration
- Climate Change Science



Nanoscale Materials Researchers Elena Shevchenko and Paul Podsialdo produced this reflected light microscopy image of self-assembled supercrystals from 4.7 nanometer of lead sulfide nanoparticles. The color variation originates from light interference.

Argonne's Eight Major Initiatives

In the coming five years, Argonne will pursue major initiatives that support Department of Energy research goals to create innovative and transformational solutions to the nation's grand scientific challenges. These initiatives have inspirational goals that will keep Argonne at the very forefront of scientific discovery and engineering excellence.

Three major initiatives emphasize the development of next-generation scientific tools and materials:

Hard X-ray Sciences

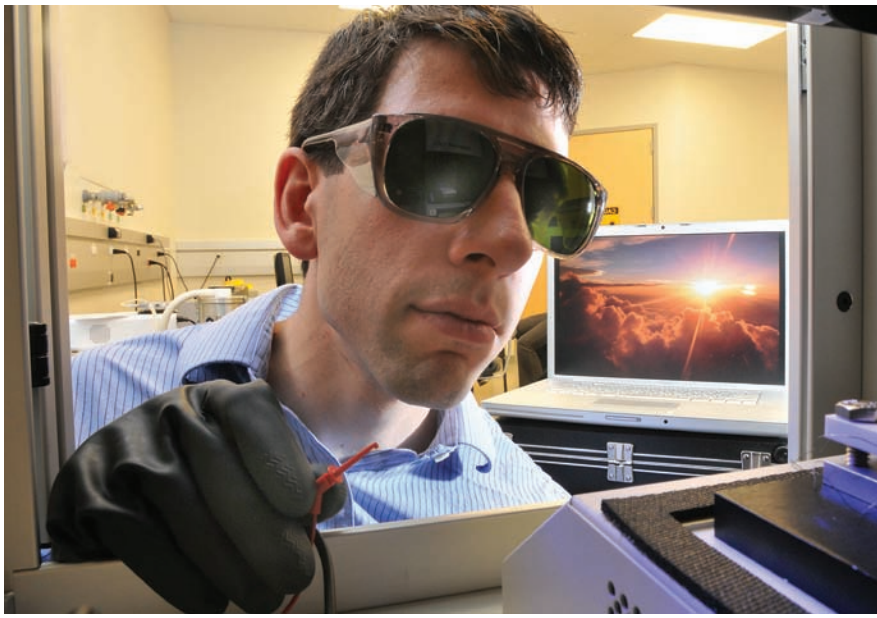
Argonne is home to one of three large high-energy light sources in the world. Each year, scientists from around the globe make thousands of discoveries while using the Advanced Photon Source to characterize both organic and inorganic materials. Argonne is pursuing the next-generation hard X-ray source, instruments, techniques, and facilities that will drive mastery of energy and information at the nanoscale, as well as characterization and control of materials far from equilibrium. Our ultimate goal is to advance hard X-ray science to enable the imaging of the very small and very fast, in real time under real conditions.

Leadership Computing

Leadership computing is widely recognized as a gateway for scientific discovery and a tool for understanding the world around us. Argonne is home to one of the fastest computers for open science, the Blue Gene/P, and has developed award-winning system software for these massive machines. The Laboratory's goal is to drive the evolution of leadership computing from petascale to exascale, lead the development of scalable codes and computing environments, and expand computational efforts to help solve the great scientific, energy, environment, and security challenges of our time.

Materials and Molecular Design and Discovery

Many solutions to pressing societal needs of today will be driven by the discovery of novel materials and molecules. The advancement of battery, solar, nuclear, electronic and fuel technologies are all dependent on these discoveries. It is Argonne's goal to produce a revolutionary advancement of the science of materials discovery and synthesis — predicting, understanding, and controlling not only where but also how to place individual atoms and molecules to achieve desired material properties.



Nanoscientist Seth Darling measures the performance of a nanostructured organic photovoltaic cell using a solar simulator that replicates sunlight under standardized conditions.

Five major initiatives directly address practical energy, environment, and security challenges:

Energy Storage

A critical enabling technology for transforming a fossil-based energy system to one driven by renewable sources is electrical energy storage. Batteries for electric-drive transportation, grid storage for intermittent energy sources, and the manufacturing processes for these materials-intensive devices all require significant advances in basic materials and molecular science and supporting applied technologies. Argonne is pursuing major advances in all of these areas with the goal of enabling widespread adoption of both vehicle and grid-based energy storage solutions.

Alternative Energy and Efficiency

The wide adoption of alternative energy sources requires major advancement of underpinning science and technologies. Argonne is developing both chemical fuels and biofuels optimized for combustion in current engine designs, as well as improved combustion schemes for future engine technologies. The Laboratory's solar energy research program is focused on devising solar-fuel and solar-electric devices and systems that are efficient, scalable, and economically competitive with the fossil energy sources in use today.

Nuclear Energy

The opportunity for nuclear energy to eclipse fossil-based sources for generation of electricity is enormous provided that safety, security and waste management concerns are addressed. Argonne's goal is to develop advanced reactor and fuel cycle technologies that enable the safe, sustainable generation of nuclear energy. The Laboratory is developing and validating computational models and reactor simulations of future generation nuclear reactors to greatly reduce the development cycle of these enormously complex systems.

Biological and Environmental Systems

Understanding the local effect of climate change requires integration of the interactions between biological systems and ecosystems with climate and human activities. Our goal is an integrated multiscale assessment of these elements, from molecule to organism to ecosystem, combined with economic and social observations. The outcome will be a regionally-focused ecological and climate assessment that will both inform government policy decisions and improve our understanding of the world around us.

National Security

Many of the sensors, detectors, and technologies used to protect and defend our country are based on the application of basic scientific discoveries. The Laboratory is committed to improving the nation's security with the inherent capabilities resident at Argonne. In particular, Argonne's goal is to develop the critical security technologies that will prevent and mitigate events with potential for mass disruption or destruction, thereby protecting the citizens of this country as well as national interests.

INTRODUCTION TO ARGONNE

As it begins its journey into the challenges of the 21st century, Argonne National Laboratory builds upon its rich history of scientific discovery and technological achievements brought about by dedicated scientists and engineers, supportive sponsors, and world-class facilities.

Argonne's vision takes it into a future in which the Laboratory continues to make significant contributions to the nation's health and well-being, and continues to deliver significant scientific achievements and technology development that are meaningful to the Laboratory's stakeholders and partners. This *Plan* presents the Laboratory's strategy for advancing its core capabilities and achieving success in a series of major research initiatives.

Two important elements are woven into this strategy: stewardship of the Laboratory's world-class user facilities, including the Advanced Photon Source, the Argonne Leadership Computing Facility, and the Argonne Tandem Linac Accelerator System; and the expansion and leveraging of the Laboratory's partnerships to advance science and technology. To ensure effective execution of the *Strategic Plan* and to achieve the ambitious goals in its vision, the Laboratory has implemented a multilevel management process throughout the organization and is working closely with its sponsors and research partners.

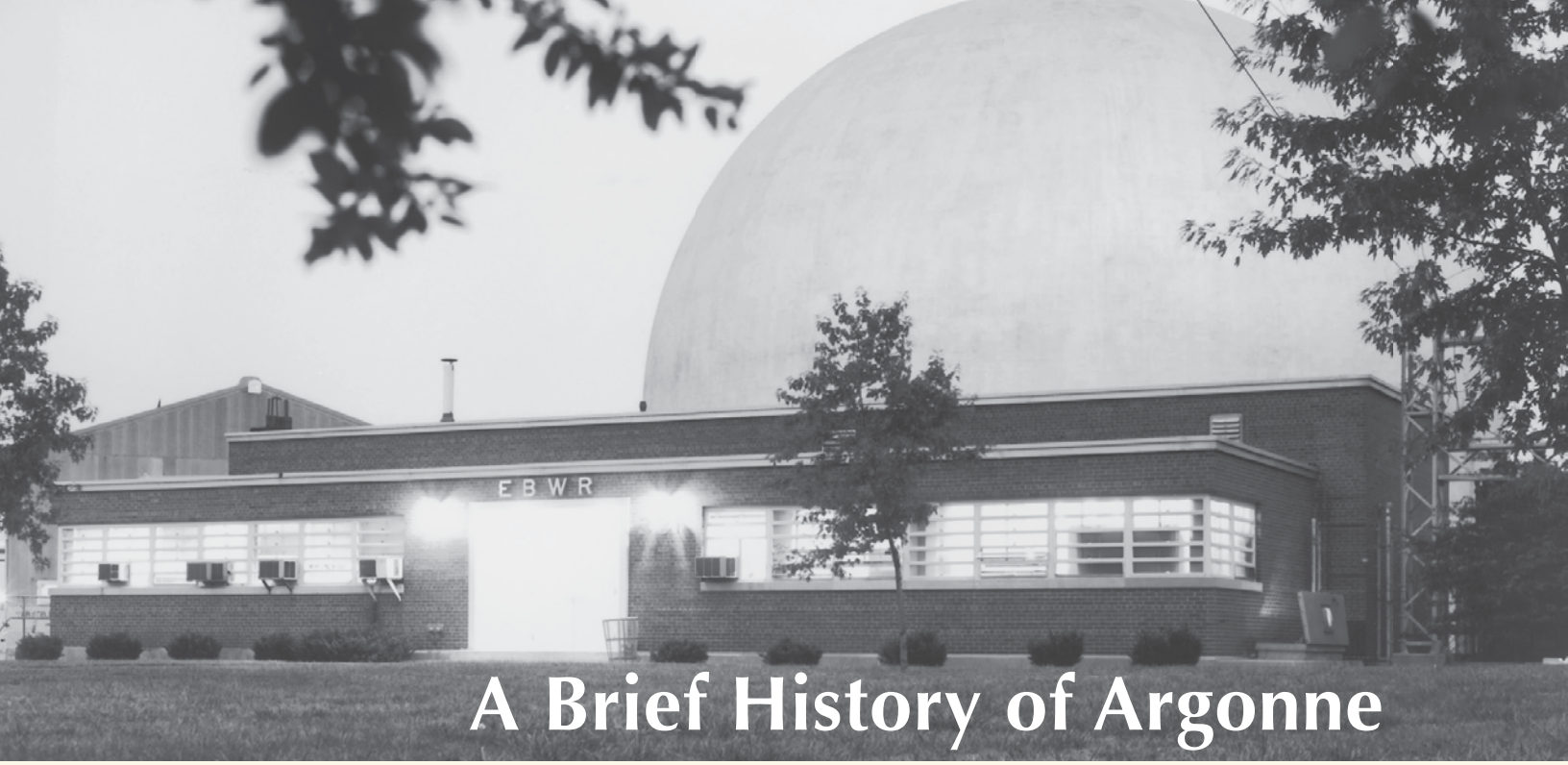
Role of the National Laboratories

The United States' national laboratory system began during a time of emergency — World War II and the ensuing Cold War. The system was intended to fill the perceived gap between universities (which were not generally set up to foster multidisciplinary approaches) and industry (which was primarily interested in developing products and services that make money) in confronting the conditions that threatened our nation at the time.

Today the laboratories as a group are engaged in a diverse set of scientific and technological challenges of national importance such as alternative energy, fossil fuels, climate change, and the future of the U.S. industrial base in an increasingly competitive global economy.

The national laboratories as a complex excel at and are committed to the continued advancement of a modern research and development infrastructure. Facility and equipment requirements are driven by the research needs of the Laboratory scientists and engineers as well as the various facility user communities. In addition to hosting facility users from other institutions, the laboratories use a wide variety of partnering mechanisms to leverage their facilities and core research capabilities. Collaborations with researchers from universities, industry, sister labs, and foreign institutions are a major factor in each laboratory's success.

When the U.S. Department of Energy (DOE) was created in 1977, it assumed stewardship of the national laboratories but continued to contract with non-governmental organizations to run them. Today, most of these "management and operating" (M&O) contractors are a consortia of universities and non-academic organizations. The DOE Office of Science oversees Argonne and nine other non-weapon, science-focused labs.



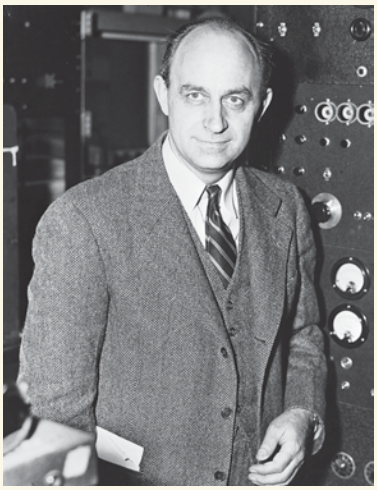
A Brief History of Argonne

Argonne traces its origins to the Metallurgical Laboratory (Met Lab) at the University of Chicago. Met Lab was established in 1942 under Enrico Fermi's leadership as part of the Manhattan Project. Fermi's group built the world's first nuclear reactor, Chicago Pile-1 (CP-1), on a squash court beneath the university's football field. There, the world's first controlled, self-sustaining nuclear chain reaction was achieved in December 1942.

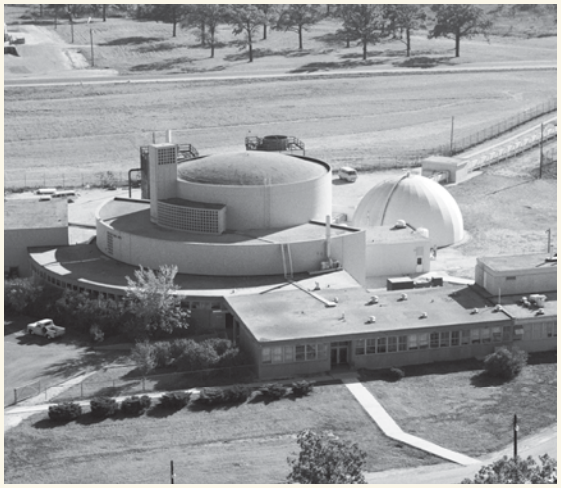
Argonne remains a vibrant research institution as it has continually re-invented itself over the years.

The Experimental Boiling Water Reactor was the first in the Western Hemisphere designed and built specifically as a pilot plant to advance nuclear power.

Enrico Fermi



Chicago Pile-5 Research Reactor



Argonne's first location, Site A, near Palos Park, Illinois

While the subsequent development of a usable atomic weapon took place at Los Alamos, New Mexico, and elsewhere in the U.S., the Met Lab group and others from the University of Chicago continued nuclear research at "Site A" in the Argonne Forest, part of a forest preserve southwest of Chicago. CP-1 was dismantled and rebuilt at Site A as CP-2, temporary buildings were erected, and the facility became known as the Argonne Laboratory. Fermi was its director until he moved to Los Alamos in 1945.

On July 1, 1946, the Laboratory — still operated by the University of Chicago — was formally chartered as Argonne National Laboratory to pursue peaceful civilian applications of nuclear energy, and within the next few years it moved to the 1500-acre site that it still occupies, about 25 miles southwest of Chicago.

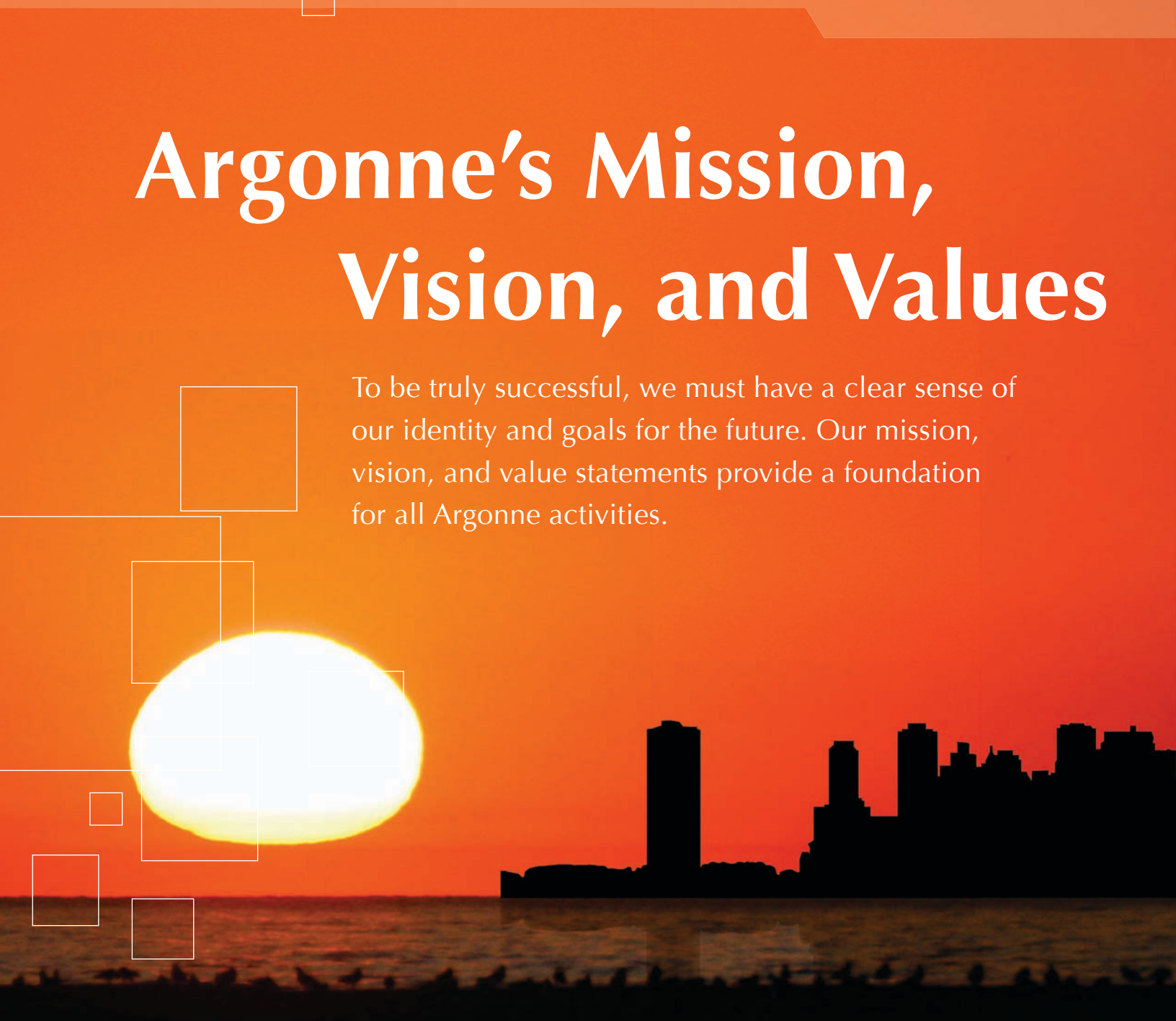
In 1949, the National Reactor Test Site (NRTS) was established in Idaho; for many years, the University of Chicago operated a second site, Argonne-West, on the NRTS reservation. Early milestones achieved by Argonne researchers include the designs for the first nuclear reactors to produce electric power (1951) and to power a submarine (1954). Argonne-led research underlies nearly every major commercial nuclear power system operating worldwide today.

Argonne remains a vibrant research institution, having continually re-invented itself over the years. In the 1950s, its focus was nuclear engineering; high-energy physics became a second focus area in the '60s and '70s, and by the '80s Argonne had made the transition to a truly multipurpose laboratory.

Since its inception Argonne has been managed by the University of Chicago. In October 2006, UChicago Argonne, LLC, a new entity formed by the University of Chicago, won the M&O contract for Argonne. The University tapped Jacobs Engineering Group to provide expertise in project management systems and facilities operations and strengthened and expanded academic and research collaborations with Northwestern University and the University of Illinois whose science, social science, and engineering programs strongly complement Argonne's capabilities.

Argonne's Mission, Vision, and Values

To be truly successful, we must have a clear sense of our identity and goals for the future. Our mission, vision, and value statements provide a foundation for all Argonne activities.



Our Core Values and Operating Principles

Discover and Innovate

We passionately pursue the discovery of new knowledge that will answer major scientific questions, address the grand technological challenges that face our nation, and deliver on the DOE mission.

Do It Safely, Do It Right

As scientific leaders, our obligation to the American people demands that we conduct our research and operations safely and responsibly. For both routine and tough decisions, we will always be ethical and do the right thing.

Closely Collaborate With Our Sponsors

We strive to exceed the expectations of our sponsors through the quality of our research, effective communication, proper fiscal management, and timely completion of awarded projects.

Our Mission

To apply a unique blend of world-class user facilities, science, and engineering that deliver innovative research and technology. Our scientists and engineers create new knowledge and technologies that address the most important scientific and societal needs of our nation.

Our Vision

To lead the world in providing scientific and engineering solutions to the grand challenges of our time: plentiful and safe energy, a healthy environment, economic competitiveness, and a secure nation.

Respect Diversity

The confluence of different backgrounds, perspectives, and ideas is one of Argonne's greatest assets. We embrace the diversity of our employees and the opportunity it affords to create a vibrant intellectual research environment.

Partner for Research

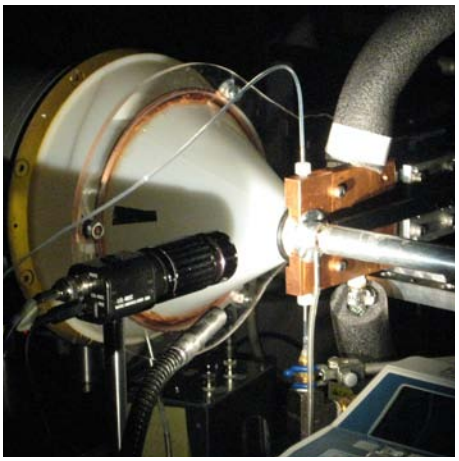
We seek out and build collaborations that break the traditional disciplinary boundaries within Argonne, and unite our expertise and capabilities with those of other leading laboratories, universities, and industry.

Prepare for the Future

We endeavor to educate and develop the careers of scientists and engineers to ensure the quality and breadth of tomorrow's workforce.

Visitors to Argonne's open house

MADMAX, a precise molecular ruler for measuring distances within a protein, is being developed with funding from the National Institutes of Health.



Stakeholders in Argonne's Success

Argonne's primary sponsor is the U.S. Department of Energy's (DOE's) Office of Science. The Laboratory also receives support from other DOE directorates, such as the Office of Energy Efficiency and Renewable Energy (EERE) and the National Nuclear Security Administration (NNSA), and from a variety of other federal agencies, such as the National Institute of Health, Department of Homeland Security, Department of Defense, and Department of Transportation. The State of Illinois has provided construction funds for an on-site hotel, the Center for Nanoscale Materials, an Advanced Photon Source beamline, and other capital projects.

The UChicago Argonne, LLC guides Argonne's strategic management and vision through its Board of Governors, which comprises 21 academic and industry leaders. The Board has established a Science Policy Council to provide strategic and scientific advice. The Council includes the vice presidents of research for the University of Chicago and Northwestern University, the vice chancellors of research at the University of Illinois at Urbana-Champaign and the University of Illinois at Chicago, and the Argonne Laboratory Director.

In addition to federal and state government sponsors, Argonne's Board of Governors, and the LLC's corporate and academic partners, many other universities, laboratories, industrial research organizations, and sponsors participate as stakeholders in Argonne's research endeavors. In the broadest sense, anyone who stands to benefit from Argonne's research activities is a stakeholder. A few of the more direct type of research relationships are discussed here.

Collaborative Research

Collaborative research relationships at Argonne take many forms, ranging from short-term between Argonne scientists and their peers at other institutions to joint appointments with major universities. Virtually all successful R&D efforts at Argonne benefit from some sort of collaboration or partnership.

User Community

The scientific user community represents an extraordinary constituency and stakeholder in Argonne's current and future success. Argonne's user facilities have hosted tens of thousands of researchers from more than 1,100 institutions worldwide. User facilities operating at the time of this writing include the Advanced Photon Source or APS, a forefront facility for materials and structural biology research; Center for Nanoscale Materials; Argonne Tandem Linear Accelerator System; Electron Microscopy Center; Argonne Leadership Computing Facility; and automotive test facilities for studies of interest to the transportation industry.

National Laboratories

Argonne also partners with other national laboratories on the design and construction of new facilities, including the International Linear Collider, the Spallation Neutron Source at Oak Ridge, the National Synchrotron Light Source-II at Brookhaven, and the Linac Coherent Light Source at the SLAC National Accelerator Laboratory.

Application Scientists

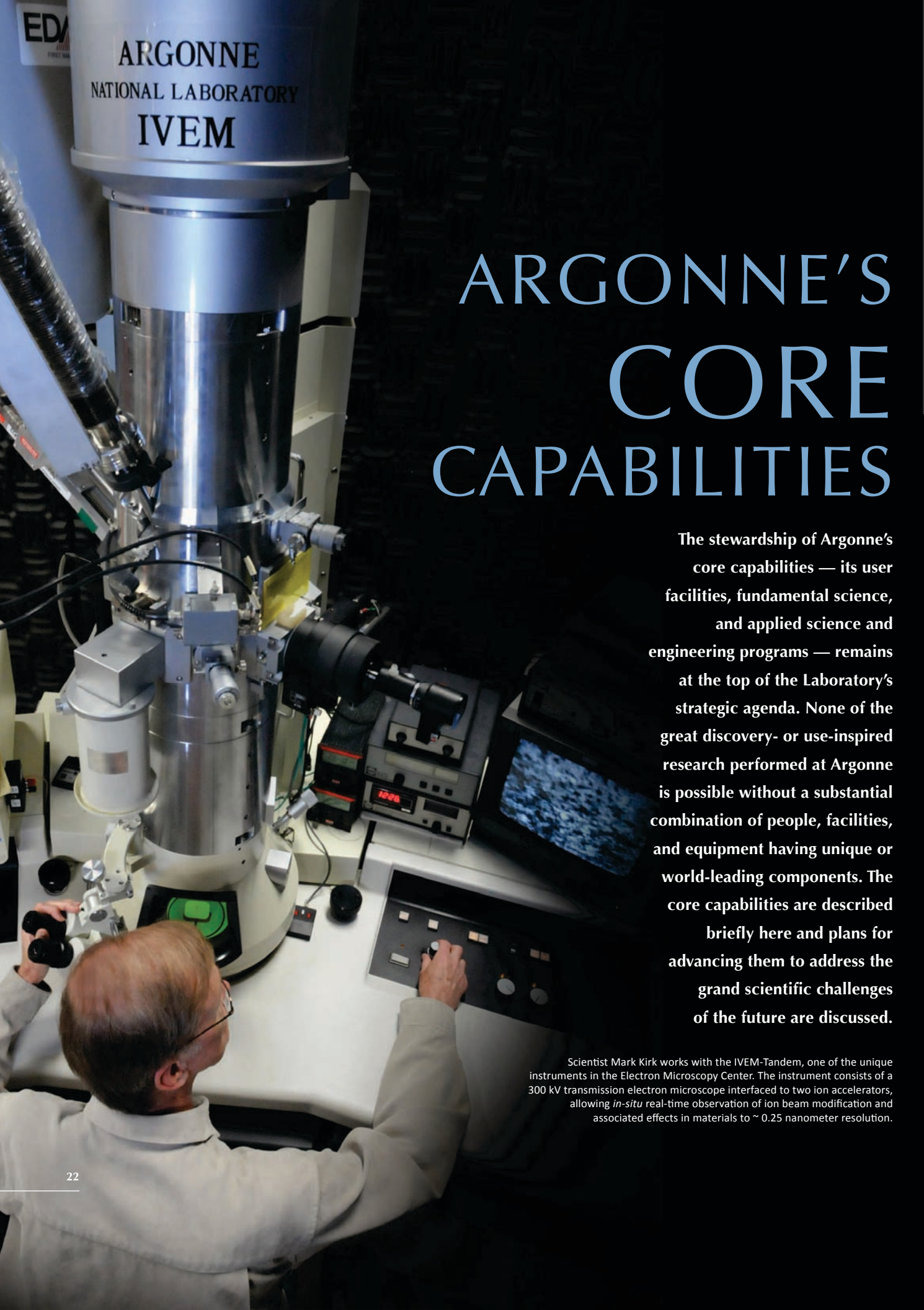
Application scientists at leading computing centers in the U.S. and abroad work with Argonne on programming models and software libraries, scientific codes encapsulating the best numerical algorithms, national and international grids, and environments for collaborative science. Computer vendors also work closely with Argonne researchers to develop the world's fastest supercomputers and the systems software to drive them, as well as standards for networking and distributed systems.

Community Residents

Argonne employees and their families, neighbors, and friends — and all residents of the surrounding communities — are important stakeholders in Argonne's research. The Laboratory maintains a dialog about its activities with surrounding communities in several ways, including direct-mail and electronic newsletters, a quarterly Community Leaders Round Table, and an Argonne open house held for the public every few years.

Major Clint Abell of the U.S. Air Force Fellows joined Argonne researchers to investigate smarter diesel engines.

Virtually all successful R&D efforts at Argonne benefit from some sort of collaboration or partnership.



ARGONNE'S CORE CAPABILITIES

The stewardship of Argonne's core capabilities — its user facilities, fundamental science, and applied science and engineering programs — remains at the top of the Laboratory's strategic agenda. None of the great discovery- or use-inspired research performed at Argonne is possible without a substantial combination of people, facilities, and equipment having unique or world-leading components. The core capabilities are described briefly here and plans for advancing them to address the grand scientific challenges of the future are discussed.

Scientist Mark Kirk works with the IVEM-Tandem, one of the unique instruments in the Electron Microscopy Center. The instrument consists of a 300 kV transmission electron microscope interfaced to two ion accelerators, allowing *in-situ* real-time observation of ion beam modification and associated effects in materials to ~ 0.25 nanometer resolution.

Scientific and Engineering User Facilities and Instrumentation

Argonne is a recognized leader in the design, construction, and operation of world-class user facilities for the U.S. Department of Energy that probe the most fundamental electronic and atomic properties of materials, advance the understanding of nuclear matter, and deliver forefront computational and networking capabilities. Together, these facilities hosted more than 4,000 users from Argonne and almost 500 other institutions in FY 2008.

Facilities and Instrumentation

The **Argonne Leadership Computing Facility (ALCF)** operates one of the largest open-science supercomputers in the world. ALCF offers user access to petascale computing for the largest scientific applications, including research in energy systems, catalysis, life sciences, and environmental and basic sciences.

The **Advanced Photon Source (APS)** is a unique national source of high-energy X-rays — the brightest X-ray source in the western hemisphere — for scattering, spectroscopy, and imaging studies. The intensity and pulsed nature of these X-rays allow time-resolved studies of dynamics over a wide range of time scales from many seconds to about 100 picoseconds. Several APS beamlines accommodate experiments at extremes of pressure and temperature, or *in situ* observations of crystal growth.

The **Center for Nanoscale Materials (CNM)** combines advanced proximal probes; a unique X-ray nanoprobe beamline at the APS that provides fluorescence, diffraction, coherent diffraction, and transmission imaging at a spatial resolution of 30 nanometers or better; organic, inorganic, biological, and digital synthesis and assembly; multiple spectroscopies, including advanced time-resolved and near-field techniques for imaging energy transduction and transfer; electron and optical microscopy; and nanofabrication — all coupled with theory and modeling.

The **Electron Microscopy Center (EMC)** provides state-of-the-art chromatic-aberration-corrected electron microscopy with applications to three-dimensional elemental imaging and *in situ* environmental studies of catalysts and other nanoscale materials.

The **Argonne Tandem Linac Accelerator System (ATLAS)** is the premier DOE National User Facility for low-energy nuclear research. Based on a superconducting linear accelerator, ATLAS provides heavy ions in the energy domain best suited to study the properties of the nucleus, the core of matter, and the fuel of stars.

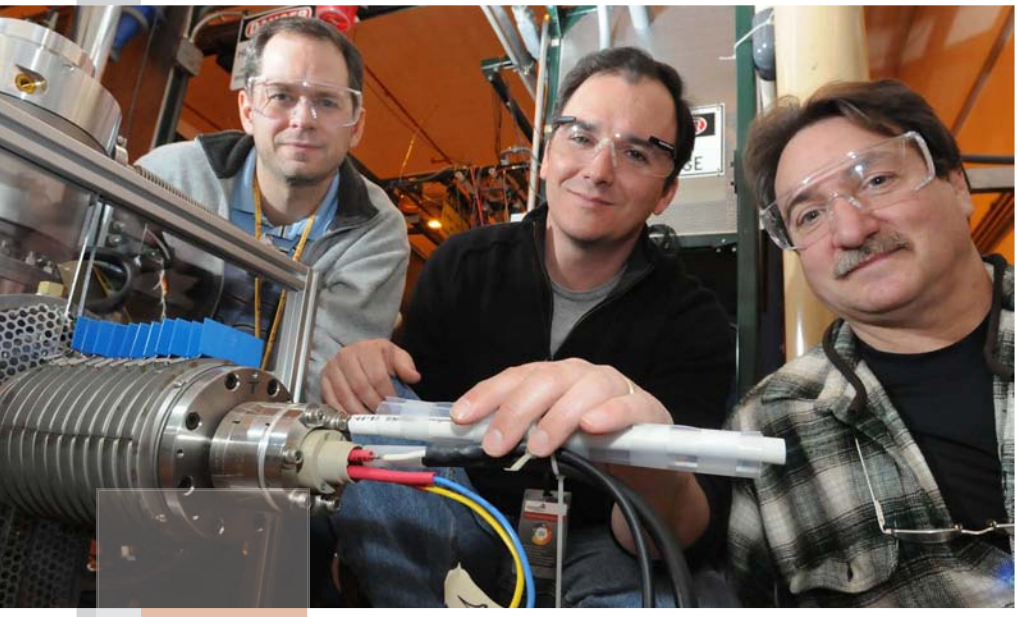
The **CAlifornium Rare Ion Breeder Upgrade (CARIBU)**, a rare-isotope injector based on a californium fission source and a radio frequency (RF) gas stopper cell, is under construction at ATLAS. Starting in 2009, it will produce unique rare-isotope beams that cannot be produced through uranium fission. Argonne also provides one-of-a-kind, custom-built detectors for use in high-energy and nuclear physics research worldwide.

Argonne's user facilities have hosted tens of thousands of researchers from more than 1,100 institutions worldwide.

The **Transportation Research and Analysis Computing Center (TRACC)**, a high-performance computing and engineering analysis research facility managed and operated by Argonne for the U.S. Department of Transportation (DOT), is being electronically linked to DOT research and development facilities, state departments of transportation, and university transportation research centers.

Argonne also provides cyber security and engineering support for the **Atmospheric Radiation Measurement (ARM) Climate Research Facility (ACRF)**, which consists of several highly instrumented ground stations in various climate zones around the world for studying cloud formation processes and their influence on radiative properties of the atmosphere.

More details about all of Argonne's user facilities and their application to the Laboratory's research programs appear in the following sections.



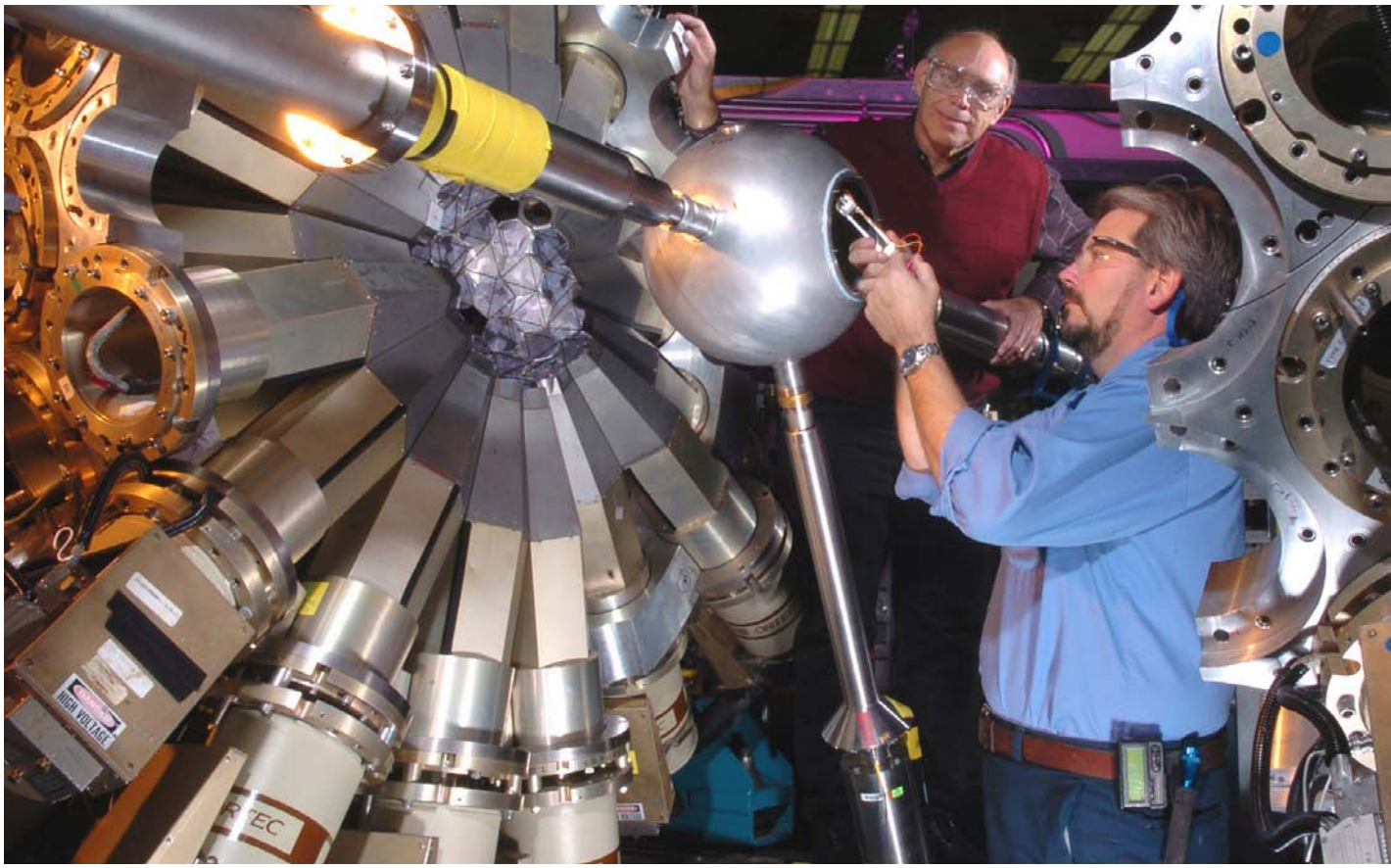
Scientific Associate Bob Scott (left), and Engineers Rick Vondrasek and Gary Zinkann, with the CARIBU surface ionization source, which provides stable beams to the charge breeder.

the future >>

Setting the standard for continued excellence in stewardship of these national resources remains a top priority for Argonne. Programmed renewal of Argonne's facilities is crucial to maintaining the Laboratory's leadership — not only in scientific applications but also in the science behind the development of the next generation of facilities. Renewals and upgrades are either planned or being planned for virtually all of the Laboratory's user facilities and major instruments.

Fundamental Sciences

Engineers Bruce Zabransky (left) and John Rohrer work on Argonne's Gammasphere, the world's most sensitive gamma-ray detector.



Argonne has an international reputation for research directed toward understanding the matter and processes that constitute the natural world. Fundamental science research at Argonne encompasses many areas of physics, chemistry, materials science, and biology. This work supports all of Argonne's major research initiatives.

NUCLEAR PHYSICS

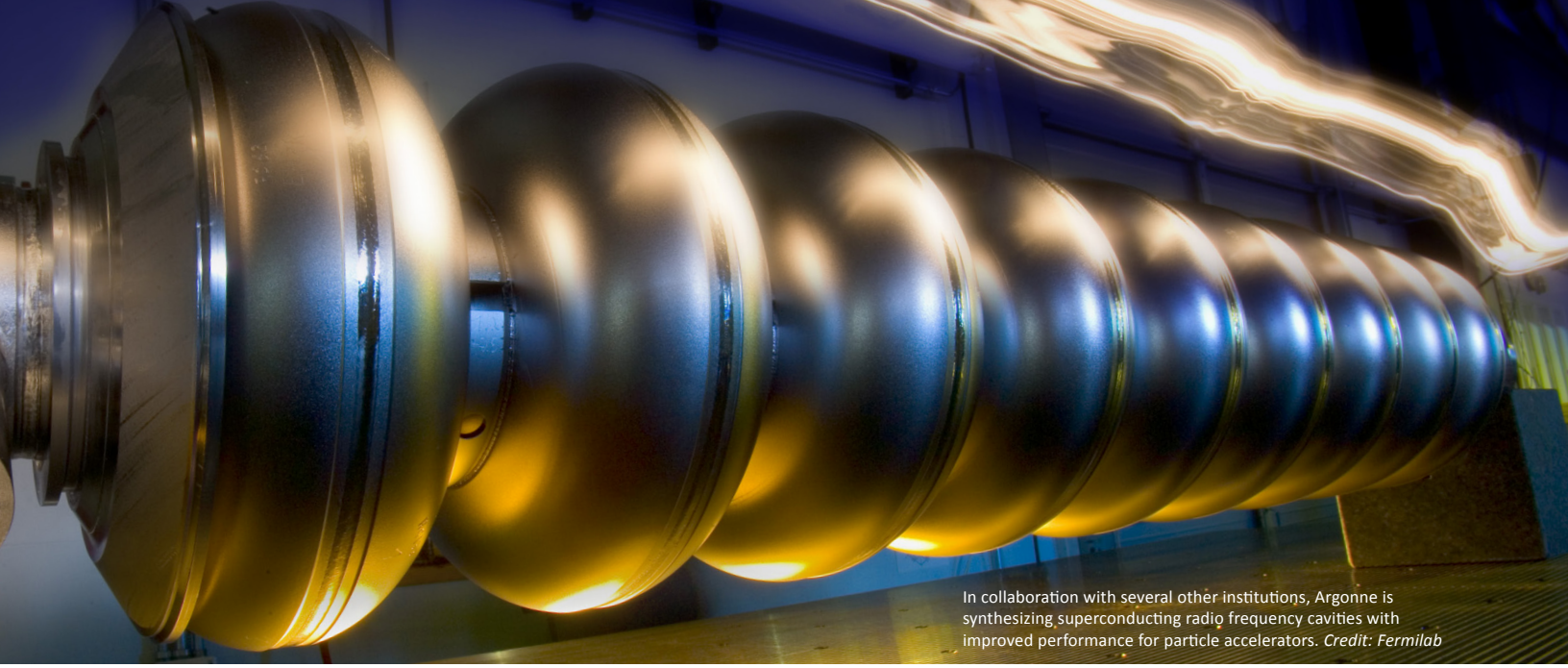
Capabilities

Argonne scientists use stable ion beams and rare (e.g., radioactive) isotope beams from the Argonne Tandem Linac Accelerator System (ATLAS) for several significant areas of research. Principally, Argonne highlights aspects of nuclear structure that are not readily apparent in stable nuclei, investigates reactions from the cataclysmic events of the cosmos, and tests nature's fundamental symmetries. The 2009 CARIBU upgrade will allow the delivery of unique rare-isotope beams for nuclear structure and astrophysics research. Argonne also seeks a deeper understanding of the underlying strong force and its basis in quantum chromodynamics as it applies to protons and neutrons (addressing how quarks and gluons assemble into various forms of matter) and to the strongly coupled nuclear many-body system. This experimental work is supported by research in accelerator science and technology and by strong theory efforts that leverage the Laboratory's advanced computer science expertise and the Argonne Leadership Computing Facility.

the future >>

An efficiency and intensity upgrade of ATLAS over the next three to four years will provide a tenfold increase in both stable and rare isotope intensities and improved beam properties required for new lines of research. Also, an advanced accelerator-based facility is being considered for the production of rare isotopes using the isotope online method. These isotopes would enable research that is complementary to studies targeted by the future university-based Facility for Rare Isotope Beams. Such a facility would also provide large quantities of radioisotopes for various applications, primarily in medicine. The Laboratory is evaluating the feasibility of support via a public-private partnership.

Argonne will continue to be a major enabler of the



In collaboration with several other institutions, Argonne is synthesizing superconducting radio frequency cavities with improved performance for particle accelerators. *Credit: Fermilab*

PARTICLE PHYSICS

Capabilities

Argonne's particle physics research focuses on understanding the properties and interactions of the fundamental particles that make up the universe, and the symmetries that underlie the fundamental forces of nature and the constituents of matter. Research teams will:

- Develop new or extend existing theoretical models;
- Develop new and unique detectors and sensors;
- Design, build, and commission large detector systems to study particle interactions;
- Design and create the software and computing infrastructure for handling very large data sets; and
- Analyze experimental data to gain new insights into particle physics.

In all these activities, the involvement of other disciplines at the Laboratory is emphasized; for example, Argonne's strong materials science capability is being leveraged to develop new materials for detectors and sensors.

the future >>

The findings from Argonne's worldwide experimental collaborations drive the direction of the Laboratory's particle physics research. Argonne will continue to be a major enabler of the ATLAS experiment at the Large Hadron Collider. Scientists will develop new dielectric-based Wakefield accelerator structures and new detector technologies, and will provide the theoretical underpinnings that help guide future particle physics research. Argonne also will look for opportunities to use the expertise and technologies associated with other core capabilities in the particle physics research and development area, and to transfer its expertise in particle physics to other Argonne research endeavors.

ATLAS experiment at the Large Hadron Collider.

Argonne-developed superconducting spoke cavities can operate at lower temperatures and at higher magnetic fields than previous designs, translating into a potential savings in the cost of a heavy-ion linear accelerator.

ACCELERATOR SCIENCE AND TECHNOLOGY

Capabilities

Argonne's expertise in accelerator science and technology supports fundamental research in hard X-ray science, high-energy physics, and nuclear physics. In the X-ray arena, Argonne excels in modeling, design, and operation of electron accelerators and free electron lasers; undulator design, fabrication, and measurement; control systems; and vacuum chamber design and construction. Software codes developed at Argonne for X-ray facility design are used worldwide.

For high-energy physics applications, Argonne is playing a significant role in research and development for the proposed International Linear Collider and for Project-X at Fermilab, which uses spoke resonators originally developed at Argonne. The Argonne Advanced Wakefield Accelerator is the only facility in the world where two-beam acceleration techniques and dielectrically loaded structures — a promising concept for linear colliders — are being developed and studied.

Accelerator activities for nuclear physics applications include the creation, acceleration, and manipulation of beams of rare isotopes and low-velocity superconducting accelerating structures. End-to-end simulations for hadrons and heavy ions are carried out with new codes that take advantage of the capabilities of the Argonne Leadership Computing Facility. Argonne is also a U.S. leader in the processing of superconducting RF cavities with techniques developed for ATLAS and its upgrades.

the future >> Materials science and other expertise throughout Argonne will be strategically aligned to focus on developing "cavity-based" accelerating structures (either superconducting or warm, made from either metal or dielectric materials), and understanding surface phenomena that currently limit performance. The Laboratory also looks to improve surfaces through standard surface treatments and new materials synthesis technologies such as atomic layer deposition (ALD), and to explore new techniques for cavity construction that combine ALD and X-ray lithography.

CONDENSED MATTER PHYSICS AND MATERIALS SCIENCE

Capabilities

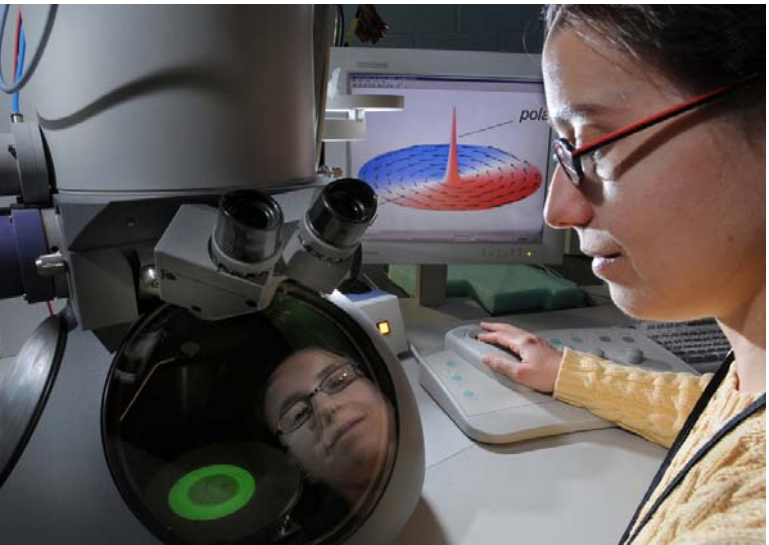
A premier core capability at Argonne is the design, synthesis, fabrication, and characterization of nanoscale materials; complex oxides and other strongly correlated systems; and other advanced materials that have the potential to transform energy production, distribution, storage, and use. Across the entire portfolio, the objective is to understand, control, and improve the properties of materials.

This capability encompasses multiple Argonne organizations from basic science through systems engineering and deployment. Argonne's strength lies in combining its strong programs in materials physics, chemistry, nanoscience, and biology with its user facilities for hard X-ray characterization down to the nanoscale, electron scattering, nanoscale materials, and leadership computing. Argonne's areas of materials science expertise include:

- Theory and computation for materials design and insight into properties;
- Synthesis for materials discovery, including bulk crystal, bio-inspired, nanoparticle, film and digital synthesis;
- Electronic, magnetic, and photonic behavior;
- Patterning methods such as electron beam lithography; and
- *In situ* characterization using scanning probe microscopies, X-ray scattering and spectroscopy, ultrafast optical techniques, and electron scattering.

the future >>

The understanding and control of fundamental interactions in highly correlated and hierarchical systems will enable the Laboratory to harness emergent functionality in bulk crystals, surfaces, and tailored interfaces to address global energy challenges. Materials design — linking research in molecules, bio-inspired and organic materials, and inorganic solids — will join *in situ* probes as foundations of this activity. Novel techniques, such as aberration-corrected electron microscopy, will be deployed to visualize the ultrasmall. State-of-the-art facilities in the new Energy Sciences Building and the proposed Materials Design Laboratory will invigorate these efforts.



Materials Scientist Mihaela Tanase observes a small magnetic disk with a transmission electron microscope. Tanase discovered a new method to control the way the atoms in the magnetic disk orient themselves to form "nanoscale vortices," which are illustrated on the computer screen.

CHEMICAL AND MOLECULAR SCIENCE

Capabilities

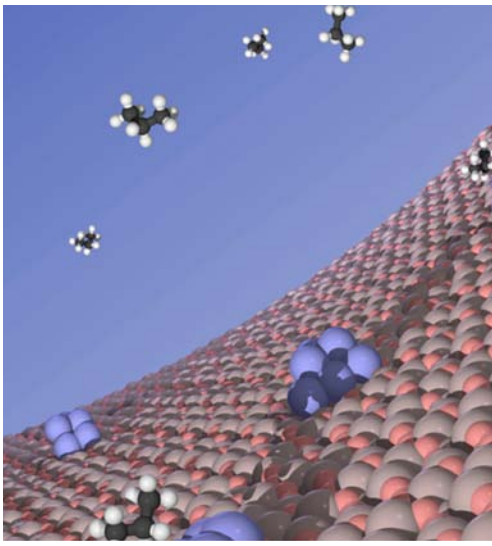
Argonne's chemical and molecular science expertise lies in the synthesis, self-assembly, characterization, and control of chemical processes that have the potential to transform energy production and use. These processes include photosynthesis, photo-induced electronic processes, catalysis, combustion, heavy-element separation, mineral chemistry, ultrafast physics, nuclear energy, and the conversion of chemical energy in batteries and fuel cells.

In addition to its broad and world-recognized expertise, Argonne possesses a mix of leading research tools for X-ray, laser, and scanning-probe studies and electrochemical analysis, as well as pioneering codes and software for computational chemistry, modeling, and simulation. Argonne's catalysis programs use state-of-the-art computational techniques — enabled by Argonne's core capabilities in advanced computer science and its large-scale computational facilities — to determine electronic structures, as well as a unique set of *in situ* analytical tools at the APS for improved understanding of catalytic systems under true operating conditions.

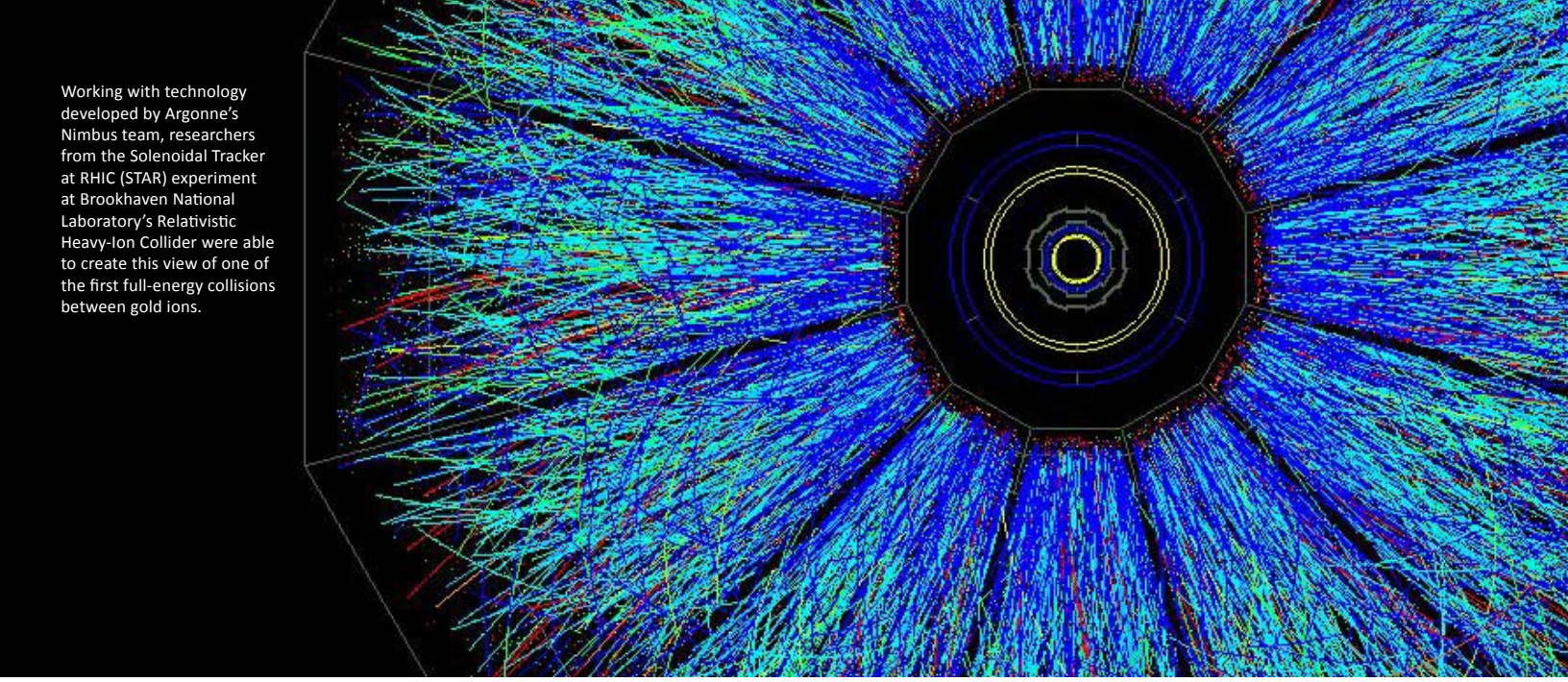
Argonne scientists apply their knowledge of photo-induced energy and electron transfer reactions in natural photosynthesis to a variety of biomimetic and synthetic systems. These studies are carried out on multiple spatial and temporal scales using state-of-the-art techniques developed at Argonne, such as ultrafast X-ray structural determination, high-field electron paramagnetic resonance, and ultrafast laser spectroscopy/microscopy imaging.

the future >>

The new Energy Sciences Building and the proposed Materials Design Laboratory will help the Laboratory's chemical science, materials science, nanoscience, and engineering efforts to focus synergistically on critical issues in energy storage, solar energy, and sustainable fuels. Argonne will develop new battery materials that will enable electric vehicles to travel as far as those fueled with gasoline. The increased understanding of how molecules are formed or destroyed by catalysts will lead to renewable production of fuels such as hydrogen and biofuels. These efforts will be part of a growing program in chemical synthesis.



Argonne scientists have discovered a new class of catalysts that may lead to energy-efficient and environmentally friendly synthesis strategies and the possible replacement of petrochemical feedstocks by abundant small alkanes. Shown here conceptually, clusters of 8-10 platinum atoms deposited in pores of an aluminum oxide membrane are highly active and selective catalysts for the oxidative dehydrogenation of propane.



Working with technology developed by Argonne's Nimbus team, researchers from the Solenoidal Tracker at RHIC (STAR) experiment at Brookhaven National Laboratory's Relativistic Heavy-Ion Collider were able to create this view of one of the first full-energy collisions between gold ions.

ADVANCED COMPUTER SCIENCE, VISUALIZATION, AND DATA

Capabilities

Argonne's Advanced Computer Science, Visualization, and Data core capability is built on the Laboratory's leadership in parallel programming models, scientific visualization, distributed computing technology, parallel file systems and I/O libraries, performance tools, large-scale data analysis, and systems software. Of particular note are the

- Access Grid, a revolutionary collaborative environment used worldwide for science and engineering applications;
- MPICH, the first portable implementation of the MPI standard and now considered the *de facto* standard for scientific research on parallel computers; and
- Globus Toolkit, which has become the *de facto* standard for grid computing.

The Access Grid, MPICH2, and the Globus Toolkit have all won prestigious R&D 100 awards.

Application groups worldwide use Argonne software, most notably in nuclear reactor simulation, computational biology, astrophysics, nuclear structure theory, and climate modeling. Argonne researchers develop software using massively parallel processors and advanced heterogeneous clusters that have novel processors and interconnects. Much of this research software is also deployed at the Argonne Leadership Computing Facility, which is used for the nation's largest scientific applications.

the future >>

Argonne is committed to continued leadership in system software, numerical libraries, and advanced analysis environments that together will provide scientists and engineers with the infrastructure and tools that enable previously unattainable science and engineering solutions. Long term, research in virtualization of resources, development of exascale infrastructure, and great advances across the scientific software stack will be instrumental in driving Argonne's science and technology forward.

Argonne's PETSc is the world's most widely used parallel numerical software library for partial differential equations and sparse matrix computations.

APPLIED MATHEMATICS

Capabilities

Researchers in applied mathematics, a core capability at Argonne since the late 1970s, now focus on optimization, partial differential equations, and computational differentiation. Argonne's optimization group has earned international renown for devising key concepts in optimization and for developing the MINPACK, Network Enabled Optimization Systems (NEOS), and Toolkit for Advanced Optimization (TAO) toolkits. NEOS, which won the 2003 Beale-Orchard-Hays Prize, processed more than 400,000 jobs in 2008. TAO, the first toolkit for solving large-scale optimization problems on advanced distributed architectures, is heavily used by academic, commercial, and government institutions.

Leaders of Argonne's partial differential equations group are recognized both for writing influential textbooks and for developing superb software. For example, the Portable Extensible Toolkit for Scientific Computation (PETSc), a 2009 R&D 100 Award winner, is the world's most widely used parallel numerical software library for partial differential equations and sparse matrix computations.

Argonne researchers also developed Nek5000, considered the best code for high-order simulations of complex fluid flows on architectures with more than 30,000 processors. Computational differentiation, which originated at Argonne between 1989 and 1992, has been cited as one of the top ten developments in scientific computing for 1970-2000. Argonne's computational differentiation group is considered the best in the world; its three major toolkits — ADIFOR, ADIC, and OpenAD — are used for sensitivity analysis and uncertainty quantification in climate modeling and nuclear safety analysis.

the future > >

The applied mathematics program will expand into new areas of interest to DOE that support the simulation of complex physical phenomena in advanced architectures. The addition of a core capability in uncertainty quantification will support, in particular, the modeling of new energy sources. A core capability in the mathematics of petascale data will address the need for algorithms and software to analyze the large data sets generated by Argonne's experimental facilities.

BIOSCIENCES

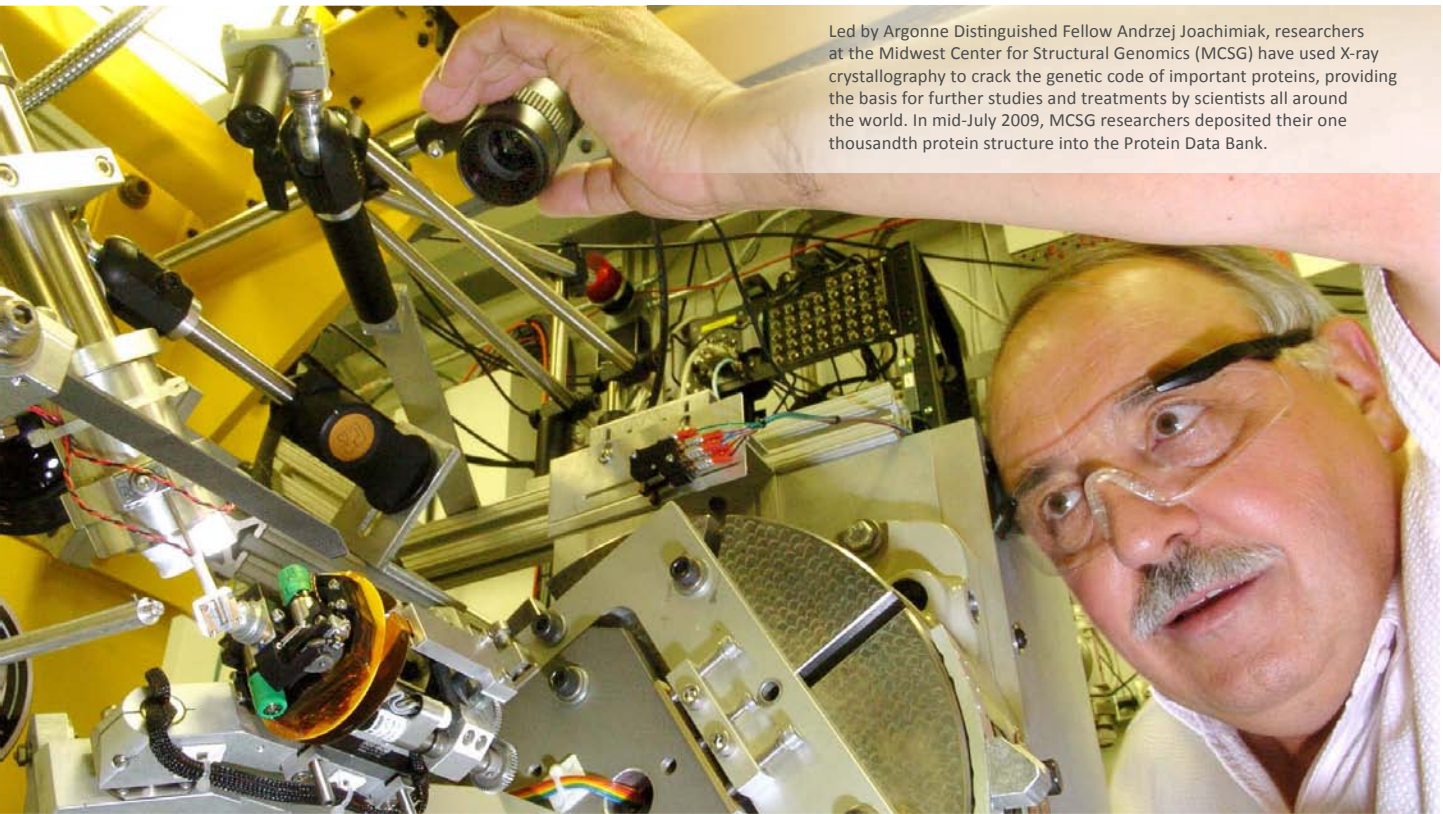
Capabilities

Argonne scientists characterize soluble and membrane proteins by using state-of-the-art molecular biology and biochemistry approaches implemented by high-throughput robotics together with the unique capabilities of the Advanced Photon Source. Their objective is to discover new biological functions and better understand known functions. The protein characterization activities are integrated with, and guided by, genome analysis, microbiology, cell biology, and field activities to address specific scientific questions.

The goal of Argonne's integrated bioscience research is to describe and understand protein systems that impact carbon management, form the basis of bioremediation strategies, facilitate advances toward alternative energy sources, and provide new therapeutics and diagnostics to improve human health.

the future >>

The high-throughput protein production, crystallization, and structure determination pipelines will be extended to include high-throughput protein function determination. The capability to predict protein function from genome sequence and then confirm it experimentally will position Argonne for the development of a Protein Discovery Center to advance molecular environmental and medical research. This Center is envisioned as a user facility supported by funding from multiple agencies.



Led by Argonne Distinguished Fellow Andrzej Joachimiak, researchers at the Midwest Center for Structural Genomics (MCSG) have used X-ray crystallography to crack the genetic code of important proteins, providing the basis for further studies and treatments by scientists all around the world. In mid-July 2009, MCSG researchers deposited their one thousandth protein structure into the Protein Data Bank.

COMPUTATIONAL SCIENCE

Capabilities

Modeling, simulation, and data analytics are employed in virtually every research division at Argonne and at a wide range of computational scales, from desktops to leadership computers. Widely recognized successes include Argonne-developed codes for nuclear reactor simulation, metagenomics, plasma processing, agent-based models, energy systems analysis, and accelerator design.

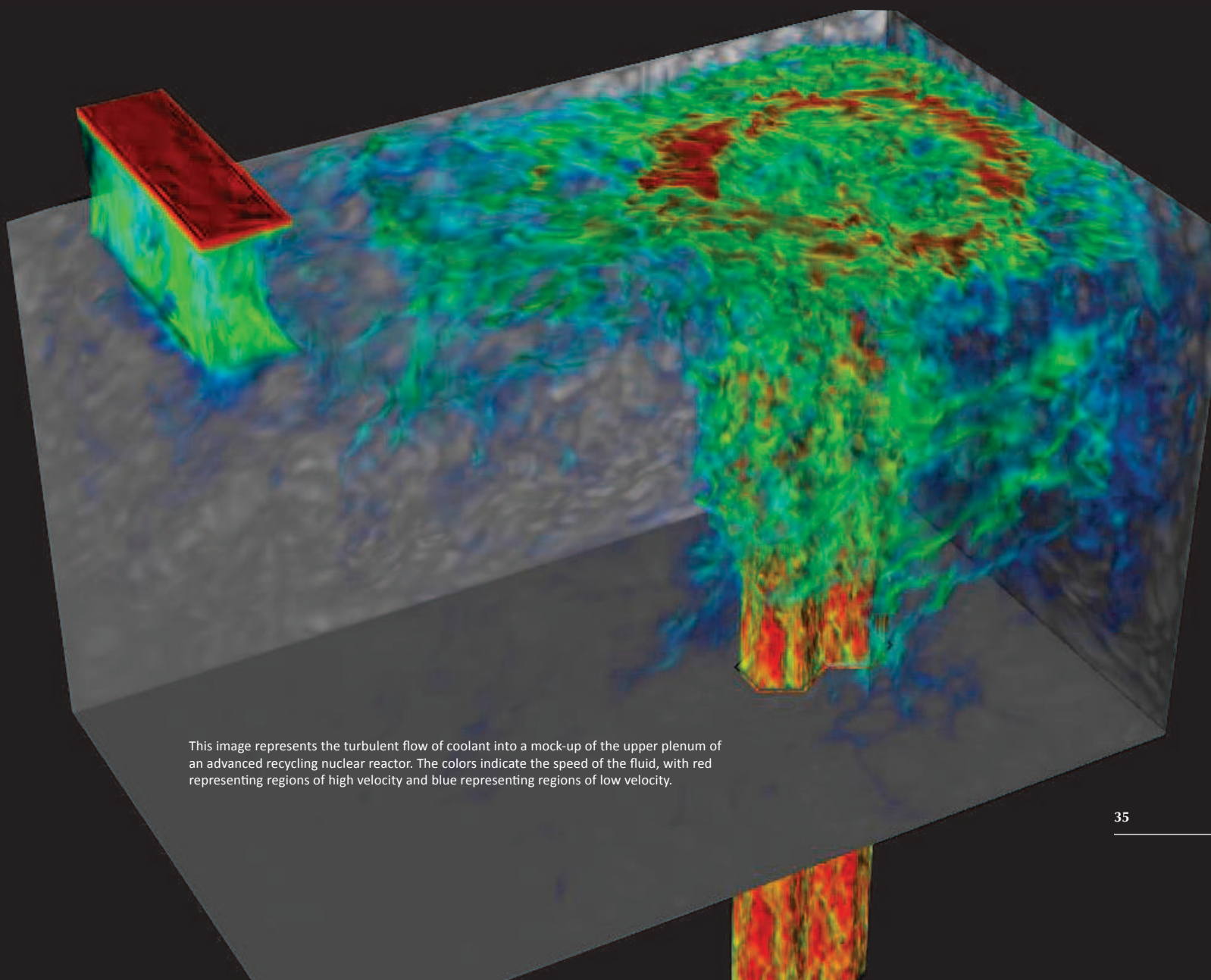
Argonne-developed tools for parallel solution of differential equations and optimization problems underpin hundreds of science and engineering applications around the world. Argonne also leads the development of applications for some of the most challenging computational problems, including computational fluid dynamics, neutronics, and coupled climate models. The deep scalable-computing knowledge of Argonne staff and members of the Argonne-University of Chicago Computation Institute, along with the Laboratory's history of building successful cross-disciplinary teams, provide a solid base for efforts in new areas.

The new Theory and Computing Sciences building

the future >>

Argonne will continue to develop modeling, simulation and analytics capabilities that advance and inspire the Laboratory's strategic initiatives, with emphasis on grand challenge problems for leadership computers. Late in FY 2009, many scattered computational efforts will be gathered into the new Theory and Computing Sciences Building, thereby enabling deeper collaboration and cross-disciplinary programs. Petascale computational programs in energy storage, biological and environmental systems, materials discovery, and nanoscale device design will be established in the near term.

Argonne-developed tools for parallel solution of differential equations and optimization problems underpin hundreds of science and engineering applications worldwide.

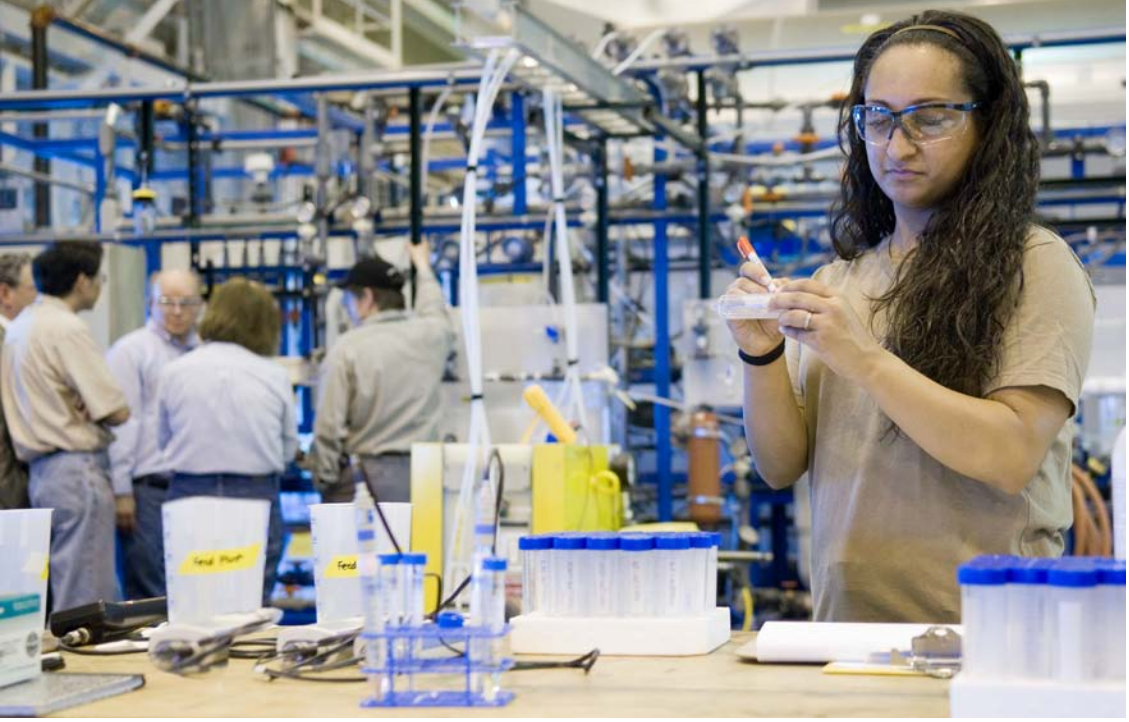


This image represents the turbulent flow of coolant into a mock-up of the upper plenum of an advanced recycling nuclear reactor. The colors indicate the speed of the fluid, with red representing regions of high velocity and blue representing regions of low velocity.

Applied Sciences and Engineering

Argonne's strong applied research program bridges the gap between fundamental science and deployable systems for sustainable energy solutions and enhanced national and homeland security. Core capabilities that underpin these efforts follow.

Chemist Jeff Elam inspects components for nanostructured solar cells. The various colors arise from thin-film coatings deposited on nanoporous membranes using atomic layer deposition.



Analytical Chemist Sabeen Ahmad labels samples from Argonne's Advanced Bioprocessing Plant.

APPLIED MATERIALS SCIENCE AND ENGINEERING

Capabilities

Significant advances in traditional and transformational energy technologies require the development not only of new materials but also of scalable processes for the production and application of those materials. Argonne's core strengths in the development, synthesis, application, and production engineering of new materials provide a foundation for advances in next-generation technologies for energy production, storage, distribution, and use. These capabilities benefit from the integration of expertise in multiple Argonne divisions; from discovery synthesis and characterization to applications in areas such as solar energy conversion, electrical energy storage, catalysis, and carbon dioxide (CO_2) capture and sequestration.

For example, Argonne is developing new materials for energy storage technologies, including advanced batteries and ultracapacitors for transportation applications, as well as membranes and systems for hydrogen production, CO_2 separation, and biofuels processing. Argonne continues to improve upon its groundbreaking, super-hard, ultrananocrystalline diamond and diamond-like carbon coatings that provide low friction and increased wear resistance for drivetrain and wind turbine gearbox components. The Laboratory is also advancing the development of manufacturing technologies needed for commercial applications of nanomaterials, including nanocatalysts, thermal nanofluids, nanolubricants, solar cells, and flat-panel displays.

the future >>

Argonne's successes in condensed matter physics, materials science, and chemical and molecular science will be translated into sustainable technologies that solve energy challenges. These will include advanced batteries and solar cells, developed through a multidisciplinary approach, and much more effective catalysts for a range of processes. Continued investment in world-class R&D facilities such as the proposed Materials Design Laboratory will enable Argonne to establish a leadership position in technology innovation for a secure energy future.

Chemistry Co-op Student Sarah Busking loads a pouch containing a lithium-ion battery cell into a test oven to evaluate its electrochemical performance.

CHEMICAL ENGINEERING

Capabilities

Argonne's chemical engineers primarily focus on developing sustainable energy resources. Research specialties range from catalysis to electrochemical systems, the nuclear fuel cycle, nuclear forensics, and environmental remediation. Argonne's advanced battery program, recognized as the leader among DOE laboratories, has been active since the late 1960s and is responsible for a large portfolio of intellectual property on advanced materials.

Argonne researchers are also developing the hydrogen production, storage, and use technologies necessary to realize the potential of fuel cells as clean, efficient power sources for automotive, stationary, and portable power applications. Advanced materials and electrocatalysts are being developed to reduce the cost and improve the durability of solid oxide and polymer electrolyte membrane fuel cells. Argonne's chemical engineering researchers continue to pioneer separations chemistry for nuclear fuel processing and are working to advance the security of nuclear processing and materials.

the future >>

Argonne will continue to develop new processes for converting resources such as biomass to transportation fuels and chemical commodities, develop and implement technologies to reduce NO_x emissions, and conduct fundamental research to improve our understanding of how catalysts promote chemical reactions. Chemical engineering will play a major role in the development, modeling, design, and demonstration of solvent extraction processes for spent fuel and radioactive waste treatment. A proposed 20,000-square-foot Battery Test Facility will provide much-needed expansion space for Argonne's testing and evaluation of advanced battery and grid-scale stationary storage systems.

APPLIED NUCLEAR SCIENCE AND TECHNOLOGY

Capabilities

Argonne has long led the development, design, and operation of advanced nuclear energy systems. Argonne is recognized worldwide for its contributions to the fuel recycle and fast-spectrum reactor technologies needed for the sustainable and safe use of nuclear energy. The Lab's nuclear engineering expertise, particularly in the behavior of irradiated fuels and materials, supports industry initiatives to extend the life and optimize the operation of existing and next-generation nuclear reactors.

Argonne's world-class capabilities in materials science, actinide chemistry, reactor modeling, and separations science all contribute to an improved understanding of reactor and fuel cycle processes. The Lab also has expertise in the components of nuclear technology that are critical for national security and nonproliferation activities, including the conversion of research reactors to low-enrichment fuels, technology export control, risk and vulnerability assessments, and information systems. Sensor and detector development expertise also supports national programs in border, cargo, and transportation security, as well as chemical, biological, radiological, and nuclear incident mitigation and management.

the future >>

Argonne will continue to advance the modeling and simulation of nuclear energy systems, providing increased assurance of their performance and safety and ultimately facilitating "numerical prototyping" of reactor and fuel cycle systems. Argonne will also team with research and commercial organizations to develop and demonstrate technologies needed for the sustainable use of nuclear energy, including fuel cycle closure and improved waste management.

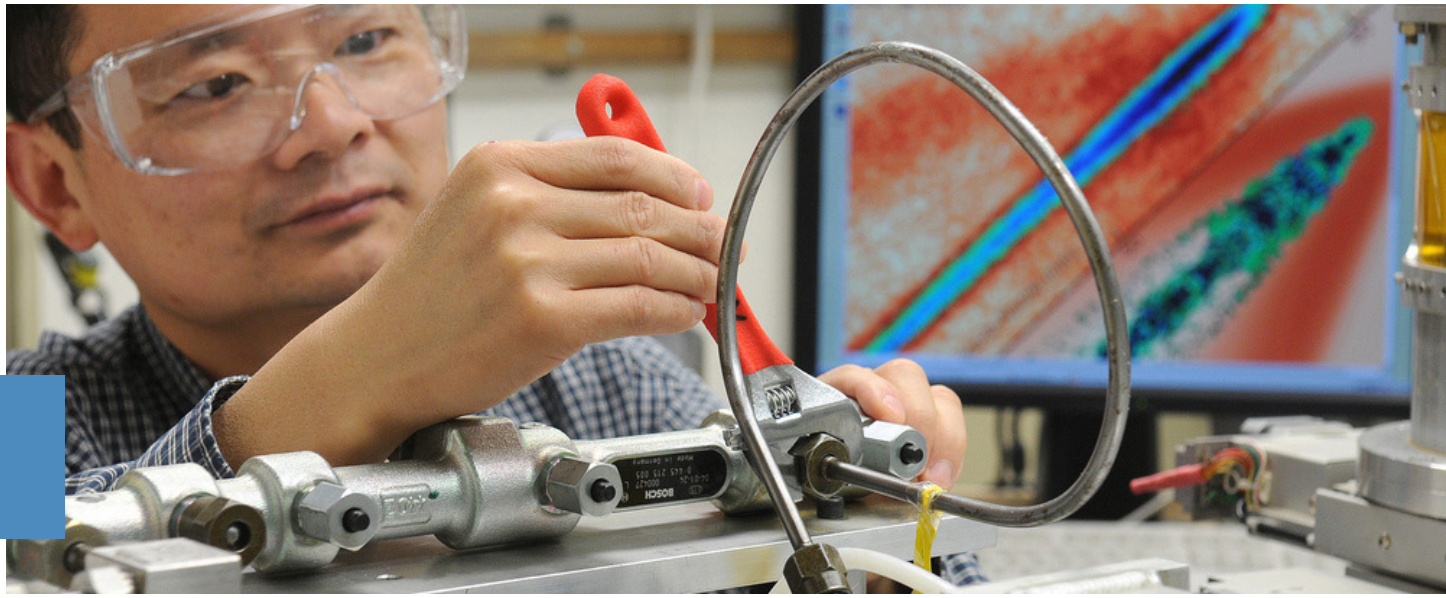
Chemist Laurel Barnes harvests uranium product from an engineering-scale electrorefiner.

SYSTEMS ENGINEERING AND INTEGRATION

Capabilities

Argonne's integrated systems approach to its research efforts is a strong core capability. The Argonne staff includes research specialists with expertise spanning a continuum from basic science through systems engineering and deployment. Teams consisting of various combinations of physical and biological scientists, engineers, computational scientists, social scientists, and decision analysts are routinely brought together to focus on the most challenging research.

In addition to a strong multidisciplinary staff, Argonne's unique facilities also enable an integrated systems research approach. For example, the APS is used to study the physics and chemistry of combustion in automotive engines, Argonne's high-performance computers are used to model engine function and performance, and Argonne's Center for Transportation Research conducts experimental research in vehicle systems and life cycle analyses. Another example of integration is agent-based modeling, a crosscutting computational technology used to address problem domains related to national security and climate change.



Physicist Jin Wang adjusts the machine used in the non-intrusive absorption experiments at the Advanced Photon Source (APS).
APS X-rays yield a highly quantitative characterization of the dynamic mass distribution in diesel and gasoline engines' fuel injector spray.

the future >> The consolidation and renewal of facilities for systems engineering activities across the Laboratory, including a user facility for homeland security research and training, will ensure the robust growth of programs supporting infrastructure assurance, power grid systems, transportation systems, and security-related activities.

CLIMATE CHANGE SCIENCE

Capabilities

Argonne is a recognized pioneer in measuring and modeling the exchange of energy, water vapor, and trace gases at the land-atmosphere interface and the dynamics of the planetary boundary layer. Our surface flux measurement capabilities are used for measuring energy and momentum flux changes at the land-atmosphere interface. A strong terrestrial ecology group conducts field and laboratory studies directed at carbon cycling in grassland, forest, and agricultural systems.

Argonne researchers investigate soil carbon dynamics and sequestration, evaluate the impact of plant-soil interactions and microbial community function on the below-ground carbon cycle, and combine state-of-the-art stable isotopic techniques with surface flux measurements to quantify the exchange of carbon between the land surface and the atmosphere.

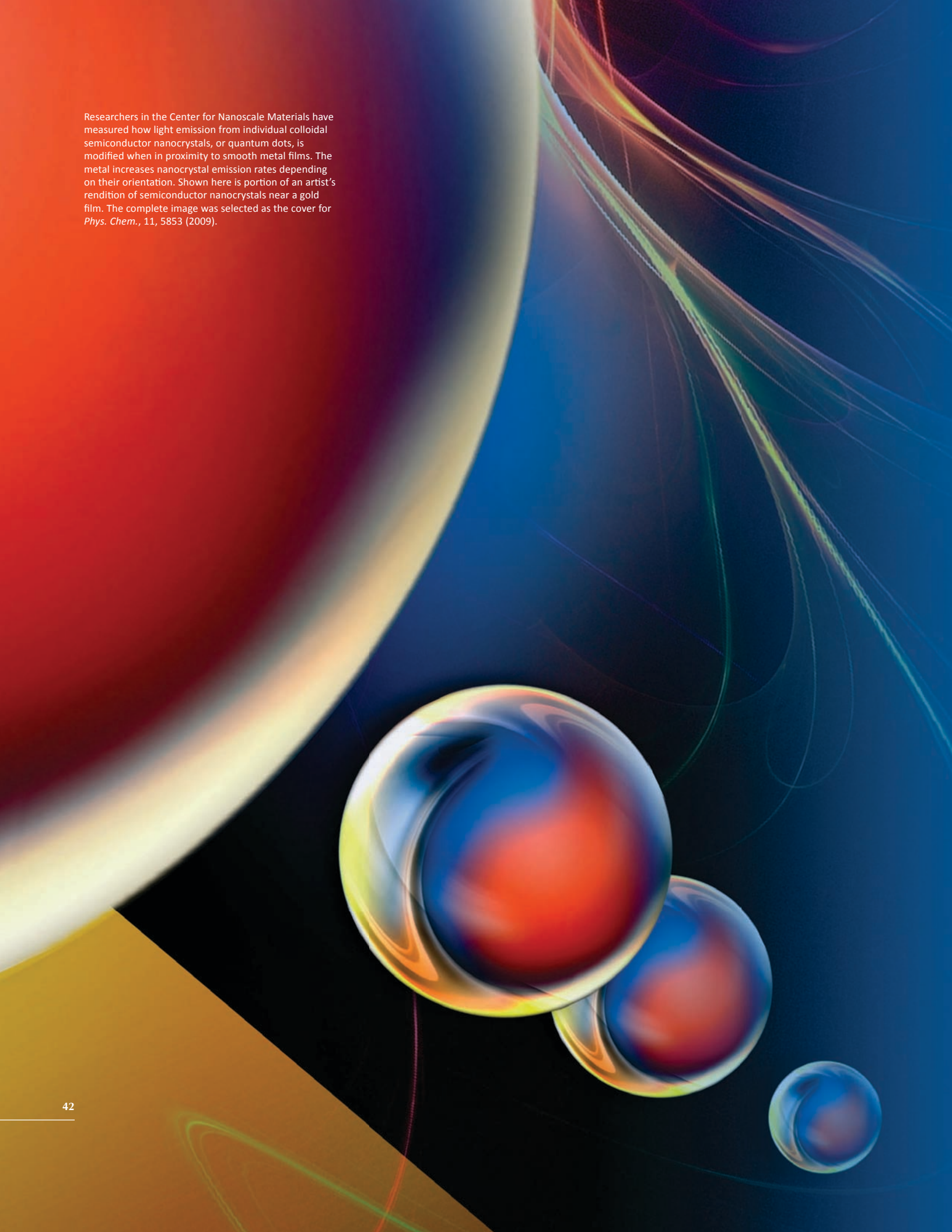
Argonne currently operates the Southern Great Plains climate observation site for the DOE Atmospheric Radiation Measurement (ARM) program and a mobile ARM facility for targeted season- to year-long measurements of clouds, climate, and radiative transfer in remote and under-sampled regions. Argonne has substantial remote-sensing expertise for probing the atmospheric boundary layer and above using laser and microwave-based instrumentation.

The Laboratory also has growing capabilities in regional scale modeling and data assimilation, and a nascent program in the development of crop model components for climate models. Argonne has world-class expertise in developing flux couplers for connecting different components of climate models, in handling large climate data sets, in applying automatic differentiation to climate codes, and in parallel computation.

the future >>

The ARM Climate Research Facility upgrade will add a diverse suite of advanced instrumentation operated at fixed and mobile sites that will support both long-term science studies (e.g., the time evolution of clouds and cloud properties) and short-term campaigns. DOE recently awarded Argonne a $2.6 million-per-year contract to expand the Laboratory's ability to make accurate, reliable measurements of cloud and atmospheric processes over the earth's oceans and other inhospitable locations.

Researchers launch a specialized weather balloon to validate and verify satellite ozone measurements at DOE's Atmospheric Radiation Measurement program's Climate Research Facility in the Southern Great Plains. Argonne has managed this site for more than 18 years.



Researchers in the Center for Nanoscale Materials have measured how light emission from individual colloidal semiconductor nanocrystals, or quantum dots, is modified when in proximity to smooth metal films. The metal increases nanocrystal emission rates depending on their orientation. Shown here is portion of an artist's rendition of semiconductor nanocrystals near a gold film. The complete image was selected as the cover for *Phys. Chem.*, 11, 5853 (2009).

ARGONNE'S MAJOR INITIATIVES AND SUPPORTING STRATEGIES

Argonne's major research initiatives build on the Laboratory's core capabilities and research partnerships to address the United States' needs for scientific discovery, sustainable energy, national security, a clean environment, and a stable global climate.

Argonne sets itself apart from many of its sister labs in its support of a multidisciplinary research continuum — from basic science to deployed technology — that encourages bold and visionary efforts. Reaching across the traditional boundaries between basic and applied science and engineering creates a fertile environment within the Laboratory for both discovery science and technical innovation.

Specifically, Argonne is pursuing eight focused major initiatives, all chosen to deliver world-class scientific and technological results:

- **Hard X-ray Sciences,**
- **Leadership Computing,**
- **Materials and Molecular Design and Discovery,**
- **Energy Storage,**
- **Alternative Energy and Efficiency,**
- **Nuclear Energy,**
- **Biological and Environmental Systems, and**
- **National Security.**

Aerial view of Argonne's Advanced Photon Source, a national synchrotron X-ray research facility funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences. The APS provides the brightest X-ray beams in the western hemisphere.

Hard X-ray Sciences

Argonne is planning for an orders-of-magnitude improvement in the hard X-ray capabilities required to advance further into the ultrafast and ultrasmall regimes and fully enable two crosscutting science drivers: mastering hierarchical structures through imaging and studying real materials in real time under real conditions.

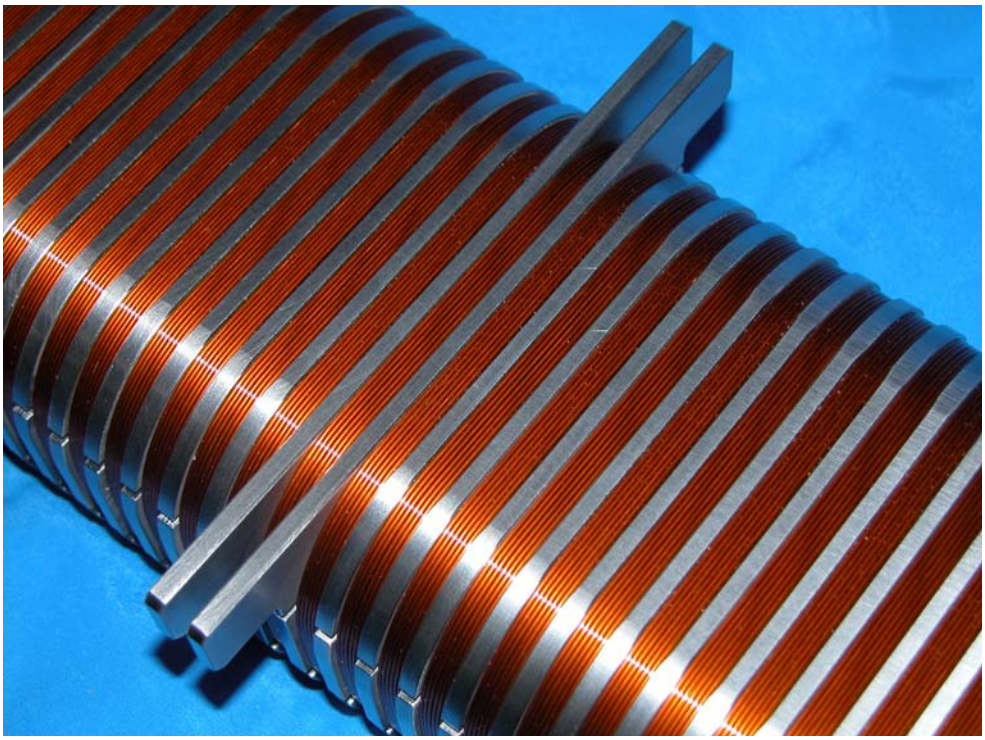
Argonne's strategy for creating these advanced X-ray capabilities consists of three interconnected elements:

- Upgrade of the existing Advanced Photon Source (APS),
- *In situ* experimentation, and
- Development of a future-generation hard X-ray source.

Next-generation plans will be further refined and proposals developed in close cooperation with DOE and through the Lab's national laboratory network.

The Advanced Photon Source storage ring is the most stable and one of the brightest X-ray sources in the world, having unprecedented availability and reliability.

Argonne is unique in the world as a large, multidisciplinary laboratory with a premier hard X-ray facility.



A superconducting undulator is a very desirable source for the highest energy applications at the upgraded APS. The short (16 mm) period superconducting undulator being developed by Argonne researchers will deliver much higher brightness at high photon energies than can be achieved with conventional permanent-magnet undulator technology. One of a pair of successfully tested 42-pole yokes wound with niobium-titanium superconducting wire is seen here.

APS UPGRADE

WHY ARGONNE? The APS storage ring is the most stable and one of the brightest X-ray sources in the world, with unprecedented availability and reliability. Its upgrade will provide experimental stations with higher-brilliance and higher-flux X-rays and user-friendly, state-of-the-art X-ray instrumentation including new optics, detectors, and data visualization and analysis software.

STRATEGY: To position the APS to support transformational science for the next decade through an upgrade of existing beamlines and accelerator and storage ring systems, and through the development of new beamlines that meet the current and future needs of the scientific user community. Program goals include:

- Obtain full program approval and funding to begin the APS upgrade effort.
- Complete upgrade of the APS and open up new capabilities to the user community.

University of Chicago Scientist Rafael Jaramillo (left) and Argonne Scientist Yejun Feng examine the element chromium at the Advanced Photon Source. Studying simple metallic chromium, the joint UC-Argonne team has discovered a pressure-driven quantum critical regime and has achieved the first direct measurement of a "naked" quantum singularity in an elemental magnet.

IN SITU EXPERIMENTATION

WHY ARGONNE? Argonne is unique in the world as a large, multidisciplinary laboratory with a premier hard X-ray facility. Hard X-ray science is fundamental to the Laboratory's mission: it impacts *in situ* investigation of materials and molecules, advanced protein structure determination, environmental chemistry, ultrafast photochemistry, and real-time studies of energy technologies ranging from photovoltaics, catalysis, and batteries to fuel injection for diesel engines.

STRATEGY: To develop the scientific foundations, communities, and techniques for the next generation of *in situ* imaging, scattering, and spectroscopy science that will enable breakthroughs in materials physics; the mastering of hierarchical structures; the discovery of novel materials and molecules; and the understanding of chemical, environmental, and biological processes. Program goals include:

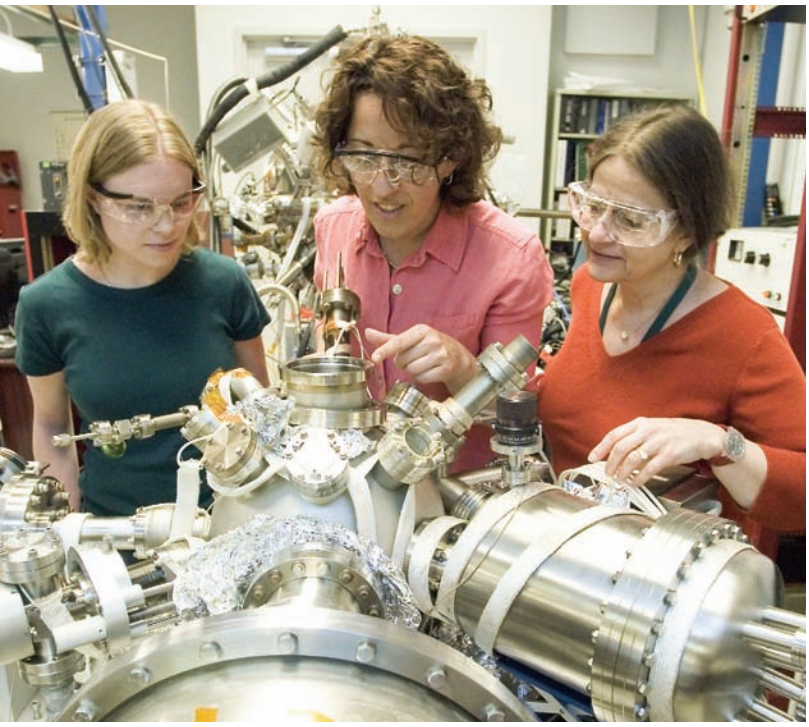
- Develop *in situ* science, including instruments and techniques, to leverage the new capabilities achieved through the APS upgrade; provide the scientific knowledge that will guide the selection of a fourth-generation light source technology.
- Organize partnerships and joint programs between Argonne and its user groups to enhance intellectual exchange and to develop scientific directions in specific research areas such as magnetism, photo-excited reactions, energy storage, catalysis, and materials discovery.
- Expand user support and integration to further develop and strengthen world-class expertise in specific areas (imaging, coherent X-rays, ultrafast dynamics, and materials synthesis); advance these techniques by enhancing experimental strategies, detectors and other beamline systems, and the computing infrastructure.

ACCELERATOR-BASED HARD X-RAY SOURCE DEVELOPMENT

WHY ARGONNE? As a world leader in the development of hard X-ray science and accelerator science and technology, Argonne's leadership role is vitally important to defining the future scientific direction of this critically important field.

STRATEGY: To begin developing a fourth-generation hard X-ray source that has the tools to visualize and quantify with unprecedented clarity the physical, chemical, and biological processes, and discover new methods to produce functional materials and devices. Program goals include:

- Strengthen research efforts in candidate source technology, such as the X-ray free-electron oscillator, energy recovery Linac, and ultimate storage ring.
- Identify scientific community needs and build consensus for the focused development of a specific source technology for a fourth-generation light source, and an approach for its design.
- Obtain full program approval and funding to begin the new facility effort.



Physicists Katherine Harkay (center) and Marion White (right) discuss a photocathode measurement apparatus with Lee Teng Intern Genevieve Boman. The goal of the research is to develop and characterize photocathodes suitable as ultrabright electron sources for future X-ray sources.

Leadership Computing

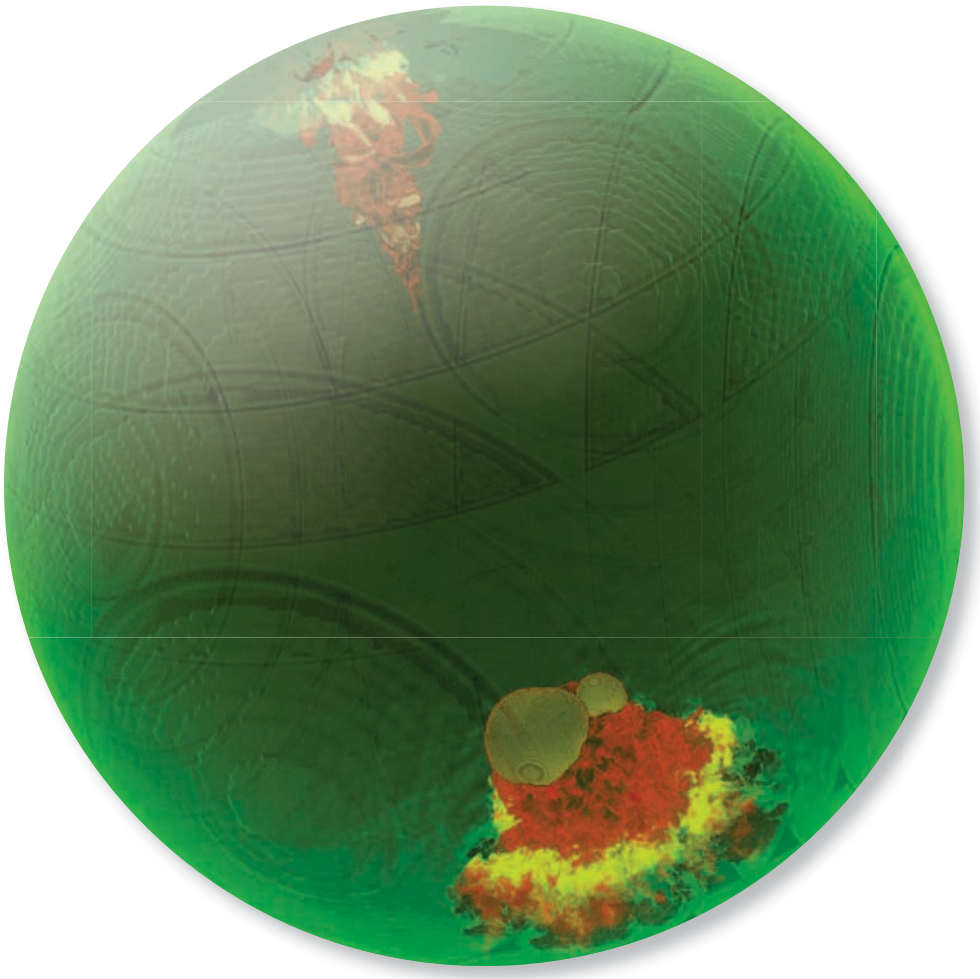
Argonne will drive the evolution of leadership computing from petascale (10^{15} flops) to exascale (10^{18} flops), while leading the development of scalable codes and computing environments for these machines. By working with users and partners, the Laboratory will enable and support extremely complex analyses that solve major energy problems and promote world-class discovery.

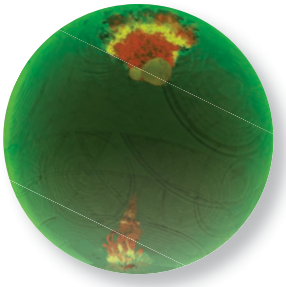
Through design/build partnerships with industry, Argonne will be the lead laboratory for developing the system software required by the most advanced computers and will ensure that emerging hardware meets the needs of the nation. Argonne will:

- Provide expert operations and support teams to assist researchers in fully exploiting leadership computing for scientific discovery.
- Integrate advanced computing across the Laboratory's scientific disciplines, continuing to strengthen its work in nuclear reactor simulation and building major efforts in such areas as energy storage, biological and environmental systems, and materials discovery.

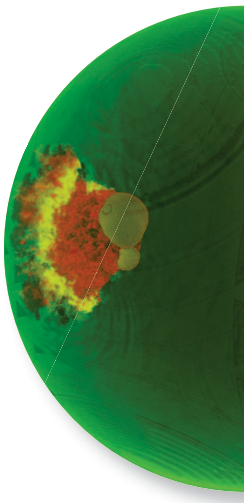
The underlying strategy is threefold, focusing on national computational facilities, exascale technology for scientific computing, and computational science and engineering.

Argonne hosts one of the world's largest open-science computers — a 557-teraflop IBM Blue Gene/P.





Argonne received two awards from DOE's Office of Advanced Scientific Computing Research for visualizations produced using Argonne's energy-efficient supercomputer, Intrepid, along with Eureka, one of the world's largest graphics processing units. One winning image, "Simulation of the Gravitationally Confined Detonation (GCD) Model of a Type Ia Supernovae for Ignition at Multiple Points," is reproduced here.

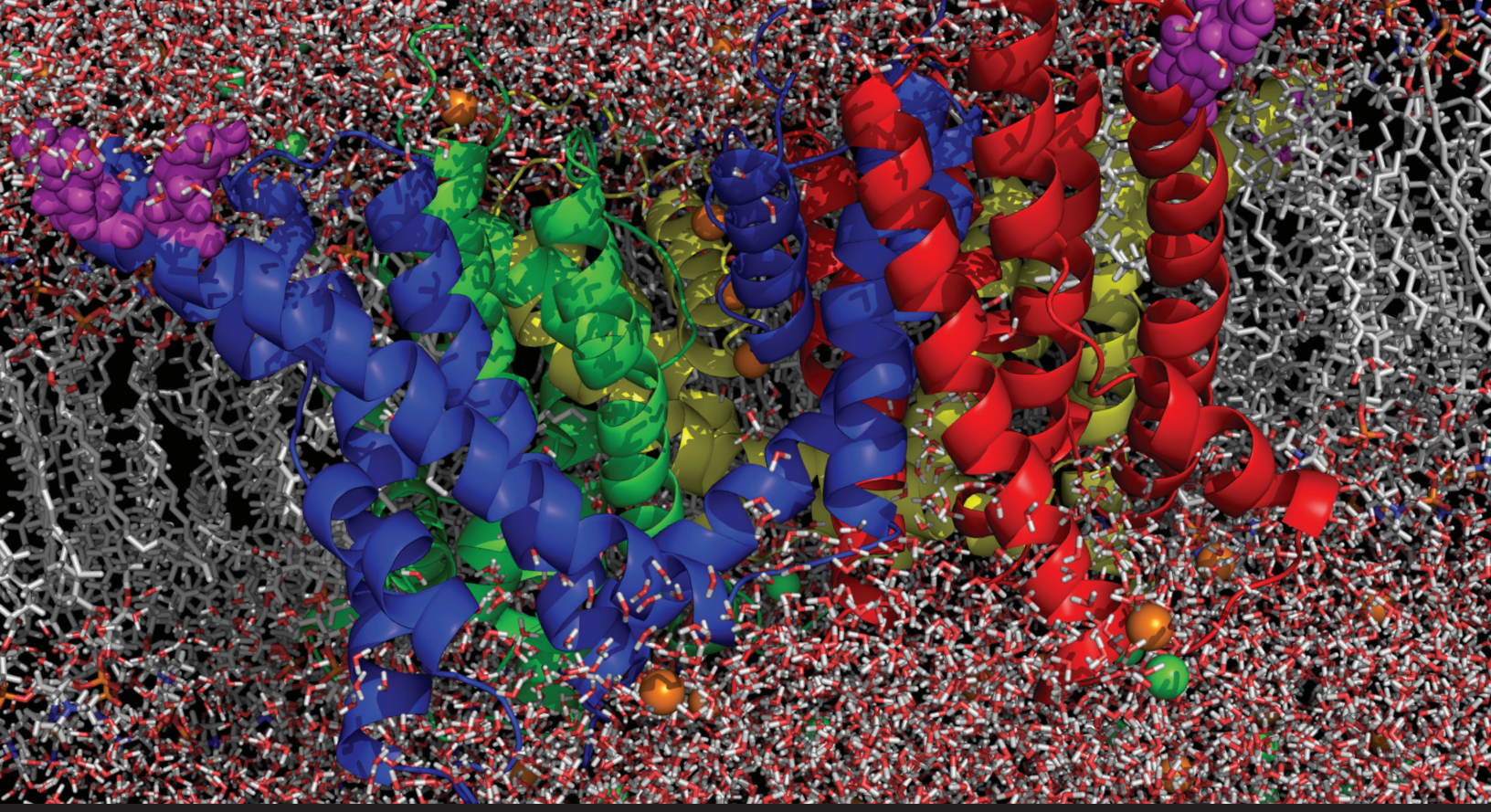


NATIONAL COMPUTATIONAL FACILITIES

WHY ARGONNE? The Argonne Leadership Computing Facility (ALCF), one of two DOE Leadership Computing Facilities, hosts one of the world's largest open-science computers, a 557-teraflop IBM Blue Gene/P. Argonne has produced world-leading systems and exemplary science results through its computer science and mathematics expertise and its design/build approach to leadership systems and strong user programs.

STRATEGY: To develop the ALCF program from petascale to exascale with innovative computer designs and high-impact science. Program goals include:

- Operate a fully functional Blue Gene/Q 20-petaflop leadership computer to meet the nation's most demanding science priorities, while creating a strong R&D program for system designs through the exascale.
- Deploy the world's first open 100- to 300-petaflop system, complete upgrades to Argonne's mid-range supercomputing capabilities, and establish a national computing facility for a new science and engineering mission.
- Deploy the world's first exaflop computer in an open scientific facility while operating a suite of advanced computer systems for high-profile science and engineering missions.
- Use mid-range supercomputer facilities at the Laboratory to create and build simulation and modeling capabilities that can scale up to leadership platforms.



The atomic model for the simulation of the KvAP channel in a lipid membrane is shown here. Dr. Benoit Roux, University of Chicago, performed the simulations using NAMD, the parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems, with up to 512 processors on the Blue Gene/L at Argonne's Leadership Computing Facility.

EXASCALE TECHNOLOGY FOR SCIENTIFIC COMPUTING

WHY ARGONNE? Argonne and Lawrence Livermore National Laboratory, along with industry partners, pioneered the highly successful design/build approach to engineering petascale computers for grand challenge science. To make the breakthroughs needed for exascale computers, the laboratories must continue to extend this approach. Likewise, Argonne is recognized worldwide as a thought leader, technology provider, and partner in advanced computer systems software, tools, and math libraries.

STRATEGY: To develop scientific computing at the exascale in support of basic and applied science through innovations and breakthroughs in hardware design, software tools, and infrastructure. Program goals include:

- Enlist a broad international community to surmount the challenges and establish the "ecosystem" needed to create exascale software.
- Launch an International Exascale Software effort that joins together industry, the high-performance computing community, and high-performance computing facilities in a collective effort to design, coordinate, and integrate software for petascale- to exascale-class machines.
- Develop an Exascale Institute with partner labs and industry to create, over the next ten years, a class of cost-effective, production computer systems capable of sustaining 10^{18} flops on a broad scientific workload.
- Operate in the long term an exascale system with open-source software stacks that support a broad range of basic and applied scientific workloads.

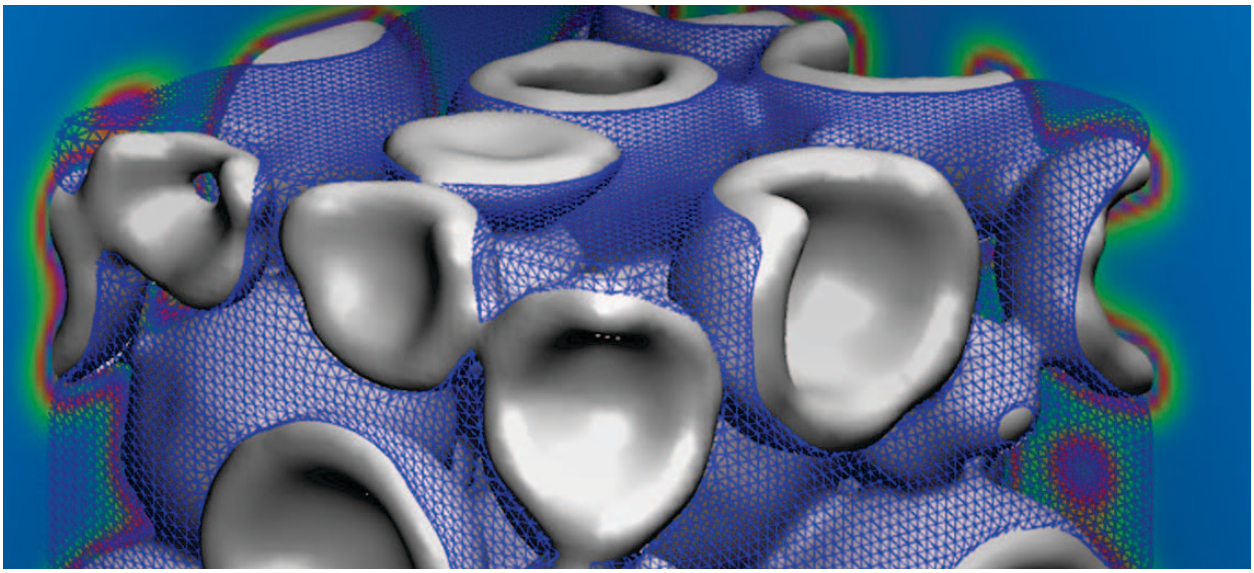
COMPUTATIONAL SCIENCE AND ENGINEERING

WHY ARGONNE? Argonne has well-established computer science leadership, the Argonne Leadership Computing Facility, the Argonne-University of Chicago Computation Institute, and extensive expertise in computational science on smaller-scale computers, with several highly successful petascale applications developed by teams of research scientists, applications developers, mathematicians, and computer scientists.

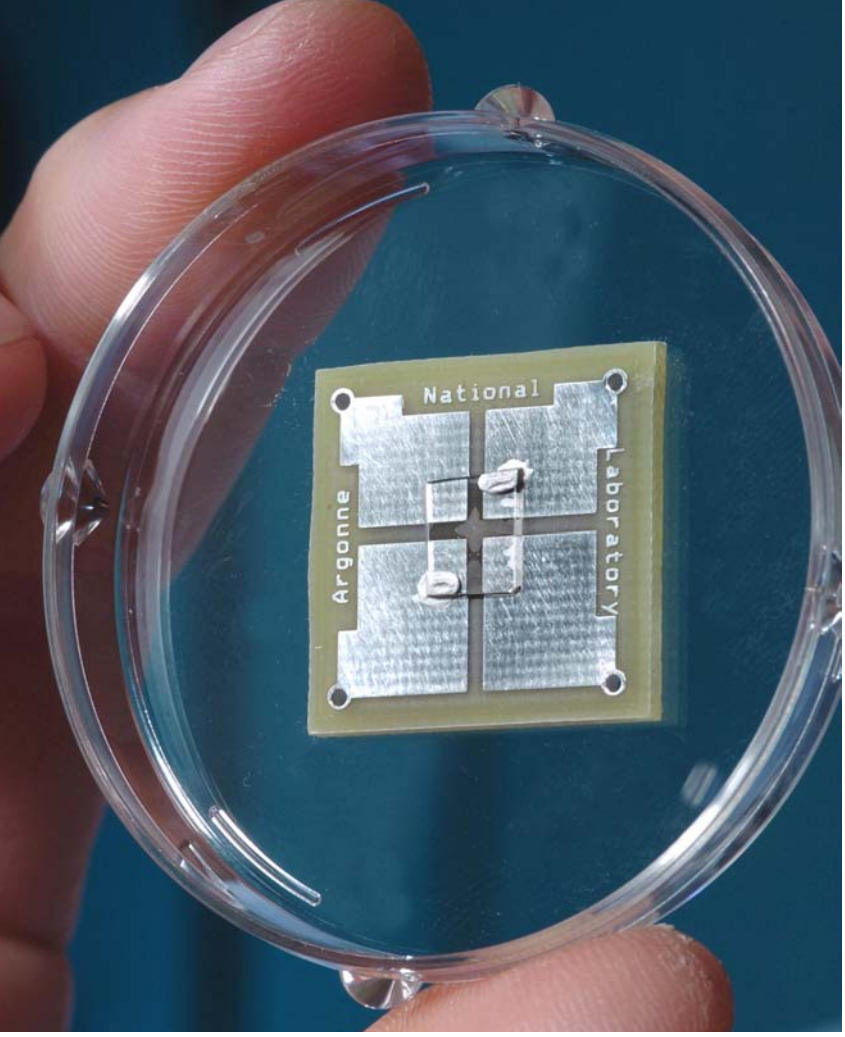
The Laboratory's major research initiatives and core capabilities require modeling, simulation, and data analytics on many different computational scales. Argonne has established computational science and engineering leadership in nuclear energy, climate change, and astrophysics. Increasingly, strong computational programs across the research spectrum provide opportunities for Argonne's growth in this key element of success for today's research environment.

STRATEGY: To develop capabilities in modeling, simulation, and analytics that advance and inspire all our major research initiatives, with emphasis on grand challenge problems for leadership computers. Program goals include:

- Create long-term computational science and engineering programs around the core basic and applied science capabilities at the Lab.
- Recruit and hire experts in large-scale computational science and engineering to augment our integrated approach to theory, computation, and experimentation.
- Continue the development of strong petascale research programs in nuclear energy, climate change, and astrophysics.
- Establish petascale computational programs in energy storage, biological and environmental systems, materials discovery, and nanoscale device design.



Proctor & Gamble researchers are using Argonne's Blue Gene/P system to investigate the molecular mechanisms of bubble formation in foams. This image represents a three-dimensional periodic mesoscale simulation of many small bubbles that exist during the early stages of foam formation. This work is expected to help P&G formulate products faster and more efficiently, thereby reducing costs for consumers.



Argonne researchers developed the world's fastest commercially producible hydrogen sensor by controlling the way nanometer-sized palladium particles self-assemble onto an insulating surface. The sensor is faster and more sensitive than competing technologies and is inexpensive to fabricate. It is being used in the fields of medicine and space exploration, in the production of industrial chemicals, and in food processing. It also holds promising potential for use in the transportation industry.

Materials and Molecular Design and Discovery

The discovery and synthesis of new compounds are critical bottlenecks both for grand challenge science and for Argonne's research strategies in energy, environment, biology, and national security. The Laboratory's innovative approaches for designing, creating, and harnessing novel, environmentally responsible molecules, and materials that exhibit revolutionary scientific phenomena or use-inspired functionality are poised to transform science and technology.

The Materials and Molecular Design and Discovery major research initiative will be an incubator for an extensive milieu of new molecular and materials concepts, discoveries, and programs at Argonne.

For example, breakthroughs in energy storage materials are essential for high-energy density batteries critical to 400-mile-range electric vehicles. In the search for alternative energy sources, new discoveries in catalytic materials are essential for converting feedstocks to chemical fuels. New architectures are essential for more efficient conversion of solar energy to electricity. Similar bottlenecks in materials restrict progress in biology and the environment, nuclear energy, and national security.

Therefore, a central element of Argonne's research strategy is to establish the framework needed to unite materials synthesis with *in situ* characterization, and theory and modeling, in order to design and create breakthrough materials and molecules.

Argonne's game-changing approach will create foundational discoveries for new materials classes, structures, and synthesis modalities.

Our design and discovery framework will integrate three approaches:

- Establish design principles through high-performance computational simulations and experimentation.
- Develop, through computation and characterization, a comprehensive understanding of links between the structure, dynamics, and functionality of new materials.
- Develop novel, "green" synthesis techniques to create the complex substances that embody the design principles revealed by the simulation and characterization efforts.

Coupling these approaches will enable not only the design of new materials and molecules but also the smart control of synthesis and subsequent steps in chemical reactions. Synthesis conditions and pathways will be harnessed to create desired products, to guide self-assembly, or to tune reactivity. Incorporation of bio-inspired strategies and bio-based assembly pathways will expand the repertoire of accessible structures.

These concerted activities will lead to sweeping improvements in energy storage, catalysis, superconductivity, thermoelectrics, photovoltaics, and other energy applications. Equally important, Argonne's game-changing approach will create the foundational discoveries for new materials classes, structures, and synthesis modalities that will lead to novel functionality.

The Laboratory will broadly apply the integrated framework of computational and empirical design, synthesis, and *in situ* characterization to all crystalline, molecular, and nanostructured materials of importance to Argonne's *Strategic Plan*. Interdisciplinary teams will develop a tailored research approach for each class of materials, supported by Argonne's state-of-the-art user facilities such as the Advanced Photon Source, Electron Microscopy Center, Argonne Leadership Computing Facility, and Center for Nanoscale Materials. The Laboratory's initial research emphasis will include complex oxides and catalysis, followed by other strategic classes of materials such as biological and bio-inspired materials, spintronic and Mottronic materials, energy storage materials, sensors, and multiferroics.

Argonne is superbly positioned to take a of novel, engineered materials including molecular

COMPLEX OXIDES AND BEYOND

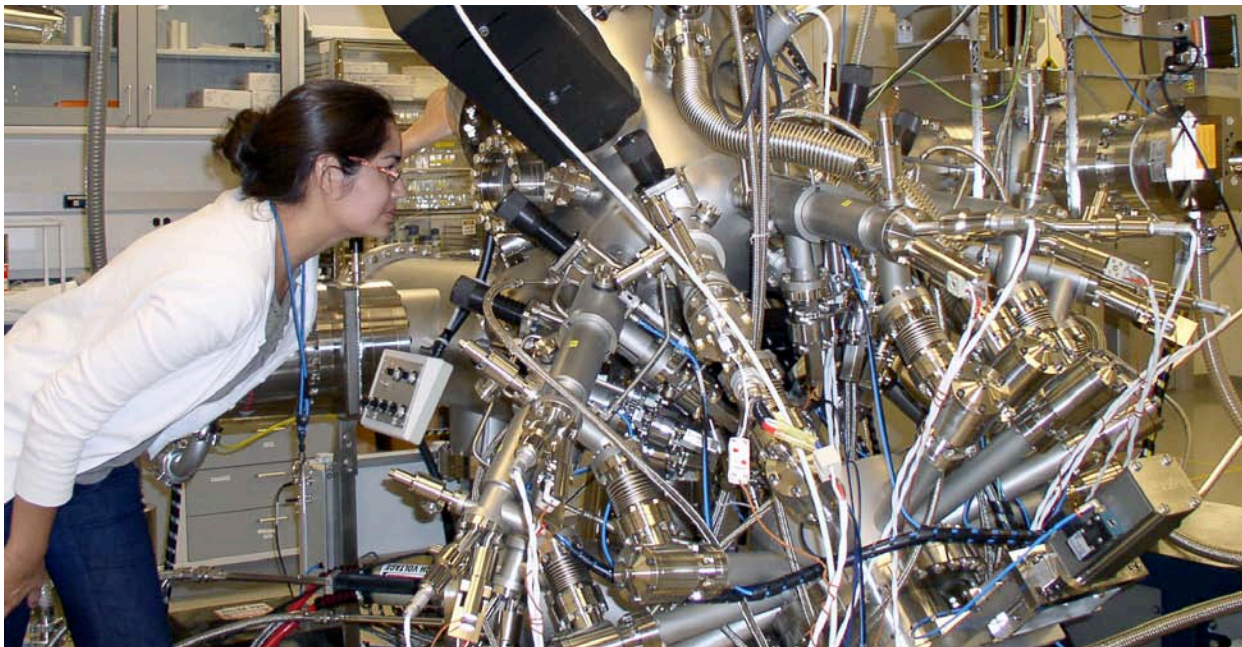
WHY ARGONNE? Argonne's well-established expertise in synthesis; nanoscience; characterization (especially *in situ*); the use of X-rays, electrons, and scanning probes; and theory — in concert with its advanced midscale and leadership computing — will lead to the creation of tools and the knowledge needed to discover fundamentally new materials. The Laboratory plans to bring a new generation of complex materials for the energy age to the level of structural, composition, and property control that was achieved for silicon during the information age.

STRATEGY: To build a comprehensive complex oxide growth and science center that will lead the world in creating bulk, film, and nanostructured crystals, and heterostructures of ternary and more complex transition metal oxides to serve as transformational platforms for next-generation energy and information technology.

The Laboratory will develop new synthesis paradigms — particularly approaches that allow Argonne researchers to create novel compounds that exist far from equilibrium — by leveraging the Lab's recognized expertise in complex oxides and seed efforts in chalcogen- and pnictogen-based systems. Insights gained from non-equilibrium biological processes will be used to help advance the frontier of the science. Researchers will pioneer *in situ* feedback techniques for process control, and model process environments to unlock the potential of nonequilibrium products such as ordered nanocomposites, digital superlattices, and complex nitrides. Program goals include:

- Develop the science for synthesizing pathways to new oxide materials that cannot be grown with today's techniques; use *in situ* experimental and computational methods to aid in the design.
- Build a nationally recognized synthesis capability with thin-film and bulk crystal growth facilities large enough to advance the priorities of both the national science community and industry partners.
- Exploit the diverse properties of complex oxides and other components in novel nanoscale conformations to produce new phenomena that combine ferroelectric, superconducting, magnetic, metallic, biological and insulating constituents, and to create new functionality for sustainable energy and information technologies.

Physicist Tiffany Santos, Center for Nanoscale Materials (CNM) Distinguished Post-Doctoral Fellow and recipient of a 2009 L'Oreal USA Fellowship for Women in Science, deposits a complex oxide superlattice structure using the CNM's oxide molecular beam epitaxy system.



leading role in the development and biochemical catalysts.

Argonne is developing alternative catalysts that can replace the high-cost platinum nanoparticle electrocatalyst currently used for oxygen reduction reaction in fuel cell technology. Seen here, Analytical/Materials Chemist Nancy Kariuki and Polymer Chemist Suhas Niyogi isolate nanoparticles from solution using a high-speed centrifuge, one of several steps in the catalyst processing.

NOVEL CATALYST MATERIALS

WHY ARGONNE? Argonne is a pioneer in the emerging field of catalytic materials design. The Laboratory's well-established expertise in synthesis, theory, and *in situ* and *ex situ* characterization for catalysis led to the discovery of groundbreaking catalytic materials. Argonne's expertise encompasses the design of electrocatalysts with dramatically increased activity for fuel cells; highly active and selective heterogeneous catalysts for breaking specific carbon-hydrogen bonds; functional understanding of biological catalysts capable of breaking and forming a variety of bonds; and leadership of a DOE Energy Frontier Research Center in catalysts for chemical transformation. Argonne's world-leading protein design and synthesis capabilities will provide a foundation for creation of bio-based catalytic systems and materials.

STRATEGY: To become a world-leading center for the design of catalytic materials with the precise control of activity and selectivity that will enable new energy technologies. Argonne's overarching strategy is to use novel design principles — including some based on modular, tightly regulated biological systems — and synthesis techniques to expand the field of catalysis into new architectures.

Materials design principles drawn from both theory and experimentation will be used to guide the synthesis of materials having desired functionalities — on scales ranging from a few atoms surrounded by ligands for homogeneous catalysis to metal particles or bionano composites of up to tens of nanometers for heterogeneous catalysis. Program goals include:

- Develop a nationally-recognized catalytic materials design workbench with strong theoretical and experimental underpinnings that is available to the scientific community and industry.
- Use materials design capabilities combined with novel synthesis techniques to develop breakthrough materials for key heterogeneous catalytic processes including carbon dioxide reduction, chemical fuels synthesis, and bond-specific activation and removal of oxygen in biomass.
- Exploit the diverse possibilities of bio-inspired catalysis to support advances in sustainable energy.
- Employ Argonne's high-throughput protein synthesis and structural biology capabilities to gain insight into extreme biological conversions and the design and construction of new optimized hybrid systems; use approaches that harness enzyme active sites and the surrounding protein matrix in new robust platforms.

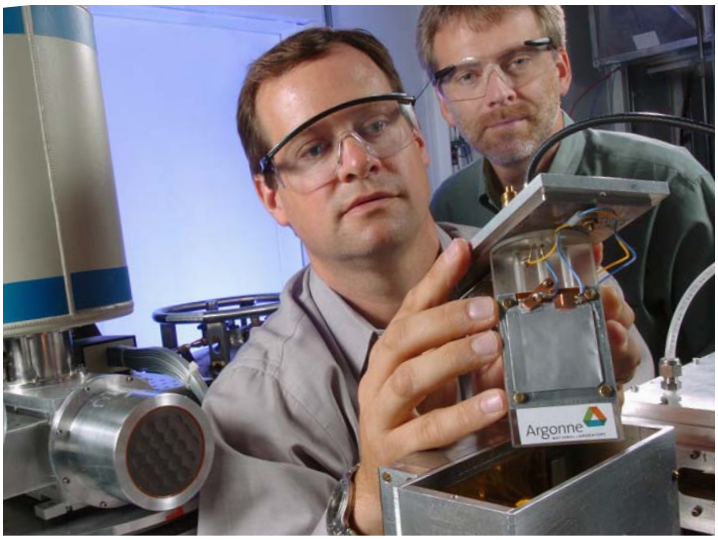
Energy Storage

The large-scale commercialization of new energy storage technologies is essential to the development of electric vehicles, as well as to distributed renewable electric power generation. To achieve the necessary transformational advances, Argonne will build upon its historical leadership in battery research to create a broad research, development, and demonstration program centered on advanced energy storage materials and systems for both mobile and stationary applications.

Initially, Argonne will focus on the development of more robust, safer, and higher-energy density lithium-ion batteries and the processes to manufacture them. In the next phase, the Laboratory will make use of its fundamental science capabilities to develop storage materials that go beyond current lithium technology to dramatically increase storage capacity and power densities for electrification of the transportation sector.

Argonne researchers will simulate the future power grid under transients with intermittent renewable energy sources, and design stationary storage systems that will balance the load and secure the system. These efforts will span the continuum from basic materials research to prototype device and systems development, and ultimate deployment by industry.

Chemist and Materials Scientist Ilias Belharouak monitors the fabrication of electrode materials for use in plug-in hybrid vehicles' energy storage systems.



Chemist Christopher Johnson (foreground) and Physicist Jeremy Kropf load a lithium-ion battery pouch into an insertion device X-ray beamline at the Advanced Photon Source (APS) in order to evaluate the stability of the electrode material structure during charging and discharging. The APS and Electron Microscopy Center are valuable research tools for Argonne's battery R&D.

Argonne has a world-class applied research program for new battery materials and a strong history of basic materials research ready for expansion.

ELECTRICAL ENERGY STORAGE

WHY ARGONNE? Argonne has more than 30 years of experience in the development of advanced battery technologies. It is the lead lab for the DOE Office of Energy Efficiency and Renewable Energy's (EERE's) applied battery research program. With a world-class applied research program for new battery materials and a strong history of basic materials research ready for expansion, Argonne is the DOE/EERE advanced energy storage materials laboratory.

The Laboratory is also DOE's leading source for independent and objective battery testing and evaluation. Argonne has unique facilities for *in situ* analysis at its Advanced Photon Source and Center for Nanoscale Materials and for computations at the Argonne Leadership Computing Facility, as well as a broad range of modeling expertise to simulate phenomena from the atomic-level to the vehicle battery pack scale.

STRATEGY: To optimize current and near-term energy storage technologies while advancing electrochemical storage materials beyond lithium-ion-based solutions to both ultracapacitors and new storage material discoveries. New storage media will be integrated into both transportation and grid-scale systems to help drive the use of renewable energy sources in the economy. Program goals include:

- Bridge the near-term energy storage performance gap by optimizing current materials and technologies to double the performance of plug-in hybrid electric vehicles.
- Develop key partnerships with academia, industry, and other laboratories to promote the development and advancement of next-generation energy storage technologies.
- Design and discover the materials and electrochemical processes to power future all-electric vehicles and provide grid-scale storage for renewable energy sources.

Chemist Joe Pomykala (foreground) and Chemical Engineer Jeff Spangenberger oversee Argonne's flotation separation pilot plant for separating plastics from mixed wastes generated by recycling facilities.

PROTOTYPE AND MANUFACTURING PROCESS ENGINEERING

WHY ARGONNE? The Laboratory has recognized expertise in materials synthesis and characterization and a proven track record in scale-up of "first-of-a-kind" manufacturing processes. Argonne is DOE's lead lab for lithium-ion battery advanced technology development, plug-in hybrid electric vehicle modeling and simulation, and end-of-life vehicle recycling. Argonne has unique facilities for materials characterization, cell and module performance testing, and onboard testing and validation of assembled modules.

STRATEGY: To enable the transition of Laboratory-demonstrated energy storage systems to commercial production. Program goals include:

- Develop manufacturing and process engineering technologies that support each segment of the energy storage device supply chain, from materials production to "power pack" packaging and delivery. Transfer these technologies to industrial partners.
- Demonstrate the processes for scalable bulk materials production to key industrial partners, thereby positioning Argonne as a manufacturing training facility.
- Develop integrated manufacturing, remanufacturing, and materials recovery and recycling process technologies and establish a least-cost integrated production model for energy storage devices. Transfer these technologies to industrial partners.

STATIONARY STORAGE AND GRID MANAGEMENT

WHY ARGONNE? Argonne is one of two national labs with distributed power generation programs and is DOE's lead lab in electrochemical energy storage research and testing. With its large-scale grid testing and modeling capabilities, Argonne is a recognized leader in power systems modeling and grid power management schemes with centralized and distributed energy storage systems.

STRATEGY: To produce large energy storage solutions through grid-level system modeling and testing using variable energy sources, thereby providing grid-level access to reliable and economic energy from renewable sources. Program goals include:

- Develop next-generation models for grid simulations that identify optimal energy storage strategies for electric power systems, including future smart grid applications.
- Develop a Center for Renewable Energy Supply and Storage using variable energy sources to research and model novel, next-generation energy storage systems.
- Demonstrate and deploy with industrial partners, future energy storage systems for power grid management that result in an economically viable, nationwide use of distributed generation and variable energy sources.

Argonne is a recognized leader in power systems modeling and grid power management schemes.

ELECTRIC TRANSPORTATION SYSTEMS

WHY ARGONNE? Argonne's internationally-recognized transportation research program remains at the forefront of electric vehicle technology development. The Laboratory's Advanced Powertrain Research Facility is the principal DOE facility for assessing advanced and hybrid-electric vehicle (HEV) technologies; companies around the world seek its use and associated expertise.

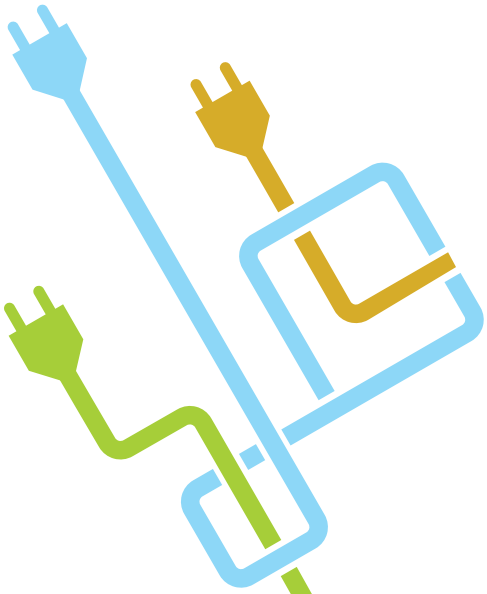
Argonne maintains a lead role in modeling and validation of HEV and plug-in hybrid vehicle (PHEV) performance. The Laboratory's Powertrain System Analysis Toolkit is the industry standard, allowing systems-level analysis of design options without prototyping.

Argonne's internationally recognized transportation research program remains at the forefront of electric vehicle technology development.

STRATEGY: To transform electric-drive powertrains and vehicle systems so these support emerging and next-generation energy storage technologies. Transfer these system technologies to industry to create commercially-viable electric-drive vehicles while providing performance feedback and traffic/grid interoperability recommendations. Program goals include:

- Characterize and evaluate the performance of Argonne-developed PHEV prototype batteries, both lithium-based and "beyond lithium," as well as ultracapacitor-based storage, providing feedback for design and material performance improvements.
- Model vehicle performance, traffic interactions, and impact on the grid (as both source and storage medium) to ensure successful deployment of new storage technologies for transportation.

Research Engineer Ted Bohn checks the battery level on Argonne's Through-the-Road (TTR) parallel hybrid electric vehicle test platform.

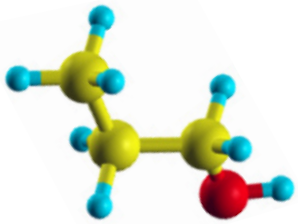


Mechanical Engineer Thomas Wallner adjusts Argonne's "omnivorous engine," an automobile engine that Wallner and his colleagues have tailored to efficiently run on blends of gasoline, ethanol, and butanol.

Alternative Energy and Efficiency

Accelerating the transition to alternative energy sources requires significant improvement in materials, chemicals, processes, and devices. To produce more cost-effective energy sources for the nation, Argonne is focused on two primary research areas:

- The development of alternative fuels and optimized engines to improve transportation systems. Novel catalytic materials, separations, biosystems, process engineering, and engine design must be integrated and optimized. The work will enable the production of a broad range of sustainable chemical and biofuels designed to operate in "smart" omnivorous engines that adjust the combustion sequence depending on the fuel. This work builds on Argonne's strengths in biological process engineering, separations, and catalysis.
- The pursuit of solar energy conversion technologies that are commercialization-ready. The discovery and optimization of new solar materials for photon absorption, subsequent charge separation, and final current collection or chemical synthesis will be pursued and integrated into components of low-cost, high-performance solar-electric or solar-fuel devices. These efforts draw on Argonne's strengths in materials synthesis, characterization, and modeling for science-based engineering solutions that can be commercialized by industry, and on fundamental research performed by the Argonne-Northwestern Solar Energy Research Center, a recently funded DOE Energy Frontier Research Center.



ALTERNATIVE FUEL AND ENGINE SYSTEMS FOR TRANSPORTATION

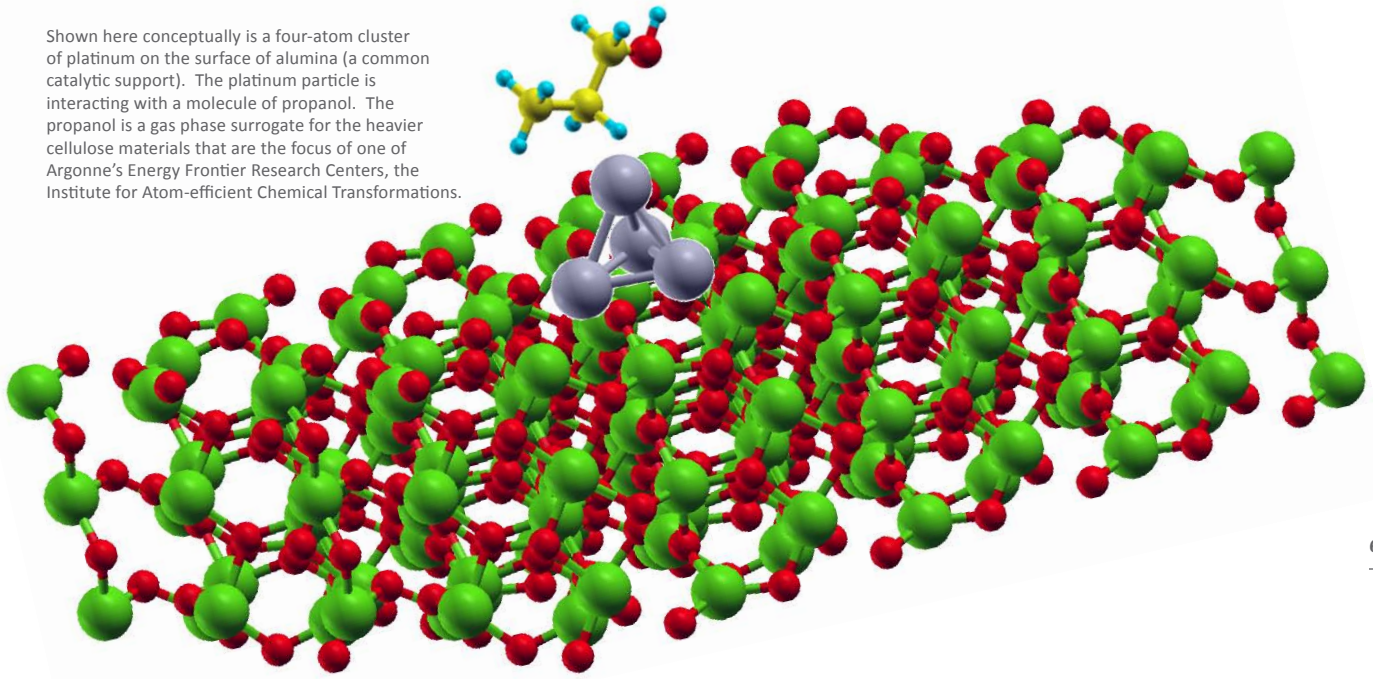
This effort has three distinct thrusts: chemical fuel development by catalytic conversion of abundant non-biological feedstock, advanced biofuel development from sustainable biomass, and fuel combustion and engine optimization for the development of advanced engines that can run efficiently and cleanly on new fuels.

Chemical Fuel Development

WHY ARGONNE? Argonne's broad capabilities in catalysis and conversion are leveraged by unique computing, X-ray, and nanomaterial user facilities that enable nationally-recognized research. Argonne recently received a DOE Energy Frontier Research Center award to establish the Institute for Atom-efficient Chemical Transformations. Expanded networks with local and regional universities place Argonne at the center of a foundation of excellence in catalytic and energy conversion research.

STRATEGY: To develop the catalytic processes for generating novel fuels from natural gas (methane) or other non-bioderived feedstock. Methane is currently converted into more useful chemicals and fuels by costly and inefficient methods that require high temperatures and pressures. In addition, many remote methane sources are untapped because of the high cost to connect them to the existing gas pipeline infrastructure. Direct on-site conversion of methane would allow the use of these reserves as a primary source for fuels and chemicals. Program goals include:

- Develop new catalysts to directly transform methane into longer-chain alkanes; perform other chemical conversions that hold promise for transportation and general energy-source use.
- Scale up promising chemical fuels for combustion testing; optimize fuel composition and production characteristics. Work closely with research partners to commercialize promising chemical fuel technologies.



Shown here conceptually is a four-atom cluster of platinum on the surface of alumina (a common catalytic support). The platinum particle is interacting with a molecule of propanol. The propanol is a gas phase surrogate for the heavier cellulose materials that are the focus of one of Argonne's Energy Frontier Research Centers, the Institute for Atom-efficient Chemical Transformations.

Argonne researchers are working with industrial partners to develop alternative clean fuels using biomass, natural gas, or coal as raw material to reduce the number of impurities such as carbon dioxide and nitrogen oxide contained in exhaust emissions. Mechanical Engineer Henry Ng is seen here with a container of diesel fuel derived from wood chips.

Advanced Biofuel Development

WHY ARGONNE? Together with its university partners who have established positions in agricultural sciences, Argonne can integrate fundamental biological research, plant modification, biologically- and chemically-based catalysis, separations, combustion modeling, and engine design and system integration analysis to develop biofuel solutions.

STRATEGY: To develop advanced infrastructure-compatible biofuels and bioenergy products that help end the nation's dependence on fossils fuels while meeting sustainability targets. Argonne's research is producing reduced, longer-chain molecular fuels for integration into the transportation sector without major infrastructure investments, as well as bioproducts that meet society's need for chemicals, materials, heat, and power. Argonne and its university partners will focus on the following cross-functional themes:

- Biological systems — photosynthetic organisms, protein expression systems, and metagenomics;
- Chemical technology — catalysis, separations, materials design, synthesis and characterization, and combustion;
- Engineering — energy efficiency, process design and engineering, scale-up, and transportation systems; and
- System integration analysis — life cycle analysis, agent-based modeling, and climate modeling.

Program goals include:

- Develop the basic research, processes, engineering, and life cycle models needed to design and produce advanced biofuels that function within the nation's current and future infrastructure and meet key performance and sustainability targets. A portfolio of biofuel products for transportation, power production, and other uses will be considered.
- Scale-up promising biofuels for combustion testing and develop improved feedstocks to meet compatibility, life cycle, and performance objectives. Argonne will consider land-use implications, consumptive water use, and emissions of greenhouse gases and other pollutants in its work.
- Work closely with research partners to commercialize biofuel technology, carefully considering the needs and priorities of the nation.

Fuel Combustion and Engine Optimization

WHY ARGONNE? Argonne has world-class programs in theoretical and experimental combustion chemistry and a well-recognized transportation program with strengths in engine characterization and testing, environmental impact analysis, and fuel development. These programs support a design-test-feedback cycle covering all aspects of fuel design and use.

Argonne's GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model is recognized as the leading software package for the life cycle analysis of the impacts of fuel production and use. Additionally, Argonne has developed unique facilities for *in situ* observation of engine combustion performance at its Advanced Photon Source.

STRATEGY: To develop theoretical and experimental combustion chemistry for optimizing clean combustion of advanced fuels and engine performance. Program goals include:

- Develop programs to support a comprehensive, integrated fuel testing feedback loop that includes generation of chemical fuels and biofuels, combustion modeling, engine and fuels testing and optimization, and systems studies of fuel generation and use.
- Use combustion chemistry, modeling, and characterization tools as part of the fuel testing feedback loop to identify and optimize potential fuels and fuel mixtures for commercial production. Optimize engine designs and operating conditions to take advantage of chemical fuels and biofuels technology advancements.

Argonne's GREET model is recognized as the leading software package for the life cycle analysis of the impacts of fuel production and use.

Engine Research Scientist Christopher Powell fits a specially designed X-ray pressure window to a high-pressure chamber used in diesel spray research. These windows allow Argonne researchers to use the Advanced Photon Source X-ray beams to probe diesel sprays under the high-density conditions found in diesel engines.

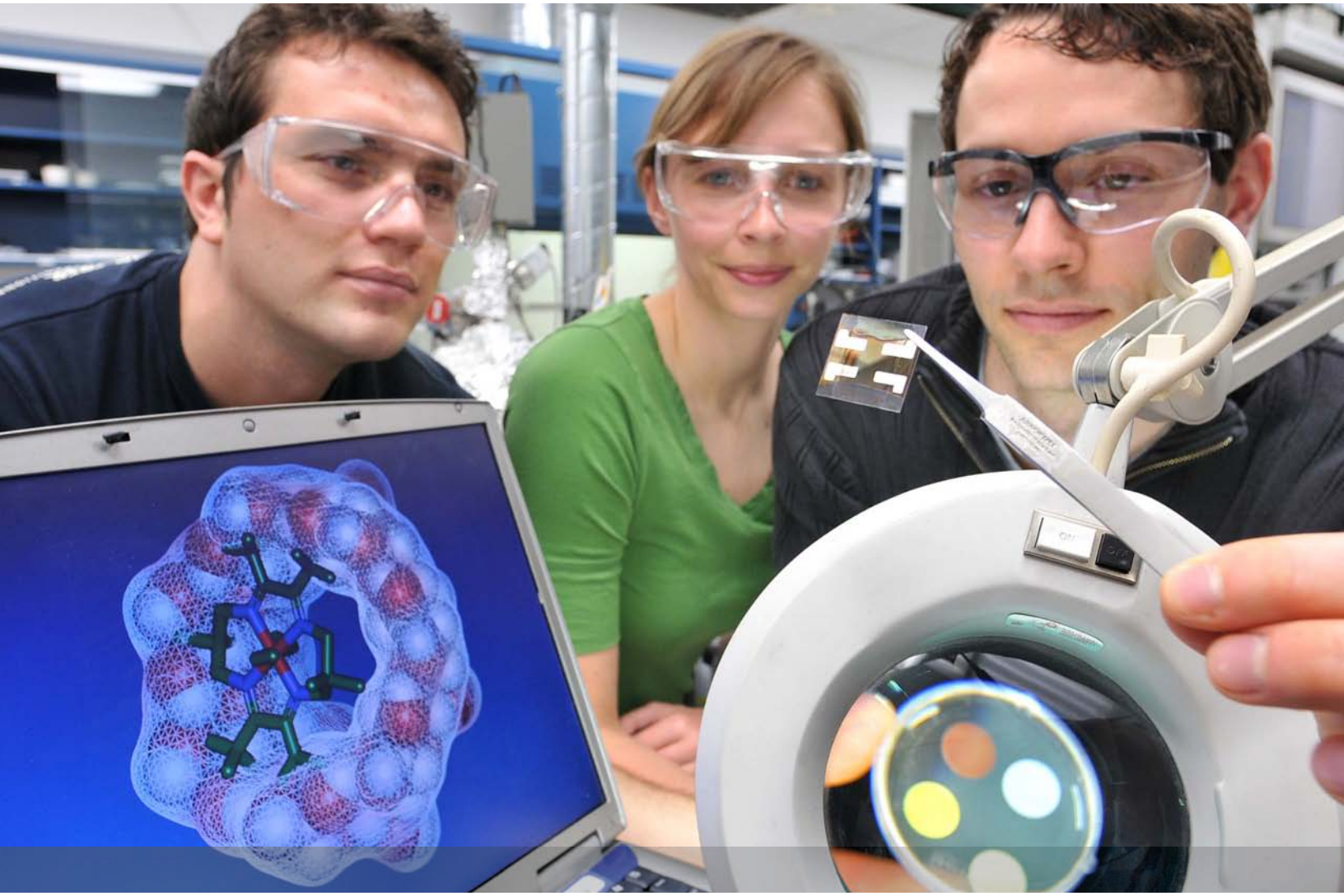
SOLAR ENERGY SYSTEMS

WHY ARGONNE? Solar energy systems design involves diverse challenges ranging from materials synthesis and characterization to device integration, energy storage, and interfacing with the grid. Argonne is uniquely positioned to assume a leadership role in an integrated systems approach to solar energy technology development. With strong research collaborations exemplified by the Argonne-Northwestern Solar Energy Research Center and the two recently-awarded Energy Frontier Research Centers, Argonne's multidisciplinary strengths in materials and molecular design and systems engineering provide the basis for success in addressing the complexities of this challenge.

STRATEGY: To develop revolutionary approaches to photovoltaic and photocatalysis technologies. Link fundamental materials behavior to novel device architectures that are integrated and scaled for use as a grid-level (solar electric) or fuel-level (solar fuel) energy source. Goals include:

- Combine computational and experimental resources to rationally design, characterize, and control the nanoscale morphology of organic, inorganic, and hybrid photovoltaic and photocatalytic systems in order to understand and optimize the internal processes that govern solar energy conversion.
- Design and couple novel solar device components, including photovoltaic and photocatalysis materials and schemes, to produce dramatic improvements in solar conversion efficiencies and to reduce the costs for next-generation technologies.
- Develop efficient system integration analysis tools that inform solar conversion research to further improve the efficiency, sustainability, and cost of market-deployed technologies. Couple these technologies with grid-level energy storage and transmission options to deliver low-cost solar-derived electric power to the nation.

Argonne is uniquely positioned to assume a integrated approach to solar energy development.



Argonne is taking a systems approach to solar energy, such as investigating the interfaces between components and devices. In one approach, Postdoctoral Appointees Ioan Botiz (left), Karen Mulfort, and Alex Martinson are exploring the possibilities for coupling solar fuel and photovoltaic devices. The monitor displays such a solar fuel complex. Martinson holds an organic solar cell with tweezers; nanostructured solar cells at various stages of fabrication (by atomic layer deposition) can be seen in the magnifier.

leadership role in an

Research Associates Julie Stevenson and Ryan Berg prepare the equipment in a glovebox for testing one of Argonne's pyroprocessing technologies.

Nuclear Energy

Today, nuclear energy is the largest non-carbon electricity production method in use, but the nation must effectively address safety, security, and waste management concerns to enable its sustained use and continued growth. Argonne's goal is to advance the safe, sustained use of nuclear energy by incorporating scientific and engineering breakthroughs in the design and operation of nuclear energy systems. Key goals are:

- Increased understanding of the diverse physical phenomena underlying reactor and fuel cycle system behavior.
- Development of advanced materials, processes, and designs for reactor and fuel cycle systems.
- Improved ability to predict system behavior through validated modeling and simulation for design, licensing, and operation.

This research is being pursued in collaboration with other DOE laboratories and universities and in partnership with industry.

Argonne has long been the champion for fast-reactor and associated recycle technology in the U.S. and currently leads the fast-reactor development program for DOE's Office of Nuclear Energy.

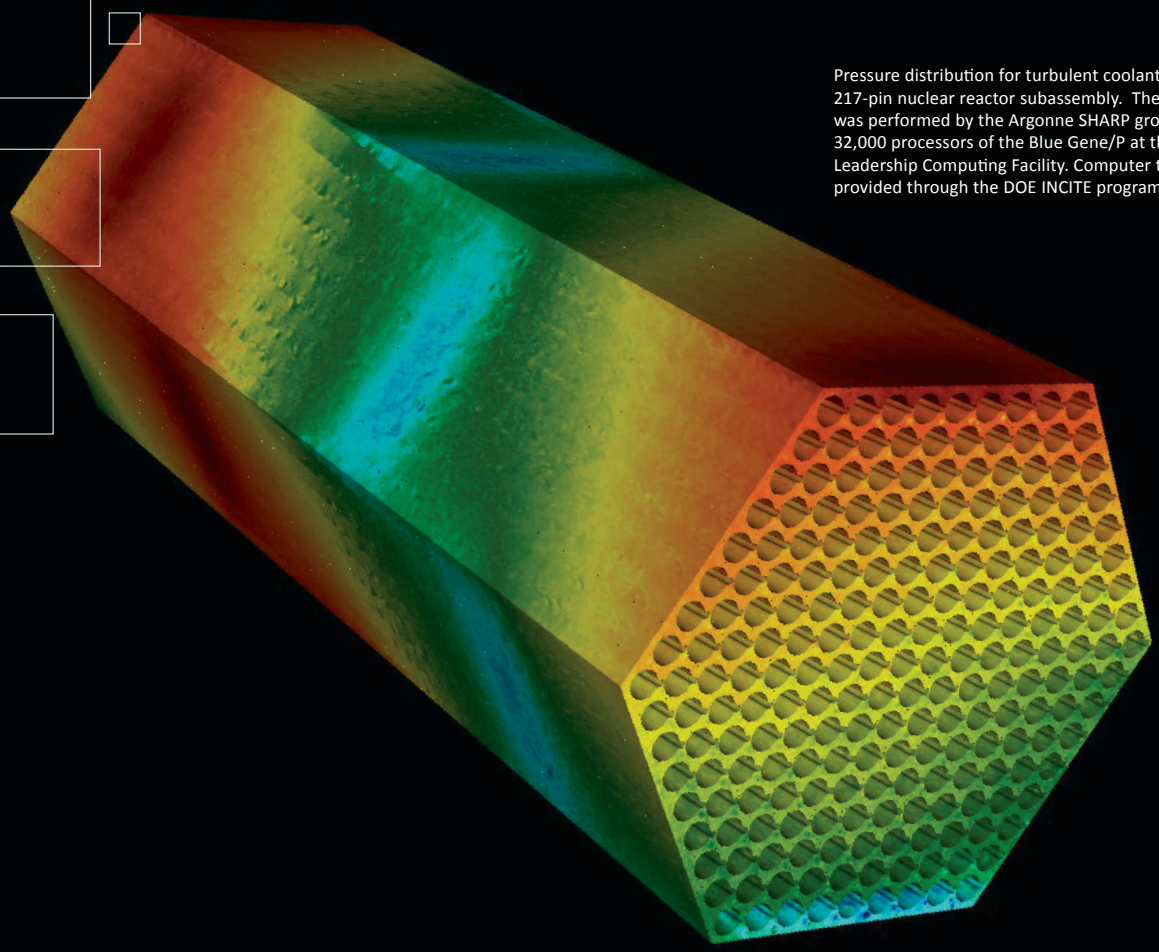
FAST REACTOR AND FUEL CYCLE TECHNOLOGIES

WHY ARGONNE? Argonne's reputation in peaceful applications of nuclear energy is well established. The Laboratory pioneered many of the nuclear energy technologies in use today and provided the vision for key technology advances. In particular, Argonne has long been the champion for fast-reactor and associated recycle technology in the U.S. and currently leads the fast-reactor development program for DOE's Office of Nuclear Energy. Significant Lab resources have been invested over the years to retain or establish unique expertise and capabilities in reactor and fuel cycle technologies.

STRATEGY: To develop and demonstrate fast-reactor and reprocessing technologies needed for fuel cycle closure and improved waste management. Goals include:

- Lead the development of advanced fast-reactor and fuel recycle technologies that meet the goals of waste minimization, safety and reliability, proliferation resistance and physical security, and competitive economics.
- Build technical consensus and a strong team of national laboratories and industry organizations to design, license, and conduct a fast-reactor fuel cycle demonstration.
- Provide technical leadership for applying the demonstration results to advance the design and operation of future nuclear energy systems.

Uranium dendrites collected during the evaluation of an advanced electrorefining technology, part of Argonne's pyrochemical process development program for treating used nuclear fuel.



Pressure distribution for turbulent coolant flow in a 217-pin nuclear reactor subassembly. The simulation was performed by the Argonne SHARP group using 32,000 processors of the Blue Gene/P at the Argonne Leadership Computing Facility. Computer time was provided through the DOE INCITE program.

ADVANCED MODELING AND SIMULATION

WHY ARGONNE? The Argonne Leadership Computing Facility, coupled with world-class expertise in nuclear engineering, computing, and nuclear computational science, uniquely positions Argonne to develop and validate modeling and simulation capabilities for design and computational prototyping of future generations of nuclear reactors. The SHARP (Simulation-based High-efficiency Advanced Reactor Prototyping) code project at Argonne demonstrates the synergistic application of these disciplines and provides a recognized basis for future advancement and growth. Partnerships with institutions who have complementary modeling and simulation expertise (e.g., for advanced fuels and separations) will provide a comprehensive modeling and simulation capability for current- and future-generation nuclear energy systems.

STRATEGY: To develop and validate advanced modeling and simulation approaches for design of innovative nuclear energy systems. Goals include:

- Develop next-generation reactor modeling and simulation methods on leadership-class computer architectures.
- Conduct key experiments to validate modeling and simulation methods, and to demonstrate their predictive capability.
- Engage industry in the improvement and validation of commercial design and licensing tools using Argonne's advanced modeling and simulation capabilities.

SCIENCE AND ENGINEERING OF INNOVATIVE NUCLEAR ENERGY SYSTEMS

WHY ARGONNE? Argonne has a rich tradition of research on the peaceful use of nuclear energy and a robust culture of creativity and innovation. The Laboratory's world-leading expertise in reactor physics and engineering, separations science, materials science, and actinide chemistry positions it well for forefront nuclear energy research and for integrating innovations and discoveries in the design and operation of future nuclear systems. Argonne's facilities, including the Advanced Photon Source, Center for Nanoscale Materials, Electron Microscopy Center, and the Argonne Leadership Computing Facility, are also major assets for discovery and improved understanding of relevant phenomena.

STRATEGY: To motivate and capture growth in scientific research on advanced nuclear energy systems. Program goals include:

- Establish Argonne as the leading national laboratory for basic scientific research, transitional research, and applied engineering in nuclear energy generation and the advanced nuclear fuel cycle.
- Develop high-performance materials, processes, and design concepts inspired by fundamental research for use in innovative nuclear energy systems.

Chemical Engineer Candido Pereira examines a sample of solvent from an experiment using a centrifugal contactor that is being tested for processing spent nuclear fuel as part of the Advanced Fuel Cycle Initiative.

Terrestrial Ecologist Julie Jastrow gathers genome sequence information from the natural environment surrounding Argonne's sister laboratory, Fermilab, to identify putative novel proteins with activities relevant to the maintenance of environmental metabolism. Such activities could be harnessed to assist with bioremediation, carbon management, and energy production.

Biological and Environmental Systems

The integration of multiscale scientific analyses with economic and social observations affords wide-ranging opportunities for discovery. Argonne's expertise in metagenomics, structural biology, coupled climate modeling, and with the University of Chicago, integrated assessments for policy guidance enables the Laboratory to bring together previously disparate research. Unification will drive an understanding of regionally-focused ecological and climate interactions and their impact on local economy and policy decisions.

Argonne's terrestrial ecosystems program is building a comprehensive metagenomics survey of each major soil and ecosystem type and mining that data for new proteins with unknown structure and function that may play important roles in the global carbon cycle. This entails the rapid end-to-end processing of novel coding sequences in DNA — from detection in a metagenomics sample to determination of the relevant protein structure and its associated functional characterization. This requires the extension of current bio-informatics capabilities to improve the quality of the sequence analysis for both genomes and metagenomes.

Success will depend on developing the ability to rapidly construct metabolic models and deploy advanced tools for data integration and reconstruction of regulatory networks. Argonne will advance systems biology methods that enable the predictive modeling of an organism's phenotype from its genotype, leading to an understanding of its role in the environment.

Current climate research efforts are inadequate to guide many important policy issues concerning impact, adaptation, and mitigation responses to regional-scale climate change. Argonne will develop new science and computational tools within the broad areas of atmospheric process development, the terrestrial carbon cycle, economic modeling, and scalable numerical methods — all with the ultimate goal of increasing the fidelity and applicability of regional climate simulations to levels that enable informed policy.

Argonne will collaborate with leading U.S. climate modeling groups to develop new versions of highly scalable Earth System Models that target existing leadership class and future multi-petaflops computing systems with 1,000,000 processing cores. Once accomplished, the U.S. will have the world's highest-resolution climate simulation capability. This work will provide a valuable and potentially revolutionary contribution to DOE's climate impact assessment capability when integrated with energy and economics models, and will lead to new insights into the impacts of climate change on human society and lifestyles.

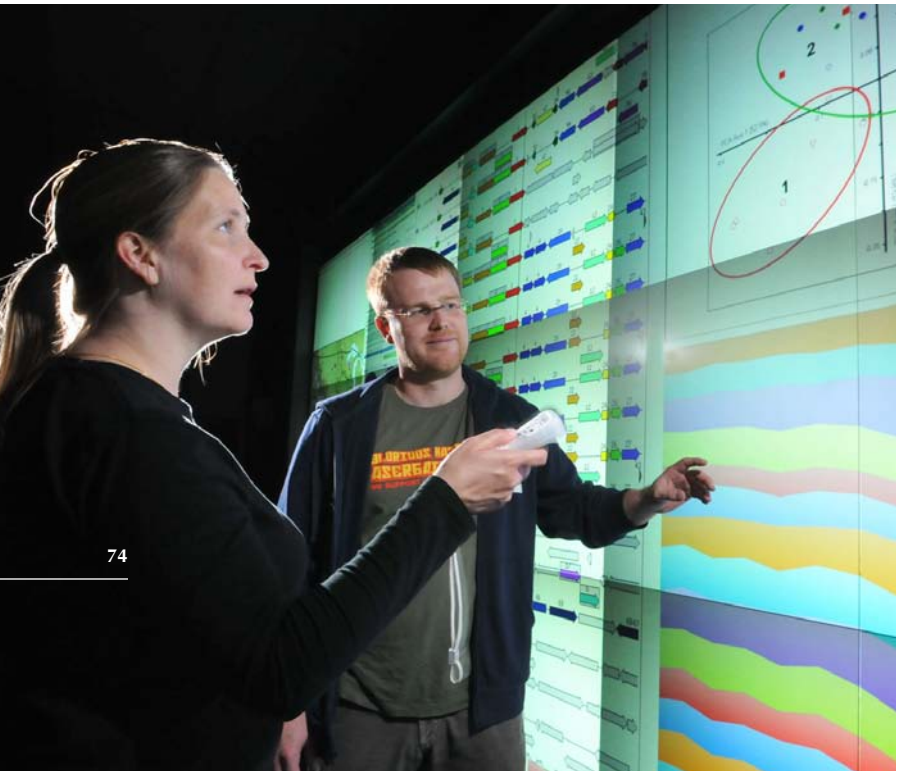
METAGENOME ANALYSIS

WHY ARGONNE? Argonne leads the world in high-throughput genome and metagenome annotation (gene function assignment), having annotated more than 4,000 genomes and more than 2,700 metagenomes in the last 18 months. More than 145 U.S. scientific institutions use the Argonne genome and metagenome annotation platform. Using metagenomics sequencing to systematically explore natural environments will produce unique insights into the metabolic foundation of the ecosystems being studied and will identify proteins that exhibit previously unknown functions.

STRATEGY: To develop computational tools and experimental methods that enable the use of metagenome sequence data to understand microbial communities and discover proteins contributing to natural processes. Goals include:

- Develop the tools and techniques to bridge the gap between metagenomics and protein analysis, while building the analysis links to various ecological systems.
- Perform systematic metagenomics analysis of wide-ranging environments, identifying protein contributions to processes driving microbial activities.

Argonne leads the world in high-throughput genome and metagenome annotation.



Scientists Folker Meyer and Elizabeth Glass analyze species and metabolic diversity from NEON soil metagenomics samples using MG-RAST (Metagenome Rapid Annotation using Subsystem Technology) on Argonne's Active Mural Display.

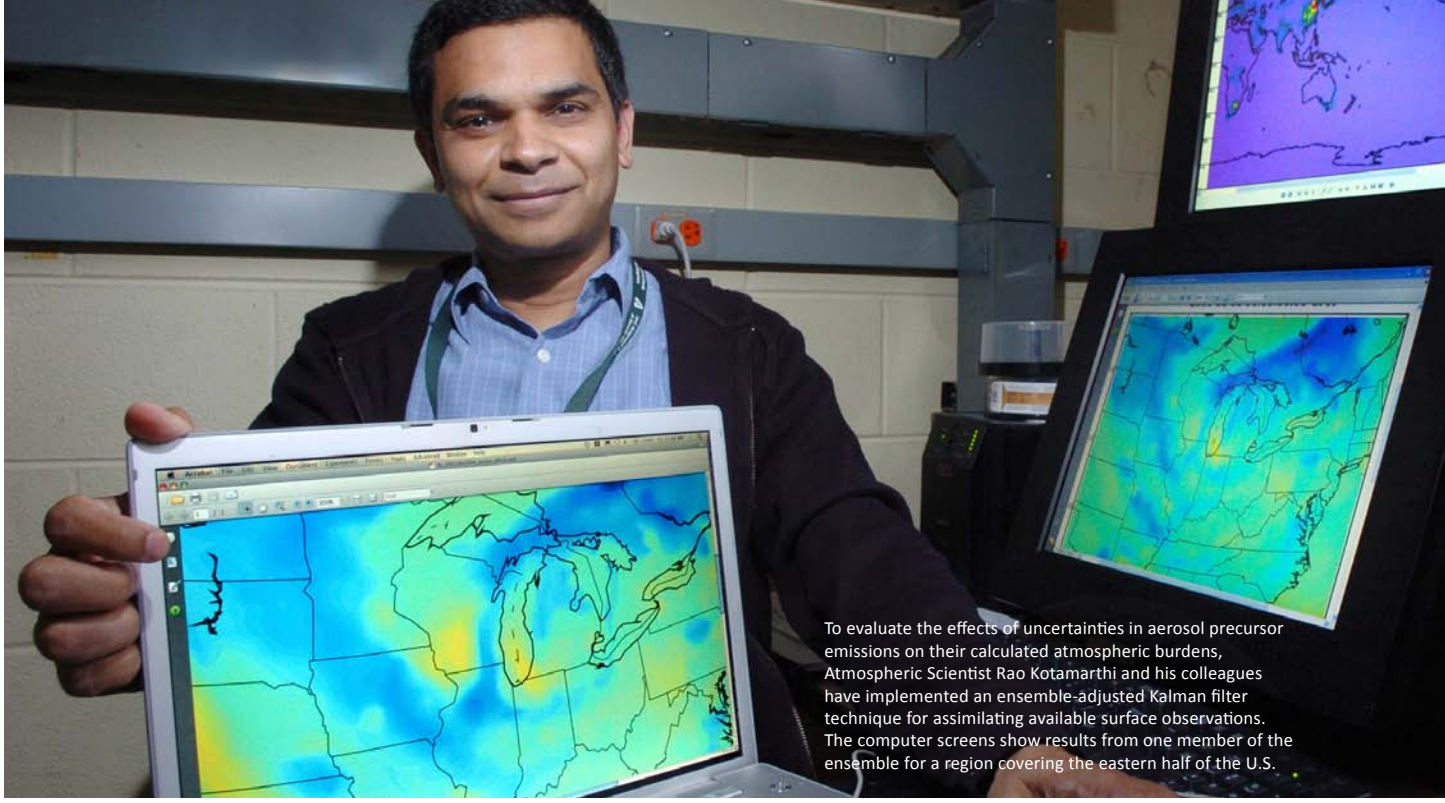
Anthrax, long feared for its potential as a biological weapon, has lost some of its mystery as scientists from Argonne and the University of Chicago recently determined the structure of a protein crucial to the virulence of anthrax bacteria. The crystal structure of the anthrax protein CabD is shown here.

PROTEIN DISCOVERY

WHY ARGONNE? Argonne is a world leader in structural biology, having contributed to the production of more high-resolution protein structures deposited in the Protein Data Bank than any other single organization in the world. The Lab is also a leader in the development of high-throughput soluble-protein expression and purification methods and has contributed a unique membrane protein expression system. This expertise, when combined with the Lab's expertise in global protein detection, metagenome and genome annotation, X-ray imaging, geochemistry, microbiology, and terrestrial ecology, places Argonne in a unique position to lead this effort.

STRATEGY: To decipher environmental metabolisms by integrating metagenome, geochemical, and ecological data with protein characterization and structure determination. This will enable the generation of sensors for *in situ* measurements of metabolic activity and computational modeling of environmental metabolism. Program goals include:

- Develop the integrated tools needed to explore and fully characterize mission-relevant protein functions and biological processes in natural environments.
- Understand environmental protein functions and related biological processes within an ecosystem and the variations that are indicative of environmental changes.
- Establish a user facility for the high-throughput characterization and optimization of environmental proteins using genetic engineering, and for the associated development and fabrication of biosensors for environmental applications.



To evaluate the effects of uncertainties in aerosol precursor emissions on their calculated atmospheric burdens, Atmospheric Scientist Rao Kotamarthi and his colleagues have implemented an ensemble-adjusted Kalman filter technique for assimilating available surface observations. The computer screens show results from one member of the ensemble for a region covering the eastern half of the U.S.

REGIONAL CLIMATE PREDICTION

WHY ARGONNE? Argonne will combine its expertise in climate models, scalable parallel computing methods and optimization with its Leadership Computing facilities to realize high-resolution climate predictions presently unavailable for regional-scale analyses. The Laboratory will draw on its highly-regarded management of the Atmospheric Radiation Measurement Climate Research Facility and its leading boundary-layer atmospheric science research to streamline the update of climate models with new data and knowledge from advanced observational networks.

The Laboratory's recognized expertise in science-based integrated environmental assessments, including recent advances toward creating a new generation of assessment models in collaboration with the University of Chicago that integrate socio-economic and environmental factors, provides a foundation for national leadership in regional policy assessments.

STRATEGY: To develop a climate modeling and observation program — including high-spatial-resolution computations and advanced observational networks — to address important policy issues concerning adaptation and mitigation responses to regional-scale climate change. The first application area is the midwest, with an emphasis on the Great Lakes basin. Goals include:

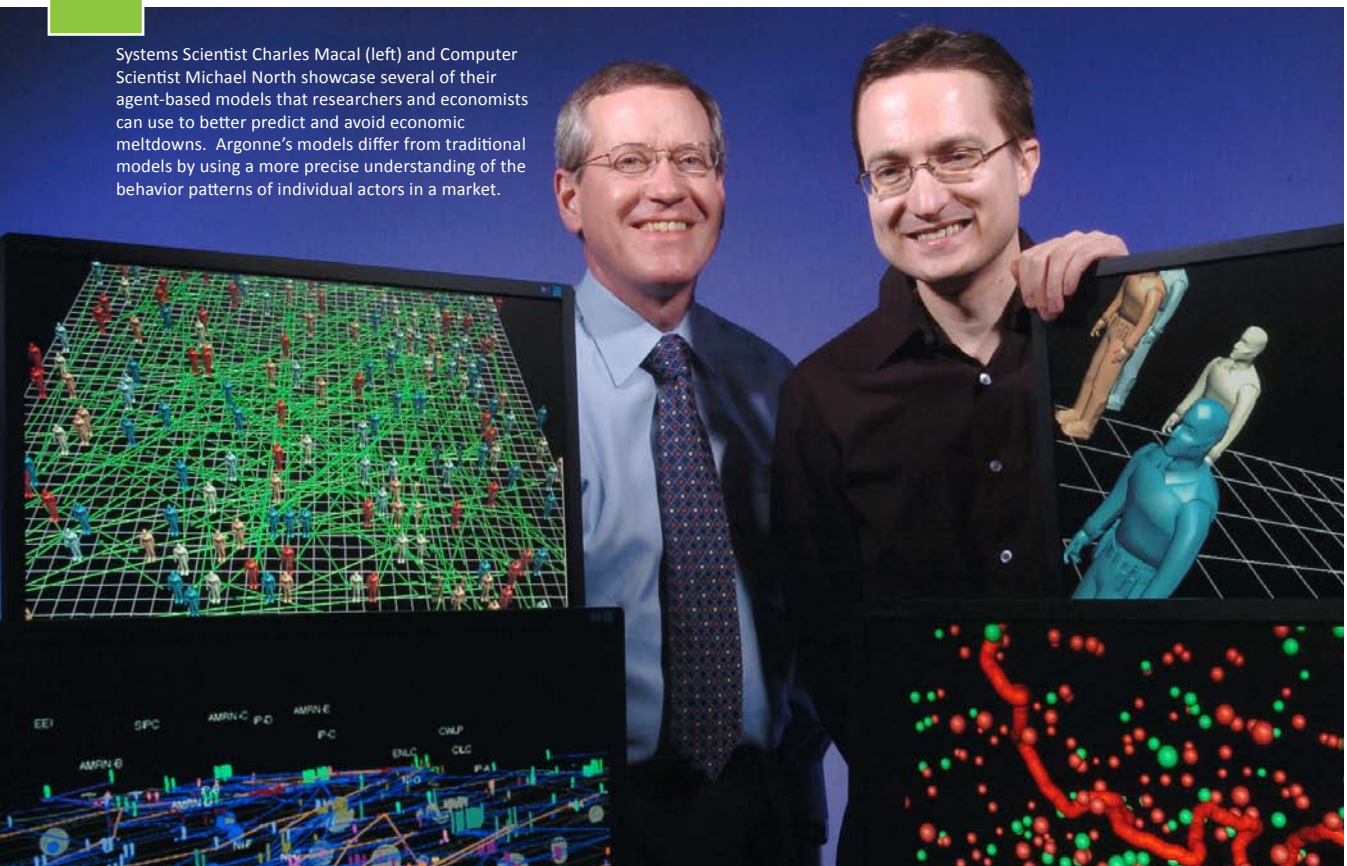
- Develop a high-resolution climate model capable of addressing regional scales that can be updated for model validation and method improvements, using data from a high-density, long-term observation sensor network focused on the Great Lakes hydrological basin.
- Apply the regional modeling paradigm and sensor network to areas outside the midwest.
- Build and maintain regionally-focused climate data sets, climate model simulation outputs, and analytical and visualization tools for input to integrated assessments.

INTEGRATED CLIMATE, ENERGY, AND ECONOMIC ASSESSMENT

WHY ARGONNE? Argonne has more than 30 years of expertise in the development, evaluation, and modeling of energy technologies and more than a decade's experience in managing large open-source communities. Through partnerships with the University of Chicago and other institutions, Argonne has unique access to expertise in economics, economic modeling, and policy. When coupled with its world-class expertise in computational mathematics and computer science (including numerical optimization, uncertainty estimation, and high-performance computing — all key topics for integrated assessment), Argonne is well positioned to forge new territory in the integration of diverse scientific, energy, and economic data sets to assist in achieving well-informed policy.

STRATEGY: To develop a program in socio-economic/environmental modeling based on modern modeling methods and data sources that will address important scientific and policy questions concerning interactions between climate change, energy systems, and economic development. Program goals include:

- Establish an open data repository for economic and energy data within an economic modeling framework as a joint Argonne-University of Chicago activity.
- Enable Argonne scientists and other teams to apply the open assessment framework to multiple scientific and policy questions. Focus on the integration of regional climate and ecological data sets to inform policy implications of climate and broader environmental changes.

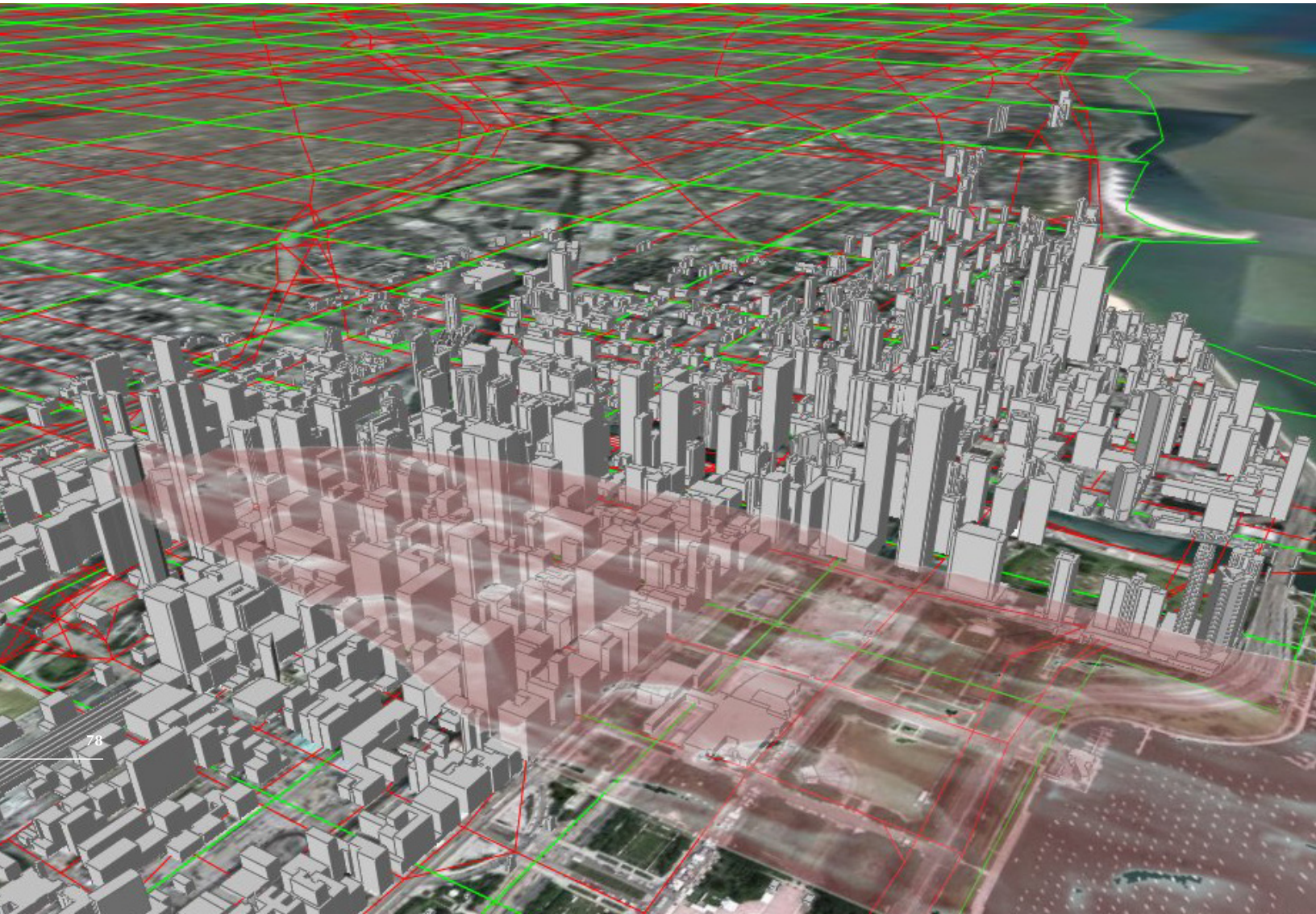


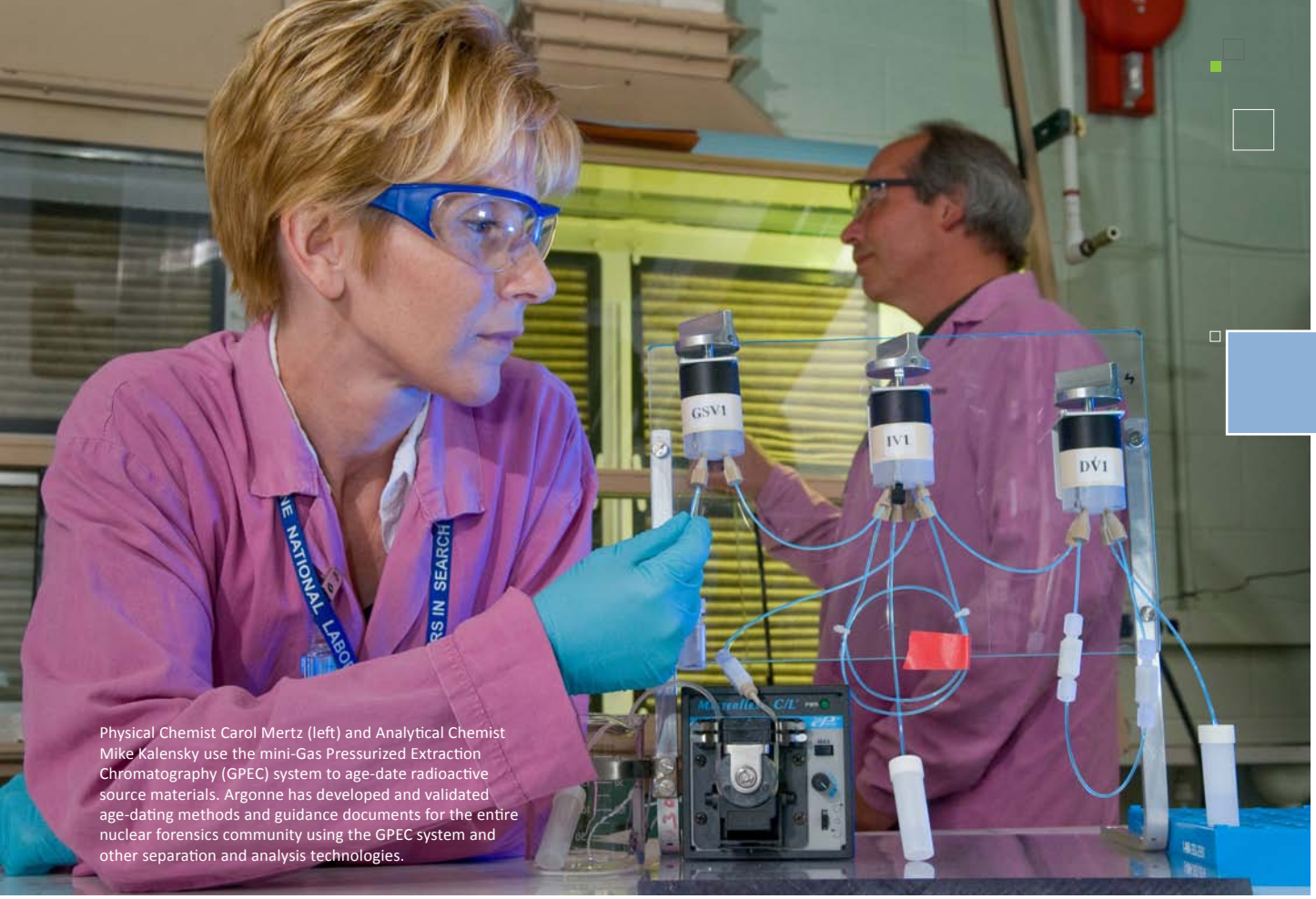
Systems Scientist Charles Macal (left) and Computer Scientist Michael North showcase several of their agent-based models that researchers and economists can use to better predict and avoid economic meltdowns. Argonne's models differ from traditional models by using a more precise understanding of the behavior patterns of individual actors in a market.

National Security

Argonne provides the nation with critical security and defense technologies that prevent and mitigate mass destruction initiated by state or terrorist activities, or caused by natural disasters. Some of our nation's most pressing security needs are being solved by Argonne's unique mix of scientists, engineers, and facilities.

Argonne's Transportation Research and Analysis Computing Center is using its high-performance computing systems and state-of-the-art software to model natural and man-made events that could require the emergency evacuation of a metropolitan area. Such a system could provide guidance to the emergency planning team in a timely fashion should the need arise. Seen here is an integrated model of the Chicago metropolitan area transportation network and contaminant dispersion.





Physical Chemist Carol Mertz (left) and Analytical Chemist Mike Kalensky use the mini-Gas Pressurized Extraction Chromatography (GPEC) system to age-date radioactive source materials. Argonne has developed and validated age-dating methods and guidance documents for the entire nuclear forensics community using the GPEC system and other separation and analysis technologies.

WEAPONS OF MASS DESTRUCTION (WMD), NONPROLIFERATION, AND FORENSICS

WHY ARGONNE? Argonne is the recognized world leader in nuclear reactor design, fuel processing, radiation detection, and radiological forensics. This enormous intellectual resource provides insight into and understanding of the use and misuse of radiological and nuclear materials and equipment around the globe.

STRATEGY: To strengthen the nation's ability to detect, prevent, and interdict proliferation of nuclear, radiological, chemical, and biological weapons through novel applications of Argonne's expertise. Goals include:

- Oversee full deployment of a completed chemical separations system for domestic production of the important medical isotope Mo-99; establish a Center for Fuel Cycle Analysis.
- Develop a fully time-dependent model, including safeguards by design, for a complete fuel reprocessing facility. Revolutionize the safeguarding of nuclear and other WMD materials by developing next-generation detectors and procedures.
- Lead domestic and international exercises to prepare the public, first responders, and decision makers for a radiological attack against the U.S. or its assets. Develop materials and procedures to allow rapid, safe, and effective cleanup after a radiological attack. Establish a Center for the Study of the Radiological Threat.

Computer Scientist Kathy Lee Simunich (left) and Systems Scientist Pamela Sydelko view the output from an air dispersion model that depicts the potential impact of a biological agent release.

DECISION SCIENCE

WHY ARGONNE? Argonne is a leading developer of decision support tools for the national and homeland security communities. These software, hardware, and assessment tools blend physical system simulation with social and behavioral analysis to assess issues of critical infrastructure protection, emergency preparedness, logistics, public health, command and control systems, and risk communication. Argonne has overseen successful application of these tools and a number of them are mandated for both U.S. agencies and abroad.

STRATEGY: To enhance and strengthen emergency preparedness of government, industry, and the public at large by continuing to develop and apply the critical decision support methods. Goals include:

- Establish a multidisciplinary National and Homeland Security Decision Analysis Center supported by an integrated, risk-based decision analysis system with broad interagency collaboration.
- Develop, field, and support an interoperable decision support backbone/architecture that connects major crisis management centers for all-source crisis decision making.
- Fully deploy this backbone/architecture across local, state, and federal agencies, ensuring compatibility and performance across disparate computing, communication, and response systems.

Scientist Yu-Sheng Chen calibrates the needle of the X-ray diffraction machine at the ChemMatCARS beamline in the Advanced Photon Source. This beamline is the only facility in the U.S. able to examine the small crystals of compounds that could one day be used for high-efficiency fiber optics and sensors to detect biological and chemical weapons at long distances.

SENSORS AND MATERIALS

WHY ARGONNE? A unique mix of applied material science and engineering, and systems engineering and integration capabilities, enables development of technologies that meet stringent security, defense, and intelligence requirements. Argonne has recognized expertise in imaging, remote sensing, and point sensing for nuclear, chemical, and biological detection, and a broad understanding of the techniques for design and discovery of novel materials.

STRATEGY: To leverage Argonne's world-class materials and engineering expertise in the development, testing, and deployment of sensors and materials that meet security and intelligence-gathering technology requirements for detection and sensing of nuclear materials and chemical agents. Goals include:

- Leverage successful imaging and sensing programs to create technologies focused on countering future-generation weapons and clandestine technologies.
- Become the recognized expert among security, defense, and intelligence agencies for meeting and exceeding requirements for materials, sensors, sensor networks, and imaging.

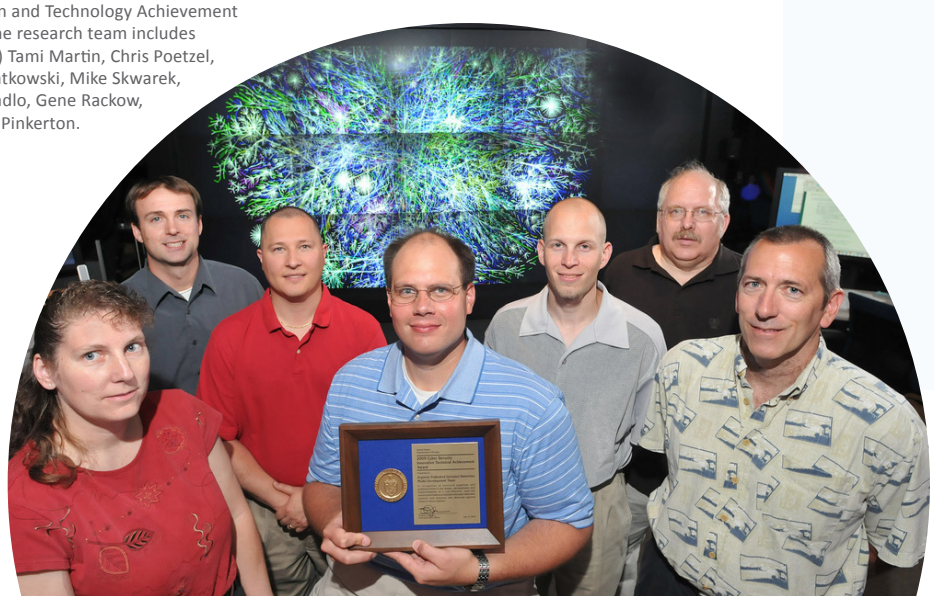
CYBER SECURITY

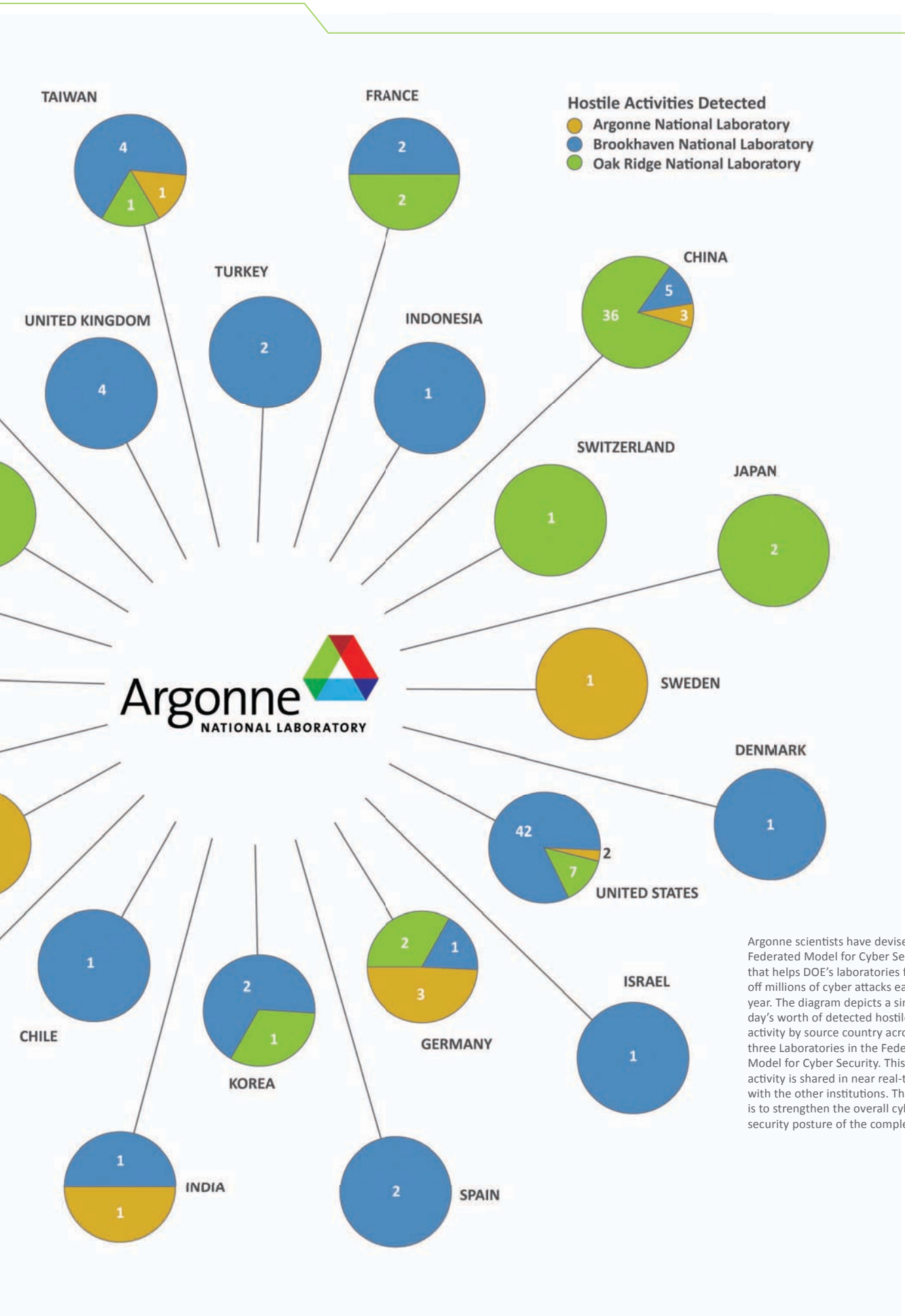
WHY ARGONNE? Current cyber security practice and policy struggle to keep pace with rapidly evolving threats and well-funded, sophisticated adversaries. Transformations in information system architecture and new capabilities are essential to rendering today's threats obsolete. Argonne's expertise in applied mathematics, decision sciences, grid and distributed systems, computer architecture, computational science, grid security, cloud/virtual-machine computing, and operational cyber security — combined with the Laboratory's leadership computing facilities and strong partnerships with industry — provides a unique capability to effect such transformation.

STRATEGY: To create science-based transformational solutions to critical cyber requirements that are not addressed through commercially available products, thereby enabling opportunities for sustainably strengthening the security of the nation's public and private sector information infrastructure. Goals include:

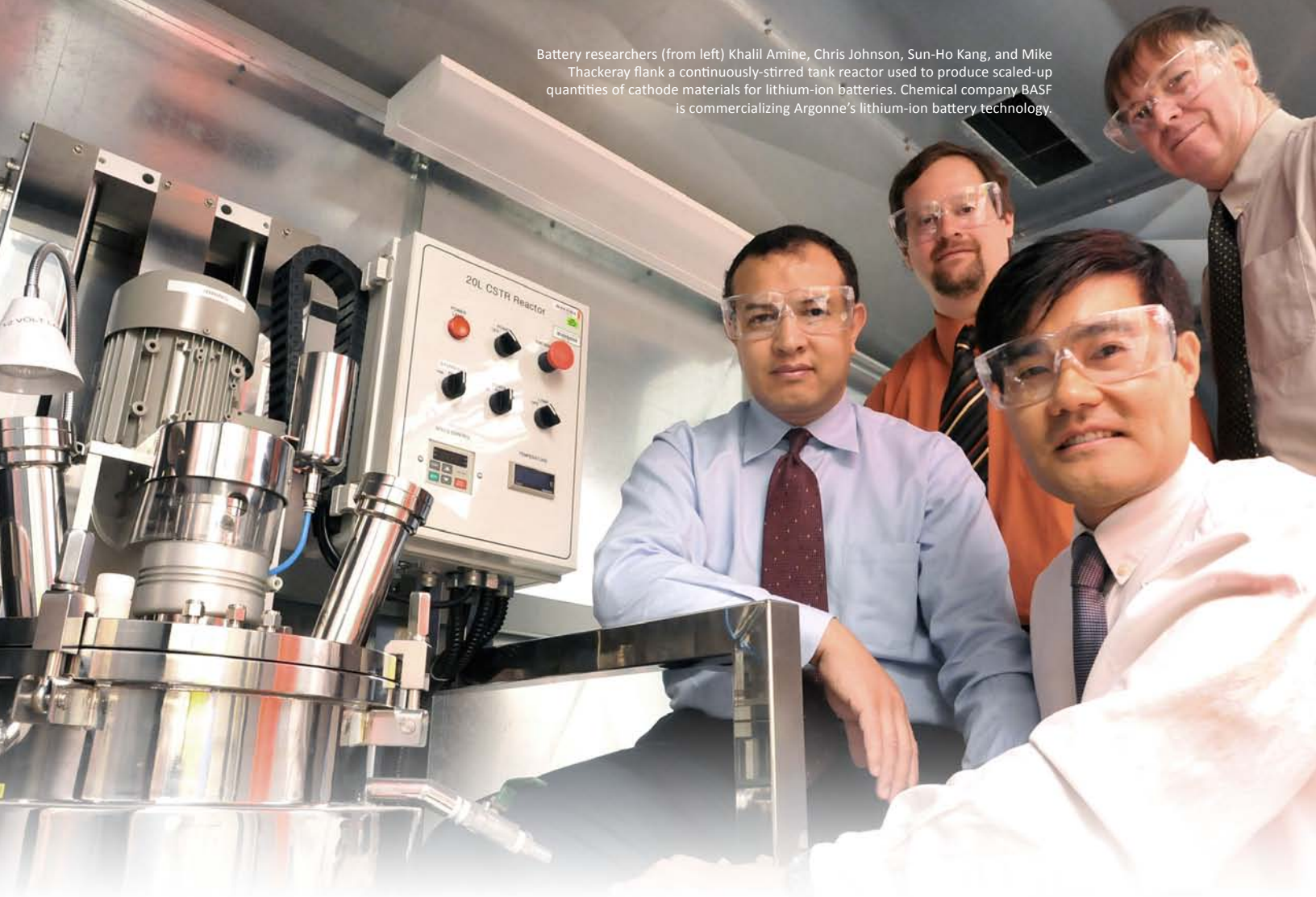
- Establish Argonne as the recognized leader in open-computing cyber security system development, with strong partnerships among the nation's security and defense agencies as well as academia, industry, and peer laboratories.
- Expand Argonne's cyber security programs to integrate applied mathematics and computation, secure hardware architectures, decision science, and data and application security.

The Federated Model for Cyber Security earned Argonne the DOE's 2009 Cyber Security Innovation and Technology Achievement Award. The research team includes (from left) Tami Martin, Chris Poetzel, Matt Kwiatkowski, Mike Skwarek, Conrad Zadlo, Gene Rackow, and Scott Pinkerton.





Argonne scientists have devised the Federated Model for Cyber Security that helps DOE's laboratories fight off millions of cyber attacks each year. The diagram depicts a single day's worth of detected hostile activity by source country across three Laboratories in the Federated Model for Cyber Security. This hostile activity is shared in near real-time with the other institutions. The goal is to strengthen the overall cyber security posture of the complex.



Battery researchers (from left) Khalil Amine, Chris Johnson, Sun-Ho Kang, and Mike Thackeray flank a continuously-stirred tank reactor used to produce scaled-up quantities of cathode materials for lithium-ion batteries. Chemical company BASF is commercializing Argonne's lithium-ion battery technology.

COMMERCIALIZATION AND TECHNOLOGY TRANSFER

Technology transfer is vitally important to Argonne's vision for the future. That is, to lead the world in providing scientific and engineering solutions to the grand challenges of our time: plentiful and safe energy, a healthy environment, economic competitiveness, and a secure nation.

To do so, the Laboratory strategically deploys technologies derived from its multidisciplinary research "continuum" — from basic science to applied science and engineering, and on to technology deployment into the marketplace. This approach is strongly linked to the success of Argonne's Office of Technology Transfer in forming partnerships with industry that result in the maturation of emerging science-based advances and introduction into commercial use. Some key areas of strategic emphasis are discussed here.

ENERGY STORAGE – Advances in anode, cathode, and electrolyte materials are being transferred to multiple licensees and the important design elements are being communicated through collaborative industry R&D contracts and Cooperative Research and Development Agreements. Argonne is partnering with the Commonwealth of Kentucky and two major Kentucky universities to establish a battery manufacturing research center in Kentucky. The Laboratory is also pursuing new research and development initiatives to deploy its capacitor technology through a venture partnership that will exploit new electrolyte materials for application to advanced vehicle systems.

RENEWABLE ENERGY – Argonne technology in continuous electrodeionization reactor design will be transferred for commercial use in biochemical processing through partnerships with a major manufacturer and a start-up company, thereby addressing different market sectors and product lines.

NANO-ENGINEERING – Argonne engineers are conducting targeted research and development in the scale-up of coatings, heat-treating, and lubrication nanotechnologies. Industrial and university partners will be identified to mature these technologies into functional engineering systems for industry deployment.

Loading engine components into the deposition system used to coat samples with Argonne's super-hard and slick material are Senior Metallurgist Ali Erdemir (left), Ph.D. Student Guldem Kartal, and Materials Scientist Osman Eryilmaz. The super-hard and slick material increases efficiency and reliability in engines used in transportation, as well as tools used in manufacturing. The technology is one of four from Argonne that received a 2009 R&D 100 Award.

Akonni Biosystems has licensed Argonne's biochip technology to commercialize a point-of-care diagnostic system for rapid treatment of infectious disease.

MATERIALS – Argonne is well positioned to exploit the economic advantage of processes that build coatings by depositing materials one atomic layer at a time. The use of this technology in flat panel displays, catalysts, and tribological applications, as well as in solar cells, will be pursued in partnership with industry in each market sector. Critical scale-up experiments are underway to illustrate the engineering advantages of our basic scientific approach to atomic layer deposition.

SYSTEMS ENGINEERING – Argonne transportation engineers are developing partnerships with automotive manufacturers to explore new hybrid and plug-in hybrid configurations. Computer modeling methods that are widely recognized as the leading approach to hybrid system development are being deployed and applied. The work will ultimately lead to design and development of advanced battery applications in future hybrid and electric vehicles.

LEADERSHIP COMPUTING – Argonne is developing partnering scenarios to enable industry to use the Argonne Leadership Computing Facility (ALCF) for both proprietary and non-proprietary research. Additionally, the ALCF will partner with key industry participants needing very high-capacity computational capabilities. The ALCF's advanced technology and capabilities will catalyze innovation within these companies to achieve the greater understanding, vision, and use of very high-capacity computing, and will help forge the path to exascale computing.

Argonne works proactively with its divisions and selected industrial partners to develop commercialization strategies, seek partners with new applications, and introduce advancements into commercial use through licenses and start-ups.

STRATEGIC COMMERCIALIZATION – Argonne has launched cross-cutting programs to accelerate commercialization in potentially all of the Laboratory's major initiative areas. Argonne has formed a consortium to work effectively with local venture capital firms – the Argonne Venture Acceleration Consortium (AVAC). It provides seasoned input and guidance for the most promising technologies evolving from Argonne's research. Argonne staff meet regularly with AVAC members to evaluate the investment potential of possible ventures and form investment teams of those interested in a particular technology. An "Entrepreneur-in-Residence" representing AVAC will be located at Argonne to help identify emerging technologies at the earliest possible time. The U.S. Department of Energy provides 50% funding support for this innovative partnership that promises to serve as a model for venture capital interactions with all DOE labs.

Argonne's use of DOE Technology Commercialization Funds to bridge the gap between the completion of research and development and the initiation of commercialization is an additional initiative to facilitate partnerships with industry at an early stage. Argonne has received funding from DOE for the express purpose of taking technologies across this gap. Over the coming year, these funds will support four to five projects that promise to have a major impact in energy storage, bioprocessing, and engineering applications of nanocoatings. In the next few years, Argonne will seek to broaden this type of support to embrace promising technologies from all of the Laboratory's major strategic initiatives.

An entire series of safety procedures are followed before, during, and after any work on the Advanced Photon Source (APS) accelerator. Senior Technician Debra Eriksen-Bubulka is seen here checking the clearance between the APS vacuum chambers and the magnets, using a set of go/no-go gauges.

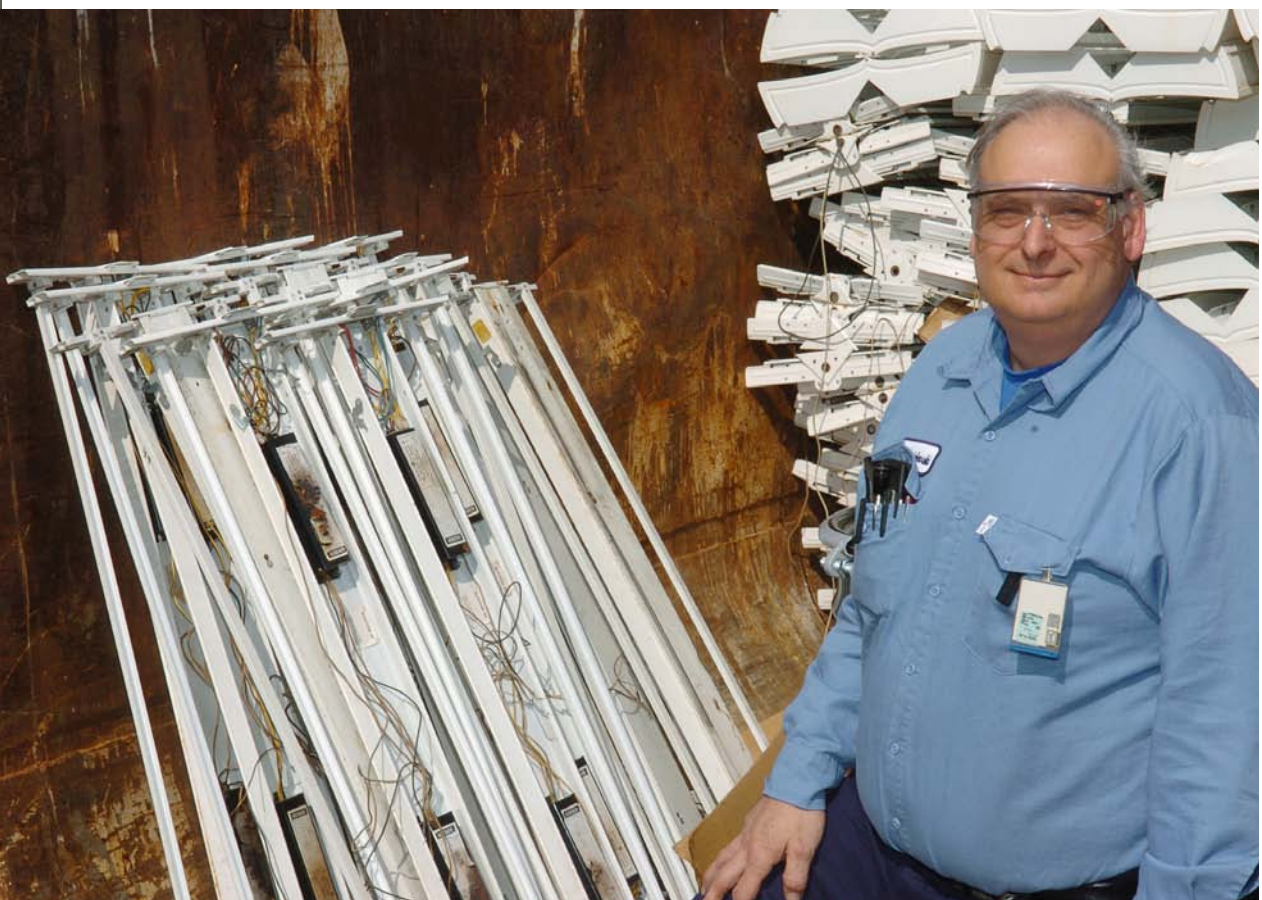
CRITICAL ENABLERS FOR OUR SUCCESS

A best-in-class Environment, Safety, Health, and Quality Assurance Program is integral to Argonne's mission.

Safety

Attaining and maintaining best-in-class Environment, Safety, Health, and Quality Assurance Program is integral to Argonne's innovative scientific research and engineering technology mission. A safe and healthful workplace is the personal, ethical, legal, and business obligation of Laboratory management. Argonne's Integrated Safety Management program is the foundation of the Laboratory's ongoing effort to protect its employees and users, other site personnel, visitors, the public, and the environment from the hazards and risks associated with Laboratory work.

Maintenance Mechanic Leon Chmielewski prevented possible worker exposure and improper disposal of hazardous materials by requesting an investigation of insulation on old wiring that was being replaced. The insulation turned out to be asbestos.



Infrastructure

Revitalizing the Laboratory's existing facilities and infrastructure to meet the current and emerging needs of our scientific missions is a major challenge for Argonne. This includes ensuring compliance with current environmental performance and safety standards, as well as the elimination of legacy waste and obsolete facilities – all while optimizing operation and minimizing maintenance costs. The U.S. Department of Energy is providing funding for the facilities discussed below, except where noted.

THEORY AND COMPUTING SCIENCES BUILDING

The Theory and Computing Sciences Building, constructed with third-party financing, provides the space and facilities to build on Argonne's strengths in high-performance computing software, advanced hardware architectures, and applications expertise. This supports the Laboratory's core capabilities in Applied Mathematics; Advanced Computer Science, Visualization, and Data; and the Leadership Computing initiative.

Construction of the more than 200,000 square-foot, seven-story-tall Theory and Computing Sciences (TCS) building was completed in late summer 2009. The building provides a much-needed infrastructure for large-scale computers, computational laboratories, a digital conference and meeting area, as well as a consolidated Argonne library.

ENERGY SCIENCES BUILDING

Construction of the 140,000-square-foot Energy Sciences Building (ESB) is to begin in FY 2010. This facility will co-locate and consolidate scientific efforts associated with three closely associated core capabilities: Condensed Matter Physics and Materials Science, Chemical and Molecular Science, and Chemical Engineering. The new building will eliminate excessive costs related to the maintenance and operation of the Laboratory's most seriously outmoded and inefficient buildings, built in the 1950s and '60s. The Materials Design Laboratory, with an anticipated FY 2012 start, will complement the ESB and enable additional consolidation.

ENVIRONMENTAL AND BIOLOGICAL SCIENCES BUILDING

Argonne is requesting funding for a 140,000-square-foot Environmental and Biological Sciences Building to support its work in sustainable energy technologies in the Biological and Environmental Systems and Alternative Energy and Efficiency mission areas, and to facilitate the removal of the existing biology facility built in 1952.

ADVANCED PHOTON SOURCE

Several smaller-scale programmatic facilities are being requested for the Advanced Photon Source, including the expansion of three APS beamlines; an interior build-out of the newest Lab-Office Module (LOM); a new APS storage building; and additions to the existing LOMs. The State of Illinois has pledged to fund the adjacent 50,000-square-foot Advanced Protein Crystallization Facility to accommodate the need for state-of-the-art experimental space for structural biology work. Construction is projected to begin by FY 2013.

OTHER FACILITIES

DOE is committed to ongoing efficiency and intensity upgrades for the target and source beamlines of ATLAS/CARIBU, including potential facility expansions. A proposal for a new Battery Test Facility is also underway.

To support growth in its Systems Engineering and Integration and Applied Nuclear Science and Technology, Argonne is evaluating non-traditional funding sources for mission-related multiprogram facilities that have special security features. To support the long-term growth of the Nuclear Physics program, Argonne is investigating an advanced accelerator-based facility to produce rare isotopes using the isotope online method. Such a facility would provide large quantities of radioisotopes for alternative applications, primarily medicine. The laboratory is evaluating the feasibility of a public-private partnership to support this effort.

In conjunction with modernization planning, Argonne has begun efforts to transfer its legacy nuclear waste, materials, and excess nuclear/radiological facilities to DOE for disposition stewardship.

Each year, Argonne sends a number of its staff to participate in the Strategic Laboratory Leadership Program to improve and develop the participants' ability to cohesively, coherently, and agilely steward and lead organizational strategy and change with the objective of becoming more effective leaders. The 2009 participants are (left to right): front row: Mark Petri, John Arrington, Thomas Gog, Will Brocker, Michael Syphers, Greg Jonas, and Roger Johnston; second row: Terry Dykhuis, Sandor Feher, Denise Keiner, Terri Bray, Julie Cross, Katherine Riley, Catherine Newman Holmes, Vaia Papadimitriou, Katie Carrado Gregar, and Jim Steimel; back row: Rao Kotamarthi, Folker Meyer, Dave Chamberlain, John Maclean, Juanita Frazier, Brendan Casey, Ian Fisk, and Amanda Petford-Long.

Workforce Development

The successful implementation of Argonne's *Strategic Plan* depends on a robust and dynamic workforce. In FY 2008, that workforce included 1,300 scientific and technical staff among a total of more than 2,800 employees. Included in Argonne's workforce are more than 160 postdoctoral appointees assigned to positions throughout the Laboratory. More than 600 graduate and undergraduate students also work and gain valuable experience at the Laboratory during some portion of the year.

The Laboratory is dedicated to hiring, developing, and retaining top-quality staff whose efforts support the *Strategic Plan*. Initiative leaders assess current expertise in their areas, identify partnering opportunities to strengthen this expertise, and determine hiring needs to close the strategic staffing gaps. Analysis of the Laboratory's overall needs leads to targeted recruiting and, in some instances, to reassignment of existing staff or strategic placement of postdoctoral appointees.

Argonne has traditionally used its own Web site and other tailored or regional sites for posting open employment positions. Additional media have been used (e.g., job search Web sites, industry journals and Web sites, and local newspapers) as a position requires. Argonne is now using Web 2.0 applications to recruit directly from talent-specific communities. These tools allow the Laboratory to reach networks of targeted, qualified prospects that can be cultivated into a self-sustaining source of engaged talent.

Argonne continues to develop relationships with university partners to enhance its recruiting and retention capability, and joint appointments are becoming a more significant part of recruiting packages — especially for strategic hires of established leaders in their fields. Senior R&D staff are often attracted to a relationship both with the Laboratory and with one of the major research universities in the Chicago area. Argonne is also exploring the feasibility of joint appointments with other national laboratories.

To remain a competitive workplace, Argonne monitors its compensation and benefits system to ensure alignment with the *Strategic Plan*. The Laboratory will also assess its current methods of defining and classifying jobs and examine its pay grades with an eye to maintaining a competitive market position. Finally, Argonne will re-evaluate whether or not it has all the compensation tools needed to attract, retain, and motivate the workforce its strategic initiatives demand.

The Laboratory sends 15 employees each year to the Strategic Laboratory Leadership Program, an executive leadership development program created through a collaborative effort between the University of Chicago Booth School of Business, Argonne, and Fermi National Accelerator Laboratory. Beginning in September 2007, the University committed to providing this program for five years. The Strategic Laboratory Leadership Program provides a great opportunity for Argonne to develop future leaders who are well-versed in strategic thinking.

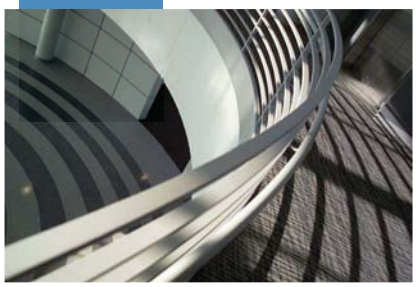
Laboratory Management System

Argonne management began a major initiative on October 1, 2006, to move the Laboratory from an organization-based management system to a process-based system and to become the first national laboratory to receive ISO 9001 and ISO 14001 certifications. The strategic motivation for the decision to follow internationally accepted ISO management practices was both to function better as an institution and to enhance Argonne's attractiveness to potential sponsors and partners.

Strategic Planning is one of the 17 Core Processes that form the framework of Argonne's Laboratory Management System (LMS). Execution plans for all our major initiatives and supporting strategies include both milestones and metrics to ensure steady progress towards achieving even our most ambitious goals.

On July 1, 2009, Argonne celebrated both its ISO 9001 and its ISO 14001 certification. ISO certification was granted after a team of independent auditors determined that Argonne's LMS was in full compliance with ISO 9001 for business systems, and that the Laboratory's environmental systems complied with ISO 14001. Certification is validation from a third party, independent source that the LMS is built and being implemented based on worldwide best practices.

On July 28, 2009, Argonne Director Eric Isaacs announced that the Laboratory has been certified to ISO 9001 and ISO 14001 international standards for business practices and environmental management, respectively, after nearly two years of work on the part of hundreds of employees. The event marks the first time a DOE national laboratory has received both the ISO 9001 and ISO 14001 certifications.



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U.S. DEPARTMENT OF ENERGY

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