ARGONNE NOW

volume 03 / issue 01 / spring 08

Argonne NATIONAL LABORATORY

mega

giga

tera

entering the petascale era

Advanced Computing Provides New Solutions

building better catalysts

a new route for transportation

a fresh vision for fission

dear friends,

Investment in basic science throughout the past 100 years transformed America into an economic and technological superpower. To continue that role, we must maintain a strong commitment to basic scientific research that will sustain America's economic security and preserve our status as a global leader in research and development. The innumerable technologies and products that form the foundation of today's and tomorrow's economies owe their existence to continued support of America's scientific enterprises.

This issue of Argonne Now highlights the growing contribution of high-performance computing to both basic and applied science and celebrates the success with which Argonne National Laboratory's many disciplines have integrated exceptional computational resources and unparalleled expertise into missions in research and development.

This magazine shows how computer scientists are fueling economic growth by reducing the amount of time and money that their experimentalist colleagues must expend on real-world testing. In this way, new technologies and better products can be brought to market more safely, quickly and cheaply. The development of detailed and precise models and simulations will hasten the innovations that strengthen our country's financial health and secure our prominence in the global marketplace.

I would like to take this opportunity to thank the Department of Energy and all of our sponsors for providing the means and resources that allow us to carry out this vital research.

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ARGONNE now

volume 03 / issue 01 / spring 08

Blue Gene/P

on the cover
Argonne’s new Blue Gene/P supercomputer, installed in the laboratory’s Argonne Leadership Computing Facility.

news / from Argonne

Left: Physicist Ulrich Welp and his colleagues created a portable source of terahertz radiation, a harmless kind of electromagnetic energy between microwaves and infrared that offers many of the screening capabilities of X-rays without the health risks.

New, safe T-ray source

A group of Argonne researchers led by physicist Ulrich Welp has developed a new, compact source of terahertz radiation, or T-rays. This new technology could be used to create T-ray scanners that can detect dangerous or contraband materials at airports or create new imaging devices for skin and breast cancers.

Previously, T-rays could only be created by using a large table of expensive equipment. The Argonne T-ray source is only a few millimeters in size, small enough for engineers to potentially use it to make a portable scanner.

The new source comprises a stack of semiconducting crystals known as Josephson junctions. Researchers can induce alternating currents of various frequencies in these junctions by applying different amounts of voltage.

T-rays present an additional advantage over their more energetic cousins, X-rays: Because they lack sufficient energy to ionize atoms, T-rays are perfectly safe for human exposure. T-rays can penetrate skin, leather, fabric, cardboard and paper but do not pass through water or metal.

Quantum dots flicker quicker

Quantum dots — tiny, colorful light-emitting particles that blink like strobe lights — have become all the rage among nanoscientists who seek to understand one of their unusual but frustrating properties.

These semiconducting nanoparticles may represent the future of light-emitting materials because the color of light that they give off can be changed by merely altering the size of the particles. This unique behavior has made quantum dots the subject of intensive investigation for potential use in medical research, as well as for new forms of lighting, lasers and solar cells.

All of these applications, though, may be compromised by the annoying tendency of single dots to flicker on and off randomly like fireflies. This

Quantum dots — small semiconducting nanocrystals — can produce a rainbow of colors depending on their size. Scientists in Argonne's one-year-old Center for Nanoscale Materials are examining the tendency of quantum dots to oscillate between bright and dark states, a phenomenon known as "blinking."

"blinking" behavior has been widely observed but remains poorly understood. Argonne scientist Matthew Pelton and collaborators from the California Institute of Technology and The University of Chicago recently discovered a previously unobserved change in the blinking of a single quantum dot viewed under a microscope during periods shorter than a few microseconds.

This result confirms a theory that the fluctuations of energy levels in the quantum dot relative to its environment cause the dot to blink. This new insight may point the way to a better way to control blinking, brightening the prospects for real-world applications of quantum dots.

Argonne helps China sprint to clean air before Olympics

Beijing, China, will play host to the 2008 Summer Olympics come this August. But the city has recently garnered a less favorable distinction for high levels of air pollution.

The air in Beijing can become especially polluted during the summer months, when a combination of high temperatures, high humidity and low wind speeds causes pollutants to accumulate in the atmosphere.

Argonne has played a leading role in helping China's scientists and policymakers improve air quality in advance of the Olympics. Since 2003, Argonne and the U.S. Department of Energy have been working with the China Automotive Technology and Research Center to promote the adoption of energy-efficient vehicles and cleaner fuels.

Scientists at Argonne have also helped to create models of Beijing air quality that have gotten the attention of Beijing's mayor, who requested that the Chinese government implement unprecedented regional control programs to ensure that the city meets its 2008 air-quality goals.

Argonne scientists have worked with Chinese scientists and officials to clean up the air of the capital, Beijing (above), which will host the 2008 Olympics.

the future of computing

Quick: What's 1,327 times 4,922? Well, don't worry about it, but how long do you think it would take you to come up with 6,531,494? A minute? Five minutes? Fifteen? Argonne's new supercomputer, the IBM Blue Gene®/P, can do that calculation, as well as another five hundred trillion or so, in a mere second.

The Blue Gene/P, installed last fall in the new Argonne Leadership Computing Facility (ALCF), is already one of the world's fastest supercomputers. When its expansion is complete, the Blue Gene/P will perform at a speed of 556 trillion FLOPS (or floating point operations per second) and spearhead the move to what computer scientists call "petascale computing."

Argonne's newly acquired access to petascale-capable hardware, combined with three decades' worth of accumulated scientific expertise, will accelerate high-impact science across the country and allow Argonne to continue its long history of cutting-edge research that broadens scientific horizons, said ALCF Project Director Pete Beckman.

Throughout this issue, you'll learn how the Blue Gene/P and Argonne's other advanced computing resources will transform research in myriad fields, from finding better catalysts (page 6) to modeling nuclear reactors (page 16) to enabling us to move around more safely, quickly and cheaply (page 10).

The ALCF provides computational power for the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, funded by the U.S. Department of Energy's Office of Science to encourage and support intensive research projects from industry and scientific research organizations. According to Argonne Senior Computational Scientist Ray Bair, the Blue Gene/P dramatically increases the amount of computing

collaborate

For general questions about the Blue Gene/P and Argonne's supercomputing facilities, please contact:
Pete Beckman
Project Director, Argonne Leadership Computing Facility
630 252 9020

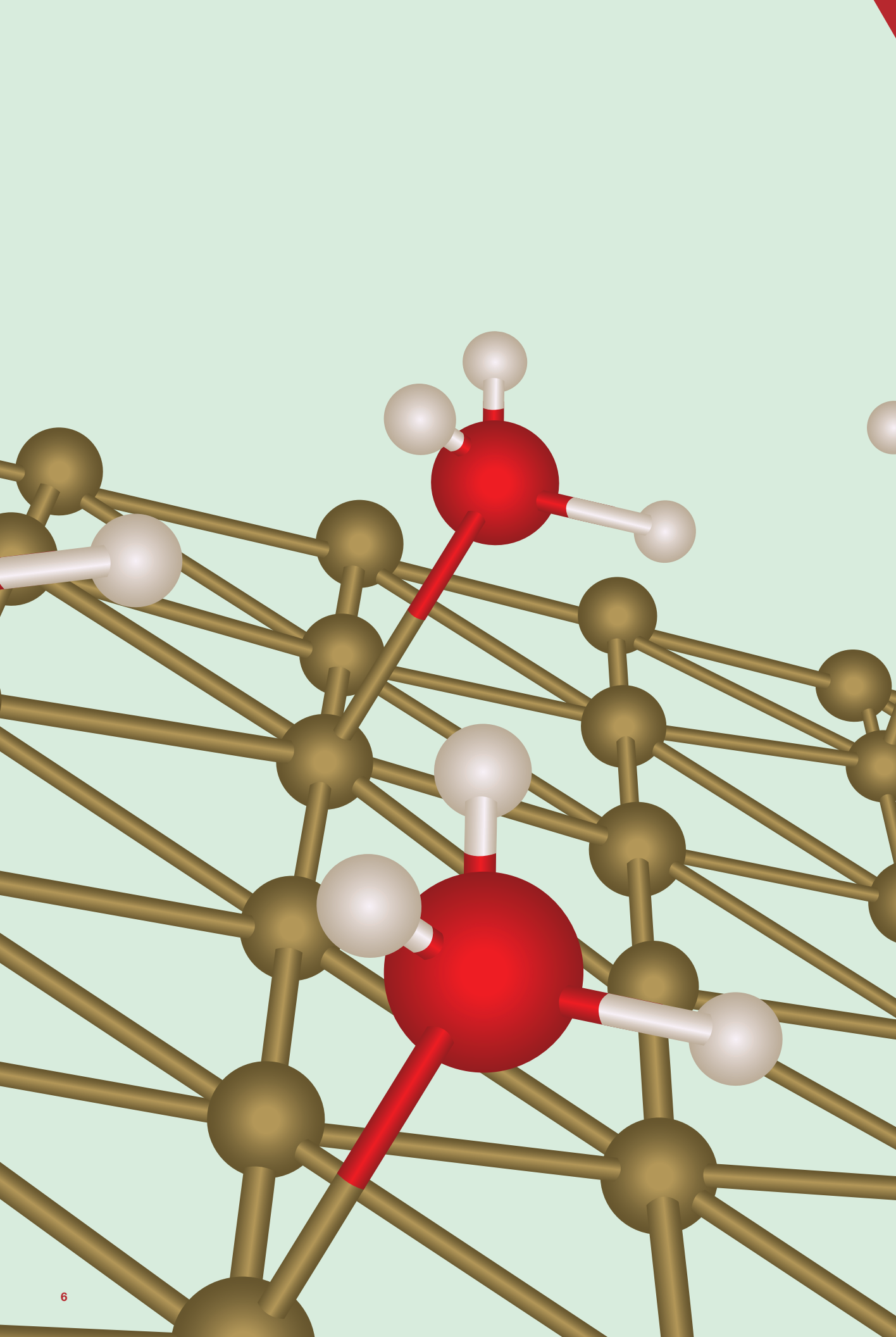
For information about becoming a user of the Blue Gene/P, please contact:
Rick Stevens
Associate Laboratory Director
Computing, Environment and Life Sciences
630 252 3378

power available to INCITE scientists and engineers. "Researchers can employ this new computing resource to attack cutting-edge problems in science and engineering at an unprecedented scale and speed," he said.

While the Blue Gene/P-equipped ALCF will be Argonne's fastest and most powerful supercomputing center, the laboratory also operates several other large computing clusters for specific scientific disciplines. Chief among these is the Nanoscience Computing Facility, a 10-teraflop system that has already enabled breakthrough research on particles less than 1/10,000th the width of a human hair. The system recently reached the 150th position on the TOP500 list of the world's fastest supercomputers.

The recent expansion of Argonne's computing facilities will provide scientists and engineers with a valuable complement to their laboratory research. By supplying scientists with the capability to construct detailed models and simulations of complex physical, chemical and biological processes, these computers will allow Argonne's experts to save time and expense while still achieving accurate and significant results.

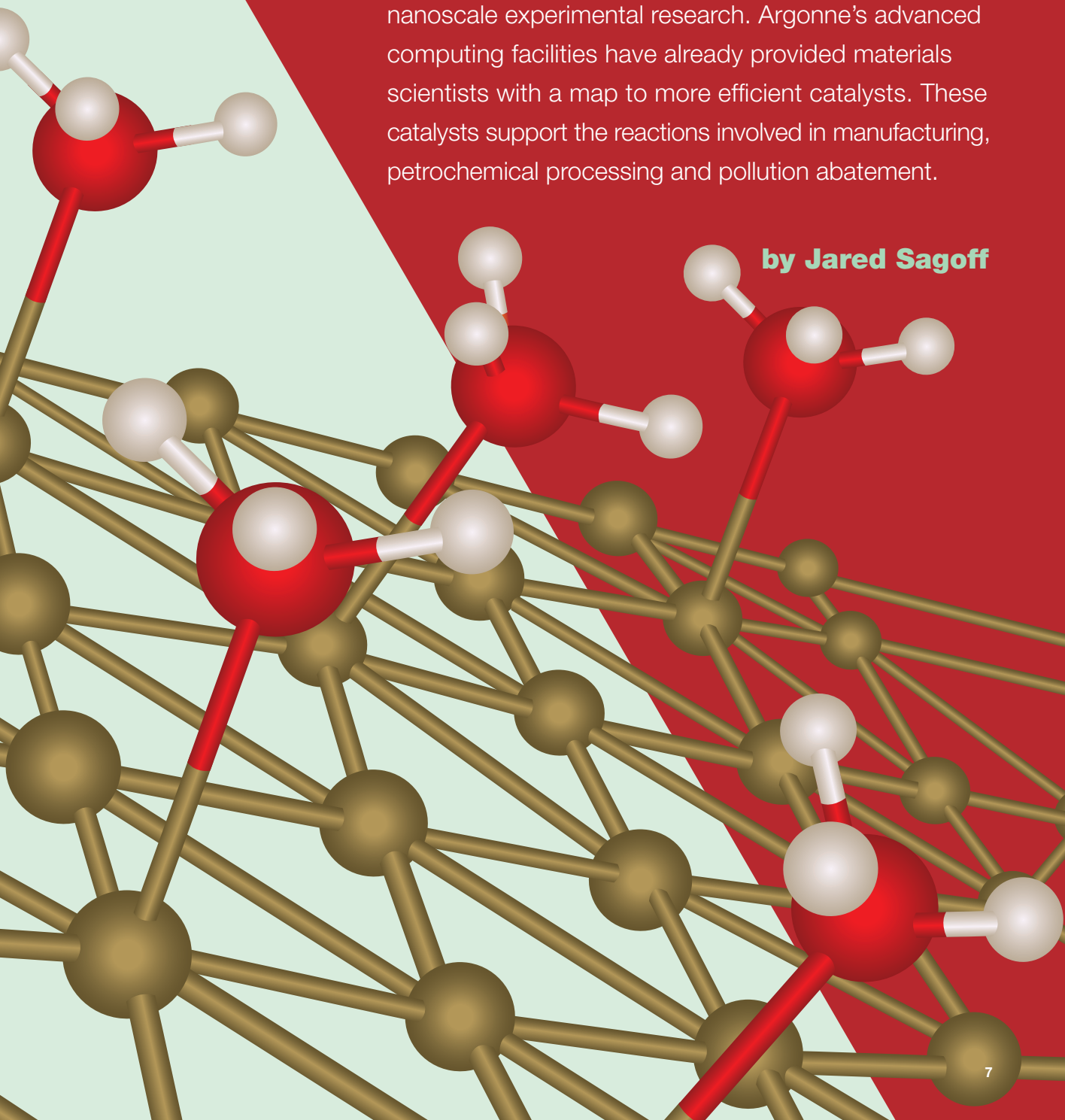
"Researchers can employ this new computing resource to attack cutting-edge problems in science and engineering at an unprecedented scale and speed."



a catalyst quest

Argonne's petascale computing capability will accelerate nanoscale experimental research. Argonne's advanced computing facilities have already provided materials scientists with a map to more efficient catalysts. These catalysts support the reactions involved in manufacturing, petrochemical processing and pollution abatement.

by Jared Sagoff



In an office at Argonne's one-year-old Center for Nanoscale Materials, materials scientist Jeff Greeley is working to find a new chemical catalyst that can transform propylene into propylene oxide, an organic molecule needed for the production of many plastics. Greeley, along with materials scientists Larry Curtiss and Peter Zapol of Argonne's Materials Science and Chemical Sciences and Engineering divisions, compiles a list of suspects and enough physical evidence to run through some of the fastest computers in the country. The way that Greeley describes the investigation sounds almost as much like forensics as pure chemistry.

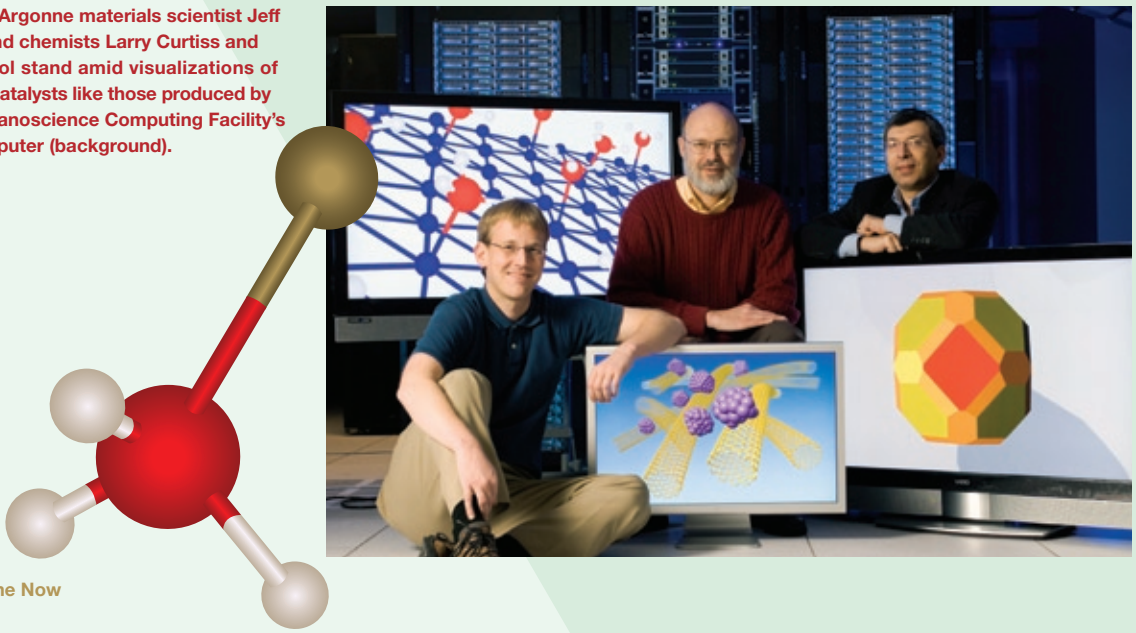
"We use a few chemical parameters as a kind of 'fingerprint' that gives clues as to how catalysts actually work," Greeley said. "Our goal is to use advanced computing to run these 'fingerprints,' so that we can help experimenters to more closely focus their synthesis and testing efforts on the most likely candidates."

Greeley's search for a new catalyst is a prime example of how basic scientific research plays a critical role in ensuring long-term economic growth. From plastics manufacturing to petrochemical processing to environmental cleanup and pollution abatement, catalysts play an essential role in many aspects of our everyday lives. According to *R&D* magazine, approximately 90 percent of commercially produced chemical products involve the use of catalysts at some point during their manufacture. Catalysts also form the core of many of the most promising future technologies, such as hydrogen fuel cells. Greeley's research is funded by the Basic Energy Sciences program in the U.S. Department of Energy's Office of Science to expand the scientific foundations for new and improved energy technologies.

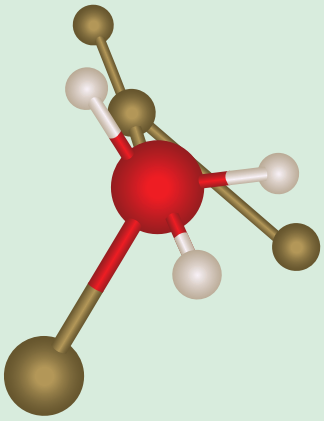
Most commercial catalysts consist of a transition metal bonded to a non-metal base. They work by reducing the amount of energy needed to initiate a chemical reaction. The best catalysts lower this quantity — known as a reaction's activation energy — dramatically, providing a shortcut from reactants to products that saves money and conserves energy. A catalyst's function also depends on its binding energy, a quantity that describes how strongly reactants attach to it.

By harnessing the combined power of Argonne's high-performance computing resources, including the Jazz cluster at the Laboratory Computing Resource Center (LCRC), the IBM Blue Gene®/P supercomputer at the Argonne Leadership Computing Facility and the new Nanoscience Computing Facility (NCF), Greeley and his colleagues attempt to predict which catalysts will have the lowest activation energies and the optimal binding energies.

These two principal quantities are relatively easy to estimate, but ensuring that they produce accurate representations of actual catalysts requires a significant amount of computing power, Greeley said. "We need our models to have predictive power; that is, we want to be able to evaluate one set of parameters for each catalyst candidate and make meaningful predictions about how fast a particular reaction will proceed, an environmental contaminant will be cleaned up or a particular



From left, Argonne materials scientist Jeff Greeley and chemists Larry Curtiss and Peter Zapol stand amid visualizations of potential catalysts like those produced by the new Nanoscience Computing Facility's supercomputer (background).



The computer models act as a sieve, allowing scientists to eliminate the vast majority of possible alloys or configurations from consideration without having to perform expensive and time-consuming tests on them in the laboratory.

fuel cell reaction will be accelerated. Then we'd like to go through and evaluate that parameter on hundreds or thousands of different alloys."

To investigate the catalytic properties of a variety of materials, Curtiss and Zapol have used the Jazz cluster to more closely examine catalysts' fundamental atomic structures as well as the mechanisms of the reactions they facilitate. Many catalysts, including those used in fuel cells, consist of a metal nanoparticle that sits on a larger non-metal support — fuel cell electrocatalysts typically use platinum active sites on carbon-based structures.

The particular geometric and electronic configuration of the catalyst on a support greatly influences its efficiency. As a result, finding the optimal atomic arrangement is as important as determining the correct component materials. In the case of propylene, for example, Argonne researchers found that small clusters of silver atoms on an aluminum oxide support helped to add oxygen to propylene's carbon-carbon double bond, converting it to propylene oxide. Later hands-on experimental research has validated that result.

"For a computational materials scientist," Greeley said, "that's the dream: to be able to make a prediction about a material that has improved properties, and then to actually test it in the lab and to find out that it works. But it takes a lot of computer power to go through all the different candidates."

The opening of the 10-teraflop NCF earlier this year has provided Argonne's scientists with enough computing power to do many more of these atomic-scale calculations than they could previously. "We used to run these calculations on smaller systems, where we'd have to represent catalysts with a smaller number of atoms," Curtiss said. "But now we can include many more. In addition, in the past many of the reactions in which we were interested were just too complex, but now we have an opportunity to study many more reactions in more detail."

Argonne's materials scientists refer to these combined approaches as "computational screening," a process somewhat like panning for gold. The computer models act as a sieve, allowing scientists to eliminate the vast majority of possible alloys or configurations from consideration without having to perform expensive and time-consuming tests on them in the laboratory.

"Our goal," Greeley said, "is to shorten the list of likely candidates so that we can give guidance to our experimentalist colleagues to help them focus their synthesis and testing efforts more closely on materials that we think have a good chance of success. Just in terms of manpower and computational expense, it would be quite costly to go through all those 750 materials and test them in a lab from the start."

Zapol agreed: "You can try different combinations much more rapidly on the computer than in the lab."

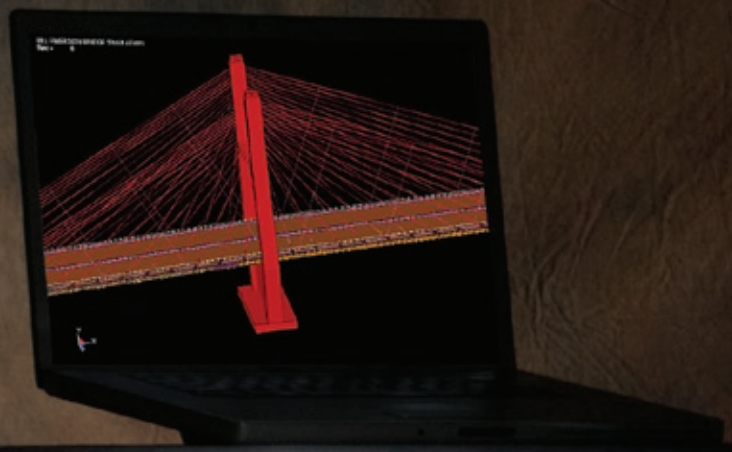
Typically, however, catalyst "gold" isn't gold at all, but rather a metal cluster, metal oxide or other composite. While precious metals like gold or silver do compose part of many of the most active catalysts, the costs of using them on a large scale provide another incentive for researchers to use computational screening to identify cheaper, but equally effective, alternatives.

In the course of his more than 30 years at Argonne, Curtiss has become widely known for his development of new computational techniques, including the formulation of highly accurate quantum chemical methods for the calculation of binding and activation energies, the two most significant parameters that scientists must consider when assessing and modeling the catalytic properties of different materials. "The availability of faster computers and new methodologies provides materials scientists with an unprecedented opportunity for designing materials with improved properties," Curtiss said.

Although Argonne's scientists do most of their computational screening of catalysts on the Argonne NCF and LCRC computer facilities, Argonne's recent acquisition of the IBM Blue Gene/P supercomputer promises to facilitate additional breakthroughs in computational catalyst modeling.

For information, contact Larry Curtiss at 630 252 7380.

transportation
moving in a new direction



As Argonne researchers consider the future of transportation, they are turning increasingly to computer simulations that can break down complex systems into millions of constituent parts. These models create an accurate and detailed picture that addresses the many challenges that face our intricate transportation infrastructure and saves time and money for the people who use it.

by Jared Sagoff

Transportation Research and Analysis Computing Center Director Dave Weber examines the bust of a person created with a finite-element model, reminiscent of Rembrandt's *Aristotle Contemplating the Bust of Homer*.

Engineer Ron Kulak stands in front of a visualization of water flowing around bridge supports. The redder colors represent faster flow rates. High-performance computing provides engineers with the ability to visualize the flow in unique detail.

In the control tower at the DuPage County Airport in West Chicago, air traffic controllers direct planes taking off and landing on the main runway. In the building next door, Argonne scientists and engineers at the Transportation Research and Analysis Computing Center (TRACC) have begun to take a more grounded approach to transportation. They focus on easing the strain on overtaxed road and rail infrastructure and on saving lives in accidents and disasters, either natural or man-made.

Under a multiyear grant from the U.S. Department of Transportation (DOT), TRACC will staff and operate a state-of-the-art, high-performance computing center that will provide the necessary computational tools and resources to address these important problems.

In a small office building in the middle of the DuPage National Technology Park sits TRACC's heart and soul: a brand new supercomputer that contains 512 processors with a combined speed of nearly two teraflops. This system will add significantly to the computational resources of the DOT's user community by providing a production-level, high-performance computing environment that also uses the Linux operating system, allowing it to run nearly any piece of commercially available software as well as software under development by the transportation research community.

"By enlisting both high-performance computing resources and technical staff with expertise in parallel computing and engineering analysis applications, TRACC represents a valuable resource for the DOT research community," said TRACC Director Dave Weber. TRACC will become a hotbed of focused computation-based research in areas of critical importance to DOT.

a bridge to tomorrow

Last August 1, during the height of evening rush hour, the I-35W bridge that spanned the Mississippi River just outside of Minneapolis, Minn., unexpectedly collapsed, killing 13 people and injuring more than 100. While bridges fail occasionally, such tragedies usually result from the impact of unusually heavy stresses: flooding, high winds or collision. The I-35W bridge, however, had experienced none of those, leaving engineers struggling to provide an explanation.

Recent research at TRACC aims to help bridge architects avoid similar catastrophes in the future. "It turns out that a lot of bridges that fail prematurely fail because of hydraulic reasons," said Tanju Sofu, an Argonne nuclear engineer who has turned his attention to constructing computational fluid dynamics (CFD) models of river beds and bridge supports.

According to Sofu, water that flows under a bridge often transports sediment that can "scour," or erode, the bridge supports. This underwater process, though gradual and invisible to normal observers, can so thoroughly wear away a bridge support that the entire structure collapses.

To prevent scour, bridge architects will have to either design their supports or redirect the current in a way that minimizes the quantity and the velocity of sediment

> "We can create as many bridges as we want on the computer without actually having to build and test them."

that washes up against the pillars. These designs necessitate scientific methodologies that can take into account large sections of the bridge structure at once.

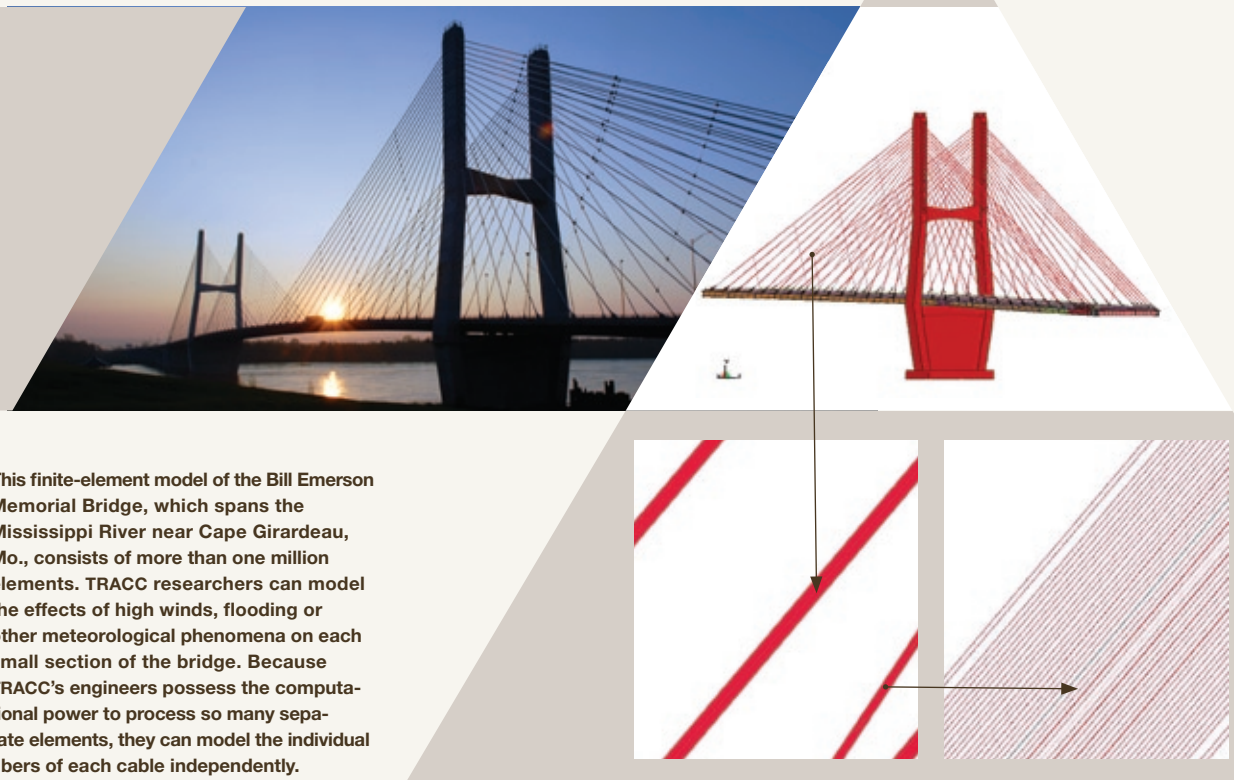
For that reason, Sofu explained, experimental testing cannot provide all the varieties of data that engineers need. "Bridge design experiments are not conducted on the bridges themselves but in controlled laboratories on a much smaller scale," he said. "Researchers are looking for a way to cut down on these experiments because they're very expensive to begin with and cannot provide information that will pertain to every single bridge."

Computer modeling, on the other hand, has that potential, Sofu said. "With access to supercomputers, we can simulate how individual bridges interact with sediment transport, local topography and changing climate conditions. We can create as many bridges as we want on the computer without actually having to build and test them."

While civil engineers consider scour one of the most insidious bridge stresses, they also study the effects of more recognizable strains. In the aftermath of the devastation wrought by Hurricane Katrina on the infrastructure of New Orleans, they have redoubled their efforts to ensure that bridges can withstand heavy floods and high winds.

While CFD models give researchers a good picture of how fluid pressures will be applied to a bridge, finite-element analysis predicts how the bridge structure will react to these pressures. Argonne engineer Ron Kulak and researchers from Turner-Fairbank Highway Research Center use models of cable-stayed bridges with hundreds of thousands of elements. That way, Kulak says, they can model the motion of every single part of the bridge,

drawing the bridge



This finite-element model of the Bill Emerson Memorial Bridge, which spans the Mississippi River near Cape Girardeau, Mo., consists of more than one million elements. TRACC researchers can model the effects of high winds, flooding or other meteorological phenomena on each small section of the bridge. Because TRACC's engineers possess the computational power to process so many separate elements, they can model the individual fibers of each cable independently.

The red lines on this map of Chicago represent the different roads modeled by TRACC's TRANSIMS software program. The model has great resolution in the downtown area, but also incorporates a network of highways and thoroughfares that extends from Milwaukee to Kankakee and from Lake Michigan out to Rockford.

down to the individual fibers of the supporting cables, as traffic, heavy winds or other meteorological phenomena stress the bridge. Computer-based research at this highly detailed level promises to prevent future bridge disasters and save lives.

finding the key to gridlock

At 8:24 a.m. on a bright September morning, a man pulls into the exit lane and turns off the Kennedy Expressway on his way to work on Roosevelt Road downtown. One minute and 17 seconds later, his wife pulls into a parking lot in Des Plaines en route to a dentist appointment. Twelve minutes and 32 seconds later, their son's school bus drops him off for the first day of fifth grade in Evanston.

It's just another Tuesday in the Transportation Analysis Simulation System (TRANSIMS), the software used by Argonne researcher Hubert Ley and his team at TRACC to simulate the "second-by-second movement of absolutely everybody during an entire day in the entire Chicago metropolitan area," as Ley puts it.

TRANSIMS tracks each of the 25.5 million automobile trips and millions of bus and train rides each day on Chicago's transportation grid, a vast network of roads that stretches from Kankakee north to Milwaukee and Lake Michigan west to Rockford.

Obviously, the program isn't psychic. TRANSIMS won't enable you to find out where Mayor Daley eats lunch or to make sure your spouse stops at the grocery store for eggs on the way home in the evening. Instead, the millions of "people" whose movements TRANSIMS follows consist of composites created by Ley from detailed census data that represent the inhabitants of metropolitan Chicago. This project provides an example of how basic research can work in the long run to improve the daily lives of millions.

This type of modeling, known in the transportation industry as "microsimulation," offers a number of advantages over older re-creations of the transportation grid that looked only at road capacities and typical loads. "It's not silly to wonder, 'why are we doing it this way? Why do we have to follow every single person at every single second if there are surely simpler methods?'" Ley said. "But the key is, although we can say 'there are 15,000 cars per hour on this road or 12,000 on that one,' only the new model can tell us if a car will turn left at the next intersection or keep going straight."

Although the results generated from microsimulation do not have a great deal of reliability at the level of a single street, the composite behavior of large numbers of synthetic "people" yields a thoroughly realistic representation of a typical day's traffic pattern in Chicago.

Ley's models work because they incorporate information compiled from surveys of Chicago-area residents that describe their movements during the course of an entire day, he said. Ley classifies the destinations of every trip gleaned from the survey as a particular "activity location," such as "work," "shopping," "school" or "home."

While TRANSIMS calculations are based on behavior patterns during a typical day, the detailed models of the traffic grid will enable researchers to better understand and anticipate likely bottlenecks during an emergency.

"It's a real challenge to try and use surveys of normal days to simulate behavior in emergency situations," said Argonne transportation researcher Young-Soo Park. "That's something that has not been done before and that we're only able to do through our micro-level simulation of individual cars."

pileups from the bottom up

There's carnage all over the road at the DOT's National

TRACC will become a hotbed of focused computation-based research in areas of critical importance to DOT.

Crash Analysis Center in Ashburn, Va. Plastic heads, legs and arms litter the asphalt tracks where transportation engineers ram Dodge Rams and roll over Range Rovers. But advanced numerical simulations conducted by Argonne and DOT researchers and run on TRACC's new supercomputer will reduce the need for hugely expensive and time-consuming real-life crash tests, while potentially saving thousands of lives—and crash-test dummies—a year.

Substituting accurate computer models for most real-world crash tests can save huge amounts of both money and time. "Maybe something goes wrong during one crash test and you don't get data, but in the end you've still wrecked a car or perhaps even several cars," said engineer Kulak, who leads TRACC's effort in computational structural mechanics.

The algorithms that TRACC uses to simulate car accidents work by breaking down a car's components into hundreds of thousands of small, but mathematically digestible, "finite elements." Each finite element, whether a little section of fender or air bag, is separately calculated, microsecond by microsecond, using LS-DYNA, an advanced simulation software package specifically designed to analyze complex physical problems and created by the Livermore Software Technology Corporation.

The crash then unfolds onscreen as the computer's 512 processors recombine the data from the separate finite elements. Each simulation typically involves between 500,000 and 2.4 million separate elements, Kulak said. The visualizations of the crash often show the cars as a collage of different colors—a navy front wheel well, a pink taillight, a maroon windshield—to indicate which processors contributed which calculations.

Kulak and his Argonne and DOT colleagues are able to perform these intricate simulations only because they have access to an enormous number of processors. A single run of a crash simulation using just the two processors of a powerful personal computer would take more than 17 hours, according to Kulak. TRACC's new computer, by contrast, can perform the same computations in roughly 20 minutes.

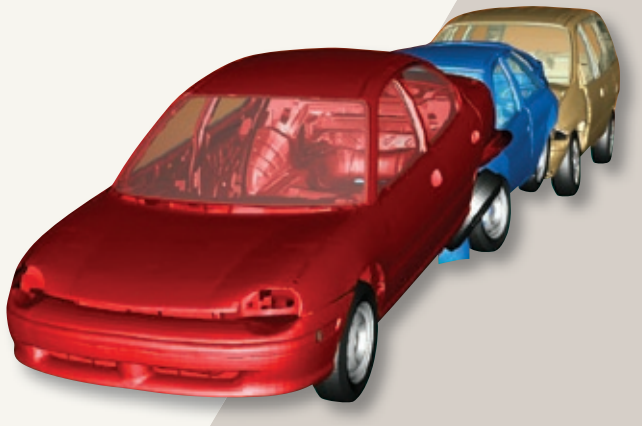
While TRACC is not the first organization to undertake crashworthiness finite-element analysis, Kulak and his colleagues at DOT hope to use the same methodology to study trauma suffered by passengers in motor vehicle collisions. "In the earlier days of crashworthiness testing, engineers only considered the damage to the vehicle," he said. "But eventually, they realized that what was important wasn't the vehicle, it was the occupants, like you and me."

Scientists who had previously tried to assess the impacts of crashes on drivers and passengers relied on simplistic representations of the human body. These early models treated each part of the body as a single entity, ignoring the complex interactions of bones, organs and soft tissues that occur during an accident.

While these re-creations provided scientists and engineers with important data and helped save lives, Kulak believes that finite-element analysis offers a more comprehensive and realistic picture of an accident victim because of its ability to incorporate biomechanical information.

With almost surgical precision, a finite-element model of a person partitions each part of the body—lung, wrist, heart, thigh, skull and others—and assigns tiny sections of them to individual processors. These processors then analyze the body's behavior during an accident and compile the data. To achieve this degree of fidelity, the simulations need to incorporate between five and ten million discrete elements, heavily taxing the capabilities of even the most advanced supercomputers, Kulak said.

For information, contact Dave Weber at 630 578 4241 or visit http://www.anl.gov/TRACC.

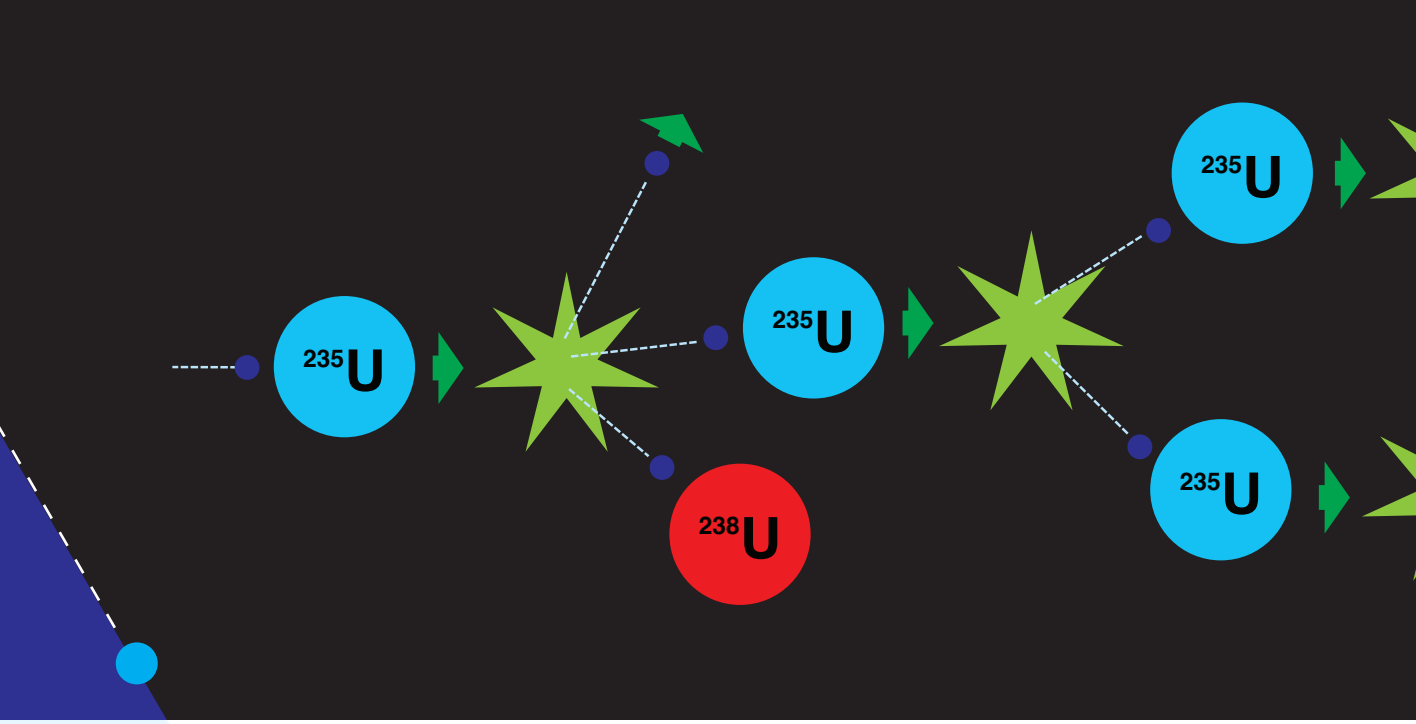


This screen shot of a three-dimensional finite-element model shows a three-car crash. In this type of simulation, separate processors compute the physics of small areas of each car but combine to determine the dynamics of the entire system.

booting up a new nuclear age

by Jared Sagoff

When it was founded in 1946, Argonne was charged with developing the technology to enable peacetime uses of nuclear energy. Now, more than 60 years later, Argonne again stands at the forefront of nuclear research as it brings its new high-performance computing facilities to bear on reactor design, enabling safer, cheaper and more efficient generation of electricity.



A fast-neutron nuclear reactor is called "fast" for a reason. The free neutrons in the reactor chamber travel at average speeds of more than 5,000 kilometers per second until they slam into uranium or other heavy nuclei, triggering the fission reaction that creates nuclear energy. But with an enormous number of neutrons zooming around and colliding with other particles, scientists have, until now, lacked the ability to tackle reactor dynamics from the ground up.

"At the fundamental level, we have a very good understanding of the neutron physics of a nuclear reactor, but we've never been able to represent all of its details at once," said Hussein Khalil, director of Argonne's Nuclear Engineering Division. "We need to resort to some models or equations that simplify the situation, but when you do that, you introduce errors and can't be completely confident that your model represents reality."

Computer models of reactors help to bridge the gap between conception and operation of new nuclear facilities. By using mathematical algorithms to process information — the reactor's geometry, composition, measured physical properties and targeted operating conditions — these models can predict how different reactors will function.

Because scientists cannot forecast exactly how a reactor will respond to variations in its configuration or the conditions under which it is operated, every nuclear facility has to be designed and operated with large safety margins, which reduces the efficiency of the plant. "The traditional tools have large uncertainties," said Andrew Siegel, an Argonne computational scientist and physicist who works at the nexus of the two disciplines. "These early models were coarse, and they represented only certain fundamental physics with a lot of assumptions and idealizations."

These old models were developed during the second heyday of nuclear research in the late 1970s and early 1980s. Back then, the stud of the supercomputing industry was the CRAY-1, a five-and-a-half-ton behemoth that could perform 100 million calculations (known to computer scientists as floating-point operations, or FLOPS) per second.

That kind of computing power far surpassed anything else available at the time, and nuclear scientists were among the first to requisition the CRAY-1's muscle for simulation work. As nuclear research fell out of favor with government and academic institutions that rationed supercomputing resources, however, other fields of study — such as astronomy and meteorology — replaced nuclear research as the preeminent uses of the available hardware. As a result, Siegel said, nuclear engineers today still have to rely on many of the design tools that resulted from work done on the CRAY-1 and machines with similar capabilities.

Although the CRAY-1's 100 megaflops capacity represented a remarkable accomplishment for the time, the nearly 30 years that have passed have seen the development of supercomputers that have made the CRAY-1 as scientifically relevant as an abacus. Last fall, Argonne became the new home of the IBM Blue Gene®/P supercomputer, which has the potential to perform at speeds of up to one petaflop — or one quadrillion calculations per second — representing a ten-million-fold improvement over the CRAY-1.

Argonne's newly acquired access to petascale-capable hardware, combined with three decades of accumulated scientific expertise, will revolutionize how scientists and engineers model nuclear reactors, Siegel said.

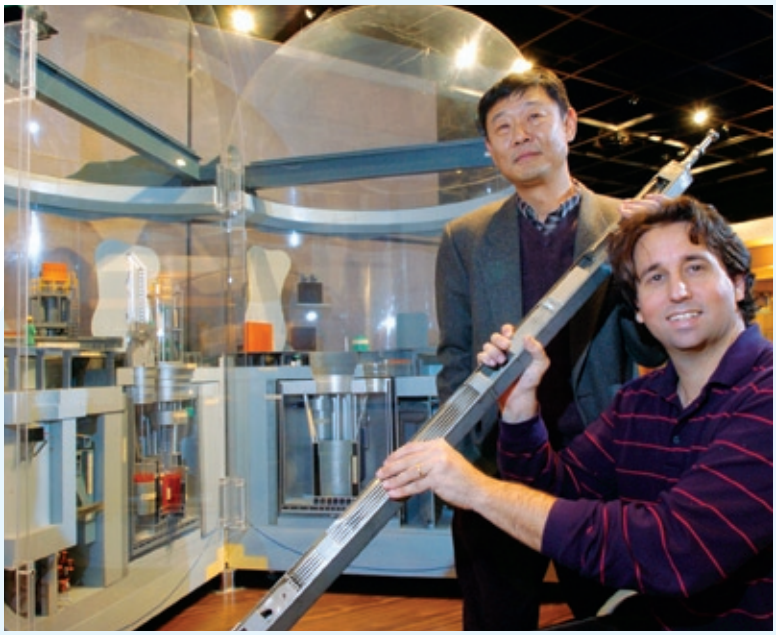
"Now, petascale computing allows us to create models that can explicitly represent a reactor's geometry," he said. "For the first time, we can resolve a great deal of the detail of what's happening in a reactor core — it's a

This diagram of nuclear fission shows a free neutron smashing into a uranium-235 atom, which releases atomic energy as it splits into large fission products and other free neutrons, which can then smash into other uranium-235 atoms, creating a chain reaction. Occasionally these neutrons hit non-fissile material, like uranium-238.

"For the first time, we can resolve a great deal of the detail of what's happening in a reactor core—it's a true paradigm shift."

true paradigm shift."

The core of a fast reactor consists of an assembly of stainless steel pins, which contain thin cylindrical rods of fuel composed of uranium or plutonium metallic alloys or oxides. Once the reactor gets going, these pins become extremely hot. In order to convert this heat to electricity and to prevent melting of the stainless steel, thousands of gallons of coolant—typically sodium—are washed over the pin bundles.



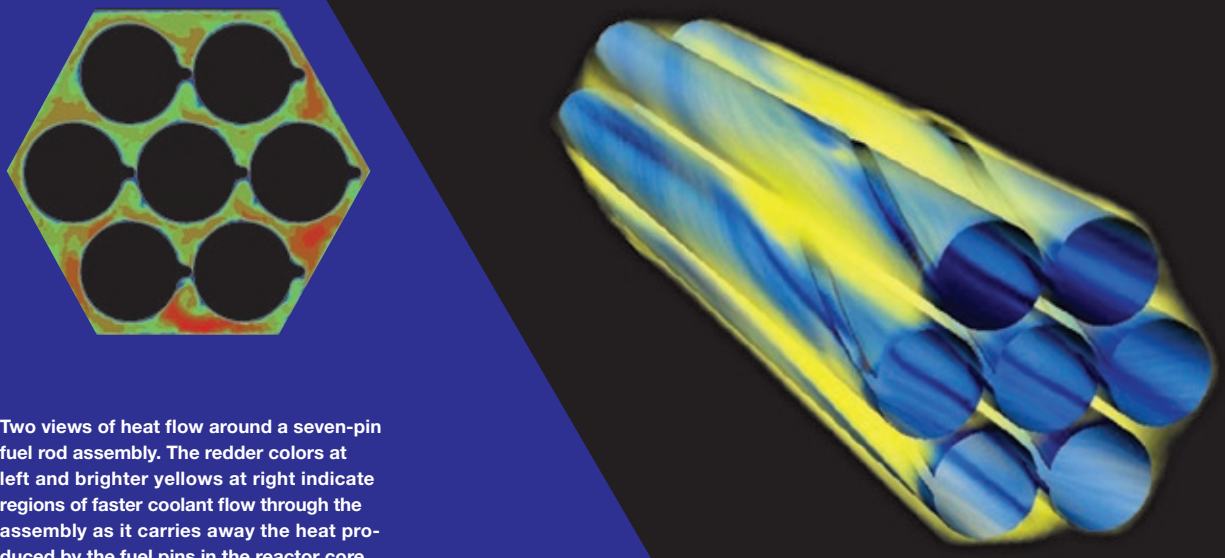
Physicist Won-Sik Yang and computer scientist Andrew Siegel hold a fuel rod assembly in front of a model of the Experimental Breeder Reactor-II, a landmark reactor built in 1964 at the old Argonne-West site in Idaho and operated for 30 years.

Altering the geometry of the pins even slightly, however, affects the neutron chain reaction and changes the dynamics of coolant flow and heat transfer. Because of the expense and potential safety concerns of testing different pin configurations experimentally, Siegel and his colleagues use computer simulations to model how the coolant flows around and between individual pins.

Reactors convert the uranium and plutonium inside each pin into energy through nuclear fission, which, when viewed at the atomic level, looks very much like a game of high-speed billiards. The "cue balls"—free neutrons—zoom around at mind-boggling speeds until they smack into uranium or other heavy nuclei. Instead of caroming off in a new direction, however, the nuclei absorb the free neutrons before splitting into a couple of lighter isotopes and more free neutrons, releasing energy. The newly freed neutrons then smash into other nuclei, continuing the chain reaction.

Millions of these collisions happen every microsecond in a fast-neutron reactor, and even with petascale-computing capabilities, nuclear scientists could not hope to represent every single one. Older models dealt with this problem not by analyzing discrete atomic events, but by treating them as continuous processes; this approach involved many assumptions and idealizations that simplified the physical realities, according to Khalil.

"What we hope to do with the more powerful computers," he said, "is actually begin the simulation at a very fundamental scale by building the model from the atomic level where the interactions are taking place. Obviously, we can simulate this degree of detail only for a very small portion of the system, but the hope is that



Two views of heat flow around a seven-pin fuel rod assembly. The redder colors at left and brighter yellows at right indicate regions of faster coolant flow through the assembly as it carries away the heat produced by the fuel pins in the reactor core.

we can then make use of this information to create a less-detailed — yet valid — model for the entire system." This research is funded by the U.S. Department of Energy's Office of Nuclear Energy to promote secure, competitive and environmentally responsible nuclear technologies to serve the present and future energy needs of the nation and the world.

To carry out this vision, Argonne's scientists base their neutron physics models on one of two types of mathematical algorithms: the Monte Carlo method or the deterministic method, according to Argonne nuclear engineer Won-Sik Yang. The Monte Carlo method, in its simplest form, involves the use of random mathematical snapshots of neutrons in the reactor, which are then integrated into a larger model of the system's behavior, a process somewhat akin to stop-motion animation.

While the deterministic method also attempts to integrate the neutron-nuclide interactions within a reactor, it does not use random numbers and will always produce the same output from given inputs. In order to remove the complexities of measured physical properties in the energy domain, deterministic models manipulate "bins" of neutrons that are grouped by energy level. Fast-neutron energies range from 1 electronvolt (eV) to 20 million electronvolts (20 MeV). Current deterministic models partition neutrons into many energy groups, the behaviors of which are calculated in several steps with different levels of spatial detail. This technique dramatically relieves the computational load while still closely describing the true character of the fission reactions, according to Yang.

"We can accurately determine the integrated qualities of the system with the Monte Carlo method," he said, "but it is still exceptionally difficult to get the local quantities with sufficient accuracy because of the many statistical fluctuations."

Because the Monte Carlo method relies on a stochastic approach, the move to the petascale will only slightly improve its performance in determining small localized quantities. However, the quantum leap in computing power will enable deterministic models to process a greater number of narrower energy bins and improve spatial resolution. "The goal is to eliminate approximation in proportion to advances in computing," Yang said.

With better models, scientists like Yang and Siegel hope to reduce modeling uncertainties and operate reactors just as safely while improving efficiency and driving down cost. "The new models provide answers in which we can have much more confidence," Siegel said. "The solutions produced by the Blue Gene/P can be directly translated into dollars saved in the operation of new reactors because we no longer have to put an enormous amount of space between what you thought the answer was and how wrong you might be."

Khalil added, "We hope that access to this technology will allow us to design higher-performance reactors and to operate them closer to their true performance capabilities."

In addition to shrinking needlessly large design and operation safety margins, these new, more flexible models could cut the costs of constructing and operating a nuclear facility even more by allowing researchers to substitute simulation for the once-obligatory experiments they performed to validate the results that the older, highly idealized models produced. "The problem is, when you do experiments, the parameters that you use are not universal," Siegel said. "So if you want to change any facet of your reactor design, you have to ask yourself, 'will my code be able to handle that, or do I have to do a new set of experiments?' With the introduction of advanced computing, for the first time the answer is likely to be that it can."

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did you know...

Argonne physicist Aneesur Rahman, known worldwide as the "father of molecular dynamics," pioneered the application of computer science to physical systems.

In 1960, Rahman successfully modeled the behavior of a cluster of 864 argon atoms on a computer that could perform only 150,000 calculations per second.

While Argonne's new IBM Blue Gene®/P supercomputer runs nearly 3 million times faster than Rahman's CDC 3600, today's scientists still base the code for their models on Rahman's algorithms.

Since 1993, the American Physical Society has annually awarded the Aneesur Rahman Prize for outstanding achievement in computational physics research.

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