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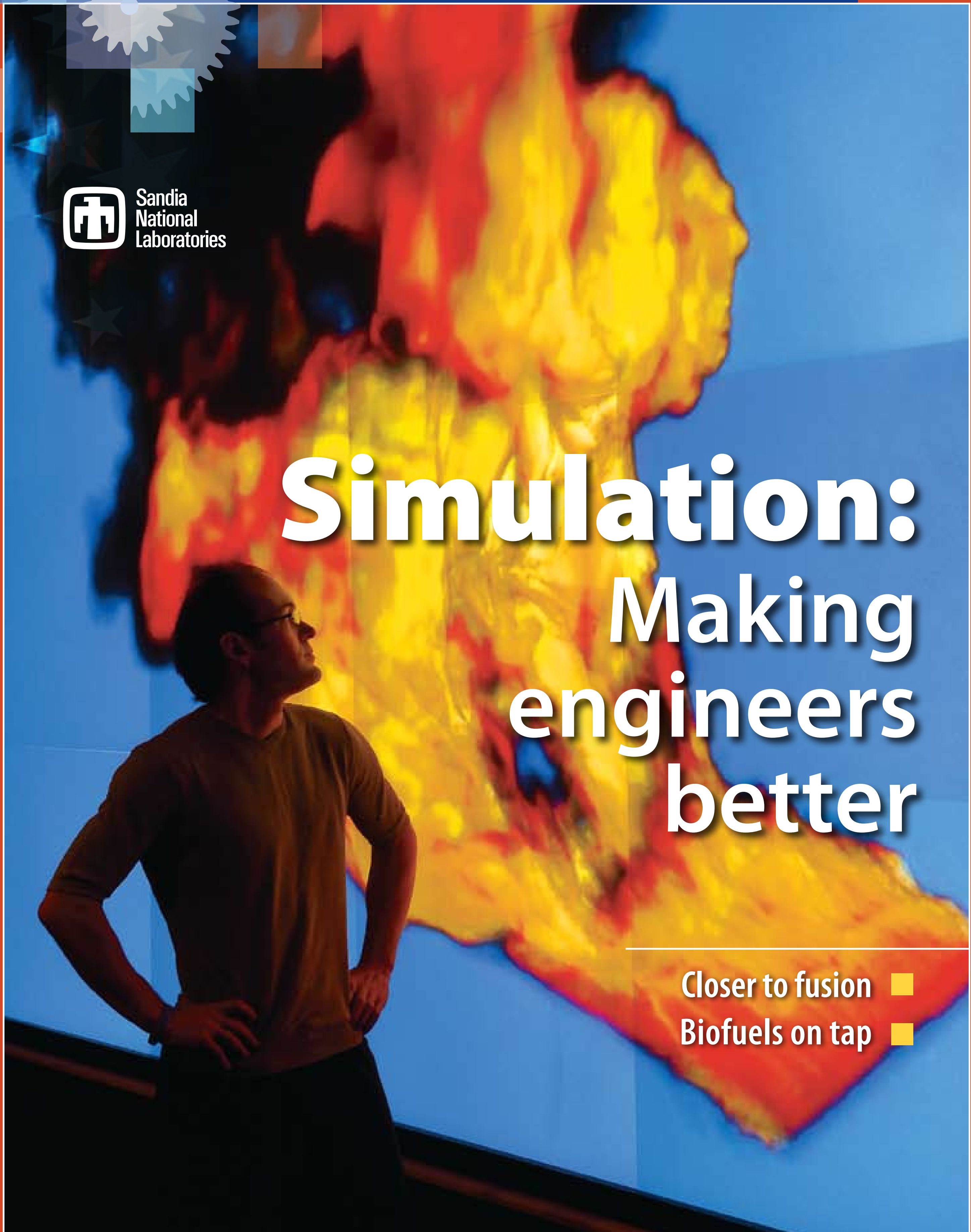

Simulation: Making engineers better

Closer to fusion

Biofuels on tap

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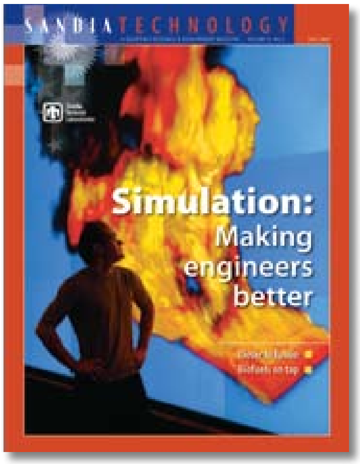
What is LDRD?

Sandia's world-class science, technology, and engineering work defines the Labs' value to the nation. These capabilities must remain on the cutting edge, because the nation's security depends on them. Sandia's Laboratory Directed Research and Development (LDRD) program provides Sandia the flexibility to invest in long-term, high-risk, and potentially high-payoff research and development that stretches the Labs' science and technology capabilities.

LDRD supports Sandia's four primary strategic business units: nuclear weapons; energy, resources, and nonproliferation; defense systems and assessments; and homeland security and defense. LDRD also promotes creative and innovative R&D by funding projects that are short term, discretionary, and often high risk, attracting exceptional research talent from across many disciplines.

When the LDRD logo appears in this issue, it indicates that at some stage in the history of the technology or program, LDRD funding played a critical role.

On the cover:



Stefan Domino studies a rendering of a simulated jet fuel fire in a cross wind displayed at Sandia's Joint Computational Engineering Lab. Running the 400 million-variable simulation occupied 5,000 processors for 24 hours on the Red Storm supercomputer. The simulation helped engineers prepare for a recent experiment at Sandia's Thermal Test Complex. *(Photo by Randy Montoya)*

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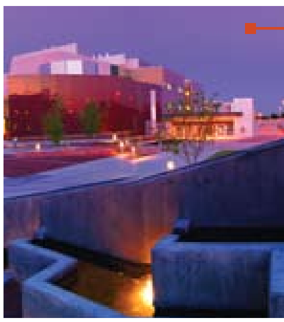


FROM THE EDITOR

Dear Readers,

Big experimental facilities, big computers, big physics, and big problems — when you put them together, as researchers at the national labs seem uniquely equipped to do, you get massive rewards. This month we look at projects in which the marriage of experimentation and simulation is making the engineer better:

- Alloys that are potentially stronger and lighter than today's metals (page 2)
- Electronics that bring us one step closer to electricity from seawater (page 5)
- A tougher long-range cannon for the U.S. Army (page 12)
- Enzymes that might make transportation fuels cheaply (page 13)
- Storage insights for the hydrogen age (page 20)

In pursuit of valuable new insights, guest contributor Hanchen Huang of the Rensselaer Polytechnic Institute calls for greater cross-fertilization between mathematicians and physicists, scientists and engineers, and experimentalists and modelers — as well as modeling that spans time and size scales (page 8).

Long before the I-35W bridge collapse in Minneapolis, a group of researchers who study the aging of metal structures — primarily aircraft — was working on better sensors to monitor the structural health of bridges and other infrastructures, as well as better repair techniques for those structures (pages 16-19).

Finally, on pages 10 and 11 we sample the colorful output of simulations. It's important to remember that these artful renderings signify physical phenomena involving millions, sometimes hundreds of millions, of variables interacting in time and space — in short, they represent substantial science in the service of national security. I hope you enjoy the issue.

John German
Sandia Technology Editor

Jason Jones and Tina Nenoff set up an experiment in a test cell at the Gamma Irradiation Facility. *(Photo by Randy Montoya)*

Metals for tomorrow

Researchers are trying to make better metal alloys using both supercomputer simulations to suggest molecular matches and radiation to synthesize nanoparticles.

Story by Darrick Hurst and John German

A Sandia research team is forging a new approach to making alloys with atomic arrangements that give the metals extraordinary properties.

By modeling on computers the complex chemical reactions that take place during the formation of nanoparticle clusters, and by using radiation to create the precise chemical conditions needed for clusters to form, the researchers believe they can construct alloys with such molecular exactness that the resulting bulk materials are stronger, lighter, and more corrosion-resistant than alloys made by conventional means.

Although the three-year project, funded by the LDRD program, is in its earliest stages, the exploratory research, if successful, could advance the science of creating alloys. That might revolutionize any number of products — aircraft engines, satellite structures, and consumer products such as bicycle frames and fuel-efficient automobiles, for example.

Cluster formation

An alloy is a material of two or more chemical elements, at least one being a metal, having properties different from its parent materials. Steel, for example, is stronger than iron, its primary component. Traditional alloy-making techniques typically involve heating and cooling, melting, annealing, tempering, and other metallurgical processes.

In the Sandia effort, the researchers start with a water-based solution into which they suspend, or dissolve, salt-like metallic particles, which are the alloy's seed ingredients. The unique twist in the work, says chemist Tina Nenoff, is the use of radiation to break up the water molecules and interact with the metal salts to produce metallic particles in a highly reactive soup.

"We're trying to form the perfect reaction conditions so the metal ions in the solution can start joining together to form clusters of nanoparticles," she says.

In these conditions, the ions begin to form metallic clumps, which then combine to form larger and highly regular alloy structures.

Transient states

The team is focusing its research on the science that happens in the "novel metastable phase spaces" — transient states of matter — that are not accessible with traditional alloy production methods such as melting, says Nenoff. Understanding these stages is important for determining what alloys are created and how they form.

Photo courtesy of Steel Industry Heritage Corporation

"The method of synthesis we're studying — known as radiolysis — breaks down the water structure allowing it to react with metal salts to form nanoparticles, a synthetic approach that is flexible and versatile for making large quantities of nanoparticle compositions that can't be easily created otherwise," she says.

Two unique Sandia experimental facilities, the Gamma Irradiation Facility and the Ion Beam Materials Research Lab, provide the radiation environments needed for the research. In them, target solutions are subjected safely to a variety of controlled radiation exposures.

Following irradiation the samples are studied using spectroscopy and microscopy to understand what effects time and experimental variables have on particle formation, size, shape, and composition.

Depending on the combination of reactants, dose, and dose rate of radiation, researchers have been able to create nanometer-sized particles of various metals, including gold, in a variety of shapes including spheres, rods, and pyramids. The synthesis principles they are testing may become building blocks for essentially defect-free alloys.

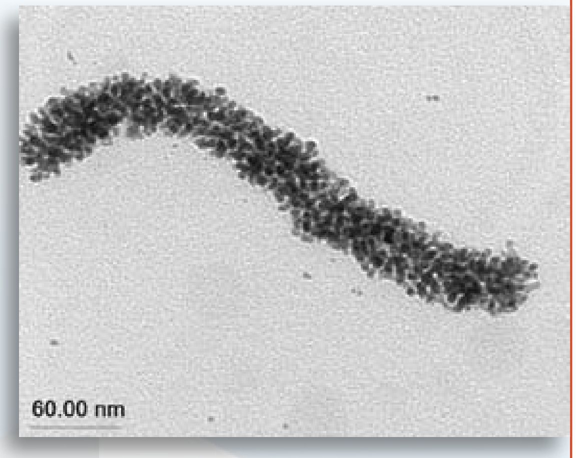
Synthesis by design

The results of the experiments are being translated into computer simulations. Kevin Leung is leading an effort to use atomistic models, along with other methods, to interpret and understand the controlling factors in cluster formation — to determine if and why certain compositions form, and to suggest promising molecular compositions.

Because the simulations involve modeling the electronic structures and various charge states of complex particles, as well as the reorganization of attached particles and water molecules around formative clusters, they are large problems requiring the use of Sandia's high-performance computers.*

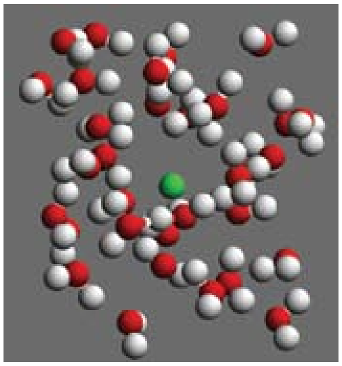
"We'll simulate the structure of the nanocrystal initiation right after radiation has been applied," Leung says. "By examining the interface between metal clusters and nearby molecules, we will be able to understand what factors govern the size of these nanocrystals at the initial stages of formation and how the radiolysis affects clustering."

"The calculations are telling us which nanoparticle compositions will be energetically more favorable than others," adds Nenoff. "We attempt to synthesize those nanoparticles and compare notes with the modeling predictions. By developing our understanding of the basic materials science behind these nanoparticle formations, we'll then be able to expand our research into other classes of materials."

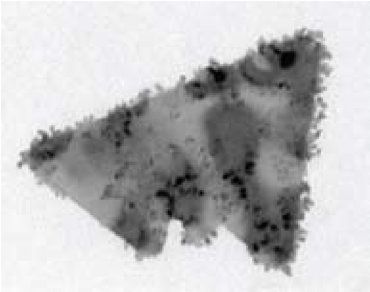


Nenoff adds that because of the novel techniques being used by the team, success of the project is not assured. "Improving on centuries of metallurgy won't be easy," she says. "But using computers to model these processes may mitigate some of the risk."

* The simulations have used Sandia's Spirit, Liberty, and Shasta computer clusters. Future simulations might be run on Sandia's supercomputers.



Desktop simulation depicting the early stages of radiolysis-assisted growth of metal nanoclusters. The radiolysis yields isolated atoms of gold or nickel within water molecules.



Gold nanoparticle crystal (above, approximately 30 nm across) and cluster (left, approximately 300 nm across) formed using radiolysis.

Gamma Irradiation Facility

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NEWS NOTE

Officials participating in the ceremonies included (from left) NNSA Administrator Tom D'Agostino, Sandia President and Laboratories Director Tom Hunter, U.S. Senator Pete Domenici, and DOE Deputy Secretary Clay Sell.

The heart of the space in which MESA's three buildings are located. *(Photo by Bill Doty)*

Fini! MESA complete

The largest project in Sandia's history is complete.

In an Aug. 23 ceremony at Sandia, top officials of the Department of Energy, the National Nuclear Security Administration (NNSA), and Congress signaled completion of the Microsystems and Engineering Sciences Applications (MESA) complex.

The 400,000-square foot complex consists of a Microfabrication Facility, a Microsystems Laboratory, and a new Weapons Integration Facility. Taken together, the complex contains optical, electrical, fluidic, visualization, and computer laboratories, as well as workspace for more than 600 scientists and engineers.

The Weapons Integration Facility, occupied in July, was the last facility in the MESA complex to be completed.

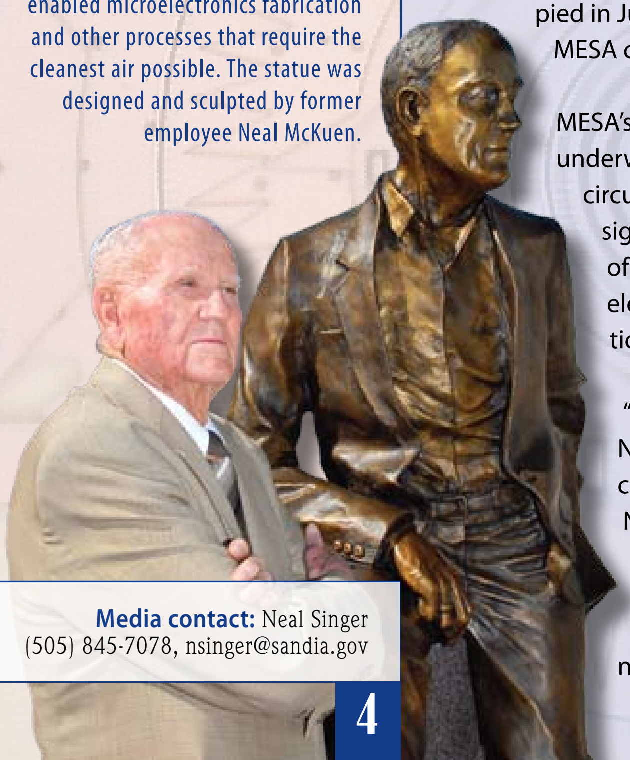
MESA's initial mission, already underway, is to produce electronic circuits and computer chips designed to withstand high levels of radiation. These "hardened" electronics are critical to national security needs.

"The MESA complex provides NNSA with a capability you can't find anywhere else," said NNSA Administrator Tom D'Agostino. "With the technology developed here, anything from our country's nuclear weapons to communications satellites will be able to withstand the worst of conditions."

Beyond its security role, MESA's combination of high-performance computing simulations, scientific research, and production capabilities in electronics and optics at the micro and nano level will make it a world leader in a new type of simulation-led engineering that will ultimately improve the quality of consumer goods.

"MESA uniquely provides a design environment and combines the power of the world's most powerful computers with the development of small, smart things that are integrated into applications of unlimited potential," said Tom Hunter, Sandia's president and director. "There is no other place like it. We are proud the nation chose Sandia for this investment."

The eight-year, $516 million MESA project was completed three years ahead of schedule and $40 million below budget.



A brass likeness of Willis Whitfield was unveiled during the ceremonies. In the early 1960s, while at Sandia, Whitfield discovered how to remove particles from air to create a dust-free environment, an advance that enabled microelectronics fabrication and other processes that require the cleanest air possible. The statue was designed and sculpted by former employee Neal McKuen.

MESA MicroLab

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One step closer to fusion power

Story by Neal Singer

Sandia's Z machine, when it fires, is already the largest producer of X-rays on Earth and has been used to produce fusion neutrons. But rapidly repeating firings, necessary for future fusion power plants, had not been thought achievable until now.

Bill Fowler tests circuits on a device capable of producing large electrical impulses rapidly and repeatedly.
(Photo by Randy Montoya)

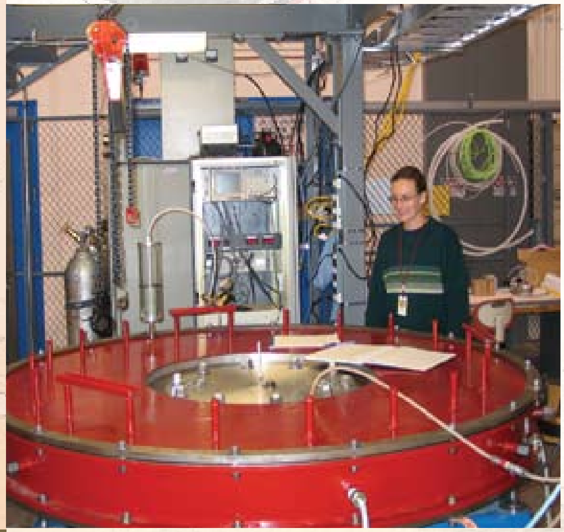
An automobile engine that fired one cylinder and then required hours to fire again wouldn't take a car very far. Similarly, a fusion machine intended to provide humanity unlimited electrical energy from cheap, abundant seawater can't fire once and quit for the day. It must deliver energy to fuse pellets of hydrogen a number of times per minute and keep that pace up for millions of shots — a kind of an internal combustion engine for nuclear fusion.

A new electrical circuit that should carry enough power to attain the long-sought goal of controlled high-yield nuclear fusion also meets the other, equally important requirement for sustained fusion energy: It can fire every 10.2 seconds in brief, powerful bursts.

"This is the most significant advance in primary power generation in many decades," says Keith Matzen, director of Sandia's pulsed power center. The circuit would replace the large capacitors used today in Sandia's pulsed power Z machine, called Marx generators, that store electrical energy and release it in microseconds to Z's center. There, pellets are compressed by X-rays generated by the electromagnetic forces.

Made in Russia

The new system, called a linear transformer driver (LTD), was created by researchers at the Institute of High Current Electronics in Tomsk,



Sandia's high current LTD laboratory

Russia, in collaboration with colleagues at Sandia. The circuit has undergone preliminary validation at Sandia.

The circuit is about the size of a shoebox. Tightly packed in groups of 20 in a circular container, and electrically connected in parallel, the aggregate of the circuits, called a cavity, can transmit a current of 0.5 megamperes at 100 kilovolts. A test cavity at Sandia has fired without flaw more than 13,000 times.

Because the cavities are modular, they can be stacked like donuts on a metal stalk. Arranged thus, they could generate 60 megamperes and six megavolts of electrical power, enough (theoretically) to generate high-yield nuclear fusion within the parameters necessary to run a power plant.

The next-generation cavity model, now being tested in Tomsk, transmits 1.0 megamperes at the same voltage and with the same rapidity. Five such units have been built; four have been purchased by Sandia and one by the University of Michigan. They, too, are performing without flaw.

New technology advantages

The new switch would eliminate the need for the hundreds of thousands of gallons of insulating water and oil in which the present Z structure is submerged. The switch would achieve this in part by eliminating Z's huge plates and extensive wiring, all of which generate magnetic fields.

Because of the proximity of the working components, there are few magnetic fields to slow the passage of current. Thus, linking the components in parallel decreases resistance and adds voltages. This allows for a powerful machine to fire very rapidly, with only a thin layer of oil bathing the rings and rows of switches.

The LTD technology is 70 percent more efficient than current Z machine firings, in terms of the ratio of useful energy out to energy in, says Matzen.

Funding for Z historically has been for defense purposes. Its experiments have been used to generate data for high-energy physics simulations on supercomputers that help maintain the strength, effectiveness, and safety of U.S. nuclear weapons.*

A powerful LTD machine would better simulate conditions created by nuclear weapons, so that

Russian scientist Boris Kovalchuk (Institute of High Current Electronics, Russia, in gray suit) demonstrates design of a new LTD system to Sandian Dillon McDaniel (left) and Tomsk pulsed power head Alexander Kim.

* Not only does modeling and simulation (of high-energy physics phenomena) benefit from experiments done at the Z machine, modeling also has played a major role in the design and integration of Z — ranging from simulations run on desktop computers that have helped design interior electric circuits and improve the performance of magnetically insulated power transmission lines, to a model of an LTD-based power plant demonstrating how such a plant could generate a fusion reaction every 10 seconds. An animation of the power plant model is available for viewing at www.sandia.gov/news/resources/releases/2007/rapid-fire-pulse.html

data from the laboratory-created explosion of a Z firing could be used with greater certainty in computer simulations. The U.S. has refrained from actual testing of nuclear weapons for 15 years.

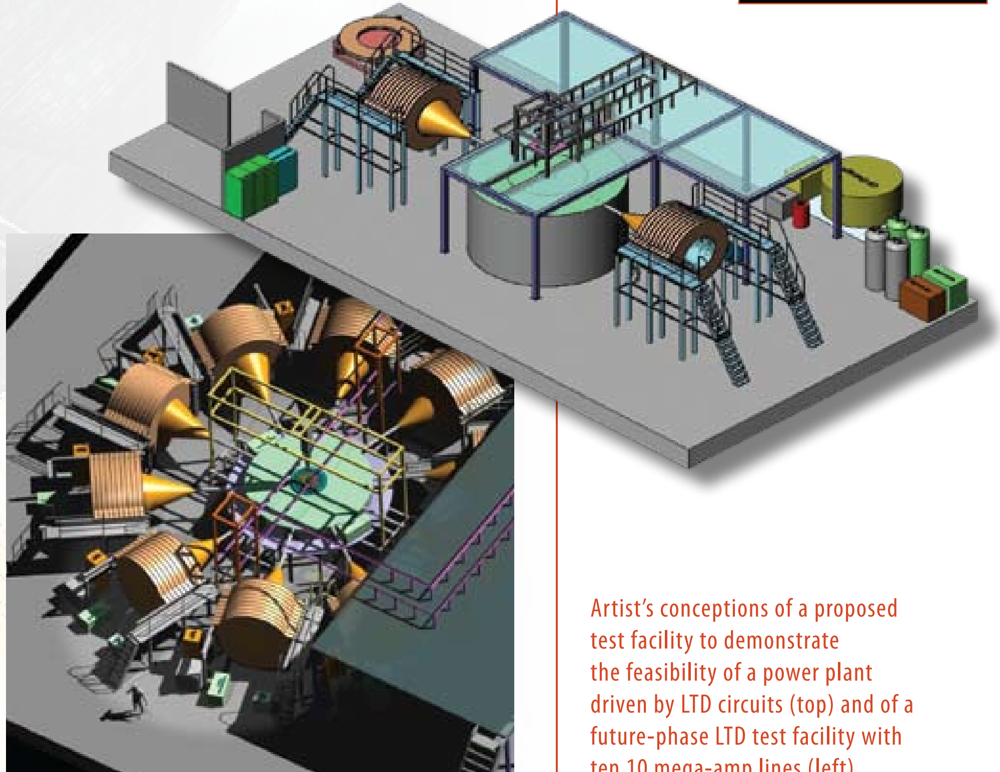
Overshadowed approach

For electricity-generation purposes, the repetitively firing fusion approach at the Z machine, known as inertial confinement, historically has been overshadowed by the technique called magnetic confinement — using a magnetic field to enclose a continuous fusion reaction from which to draw power.

But fired repeatedly, the revamped Z machine could well form the basis of a fusion energy plant. To confirm the new Z concept would cost $35 million over five to seven years using a test bed with 100 cavities. If successful, future generations of Z-like facilities would be constructed with LTDs.

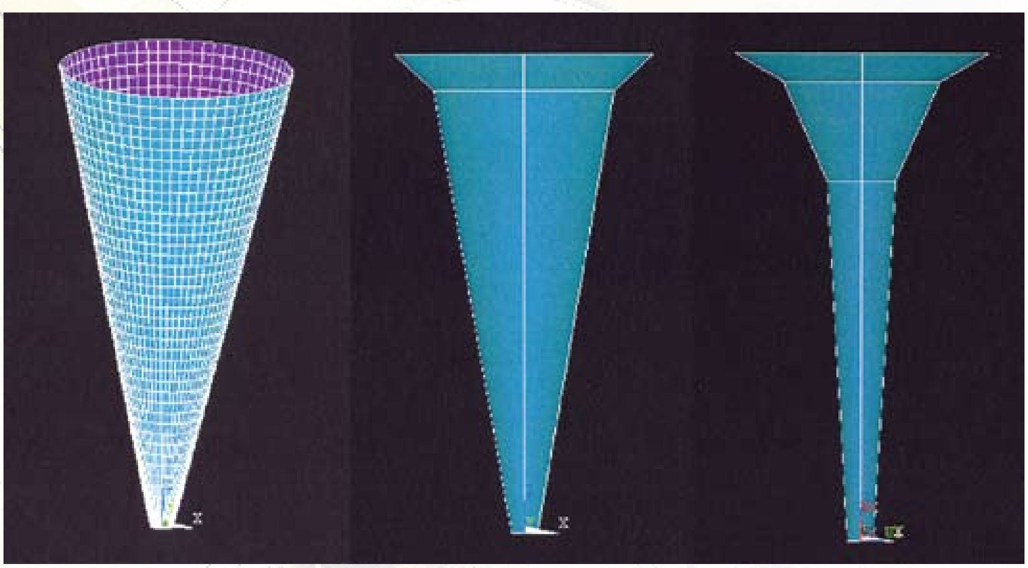
Funding thus far has come from two U.S. congressional initiatives, Sandia's LDRD program, and Sandia's inertial confinement fusion program.

"We think we need 60 megamperes to make large fusion yields," says Matzen. "But though our simulations show it can be done, we won't know for certain until we actually build it."



Artist's conceptions of a proposed test facility to demonstrate the feasibility of a power plant driven by LTD circuits (top) and of a future-phase LTD test facility with ten 10 mega-amp lines (left).

The device was designed by Tomsk pulsed-power head Alexander Kim, with the switch developed by Boris Kovalchuk. The work was led at Sandia and Tomsk by Sandia's Mike Mazarakis. Sandia has filed a U.S. patent application on a high-power pulsed-power accelerator invented by William Stygar that can use an LTD as the primary power generator to replace the conventional Marx generator.



Simulations provide design options for strong but low-mass recyclable transmission lines (RTLs), which focus power flow in an LTD accelerator. Small RTLs have been fabricated, tested, and modeled at Sandia.

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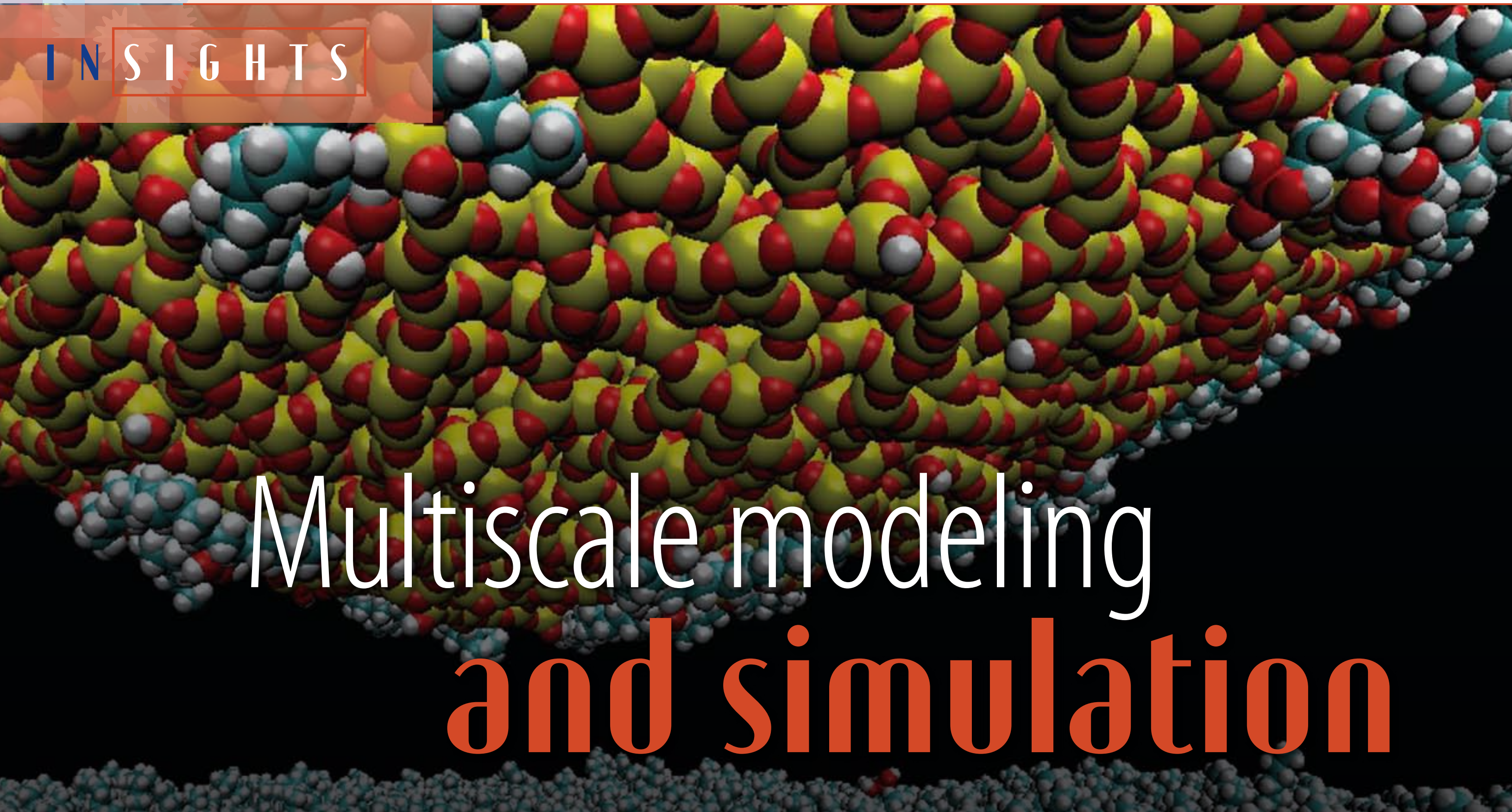


Multiscale modeling and simulation

By Hanchen Huang
Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute

Modeling and simulation will continue to play an important role in science and technology as engineers tackle problems over multiple scales — from very large problems involving engineered machines or durations of years (or longer) to very small problems involving phenomena of matter occurring in an instant.

Large machines, such as airplanes and nuclear reactors, are many meters in size and operate for many years, yet their performances depend on the fundamental mechanics of atoms and electrons. This dependence is even more pronounced for machines made of nanostructured materials. Therefore, modeling and simulation of engineering problems must address multiple scales in both size and time.

To fully realize the greatest potential of multiscale modeling and simulation in science and technology requires synergies in three aspects.

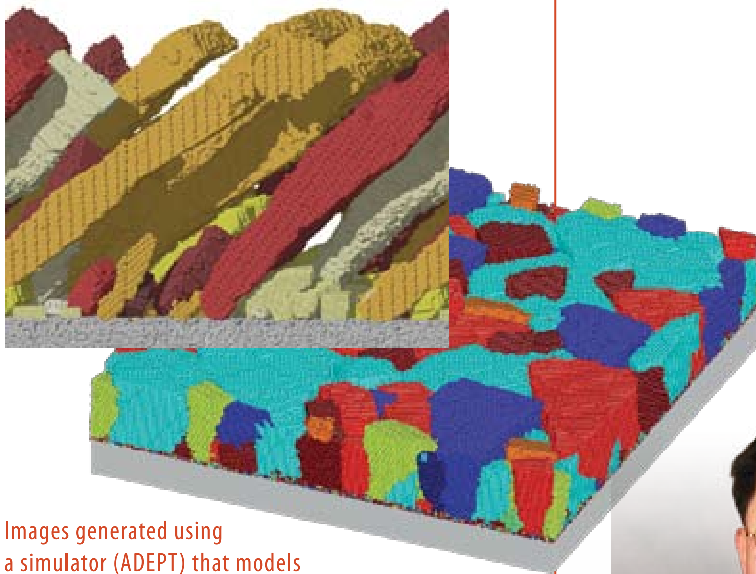
The first synergy is among researchers of mathematical and physical (or biological) sciences. The advancement of modeling and simulation methods relies on smart mathematics for realization in computers, and on physics for meaningful representations of reality. Professional societies such as the U.S. Association of Computational Mechanics and federal agencies such as the National Science Foundation (NSF) have actively promoted cross-fertilization between computational mathematicians and physical scientists. Continuing and strengthening such cross-fertilization will be very beneficial.

The second synergy is between scientists and engineers, and it has been in practice among the modeling and simulation teams at the U.S. Department of Energy national laboratories. The integration of mission-oriented engineering research and discovery-oriented scientific exploration maximizes the potential impacts of multiscale modeling and simulation.

The third synergy is between modelers and experimentalists. The term “computer experiments” may have been coined with good intentions. However, modeling and computer simulations offer their greatest potential when accompanied by experimental validation or when motivated by experimental observation. The engagement of experimentalists in multiscale modeling and simulations deserves particular attention and cannot be overemphasized.

Augmenting these synergies is computational capacity. Having the world’s eight most powerful computers, the U.S. should undoubtedly be in the leading position. Indeed, supercomputers such as Red Storm at Sandia and the IBM Blue Gene at Rensselaer Polytechnic Institute have proven to be enabling tools for multiscale modeling and simulation.

Equipped with the three synergies and the necessary computational capacity, the modeling and simulation community will be in a good position to address the challenging issues of both time and size scales. The issue of multiple time scales is probably the most challenging and can also be the most rewarding. The issue of multiple size scales has been the focus of intensive efforts, and the moment is ripe for the transition from demonstration of methods to their application in realistic engineering environments.

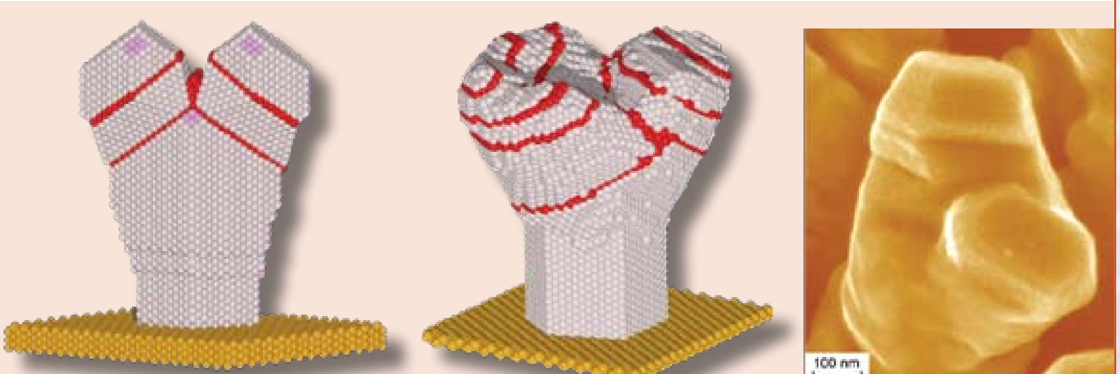


Images generated using a simulator (ADEPT) that models fabrication processes at the atomic level, in real time, and in three dimensions. Shown are renderings of textured nanocolumns (left) and a thin film structure (right).

(Reference: Huang, Texture Evolution during Thin Film Deposition, in Handbook of Materials Modeling, Springer Science and Business Media, 2005)

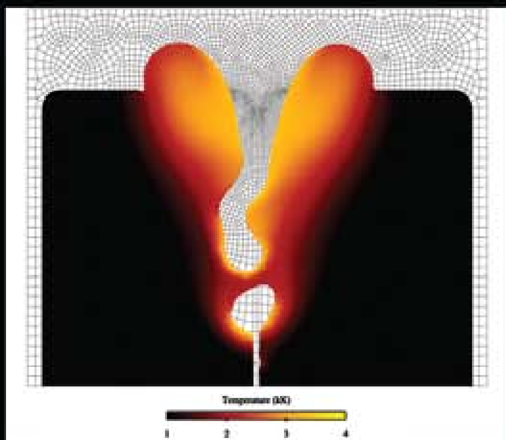
Although its full potential has yet to be realized, modeling and simulation has an important future role in the advancement of science and technology. Its impacts should be at three levels. At the first level, it provides interpretation to experimental tests and observations. At a higher level, it offers insights to scientific and engineering exploration. At the highest level, multiscale modeling and simulation is predictive and leads to scientific discovery and science-based engineering and design.

Hanchen Huang is professor of mechanical and nuclear engineering at the Rensselaer Polytechnic Institute. His research group studies the evolution of nanostructures during fabrication, mechanical deformation, radiation exposure, and aging. The research relies on atomistic simulations augmented by experimentation. With more than 90 published journal papers to his name, Huang is considered an authority in computational science that makes use of experimental insights. He has been an invited speaker at more than 50 conferences and university seminars, has served as guest editor of several materials-related publications, is an assessor of research proposals for the National Science Foundation, Department of Energy, and several other science organizations, and is co-chairman of the U.S. Association for Computational Mechanics’ Nanotechnology Committee. He holds a Ph.D. in applied plasma physics and fusion engineering from the University of California at Los Angeles. (www.rpi.edu/~huangh)

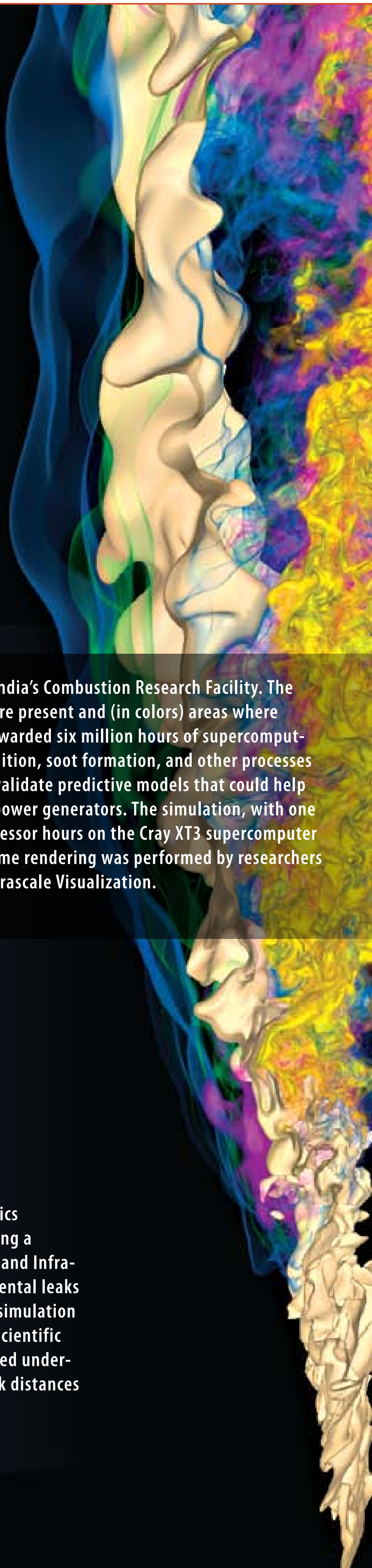


These RPI images, showing self-organized branching that occurs during materials synthesis, illustrate science-based conceptualization (left), a rendering based on predictive simulation (center), and experimental validation (microscopy image, right).

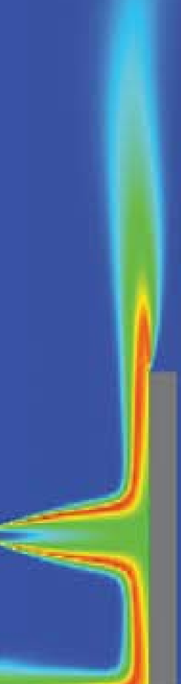
(Reference: Wang, Huang, Kesapragada, and Gall, Nano Letters 2005)



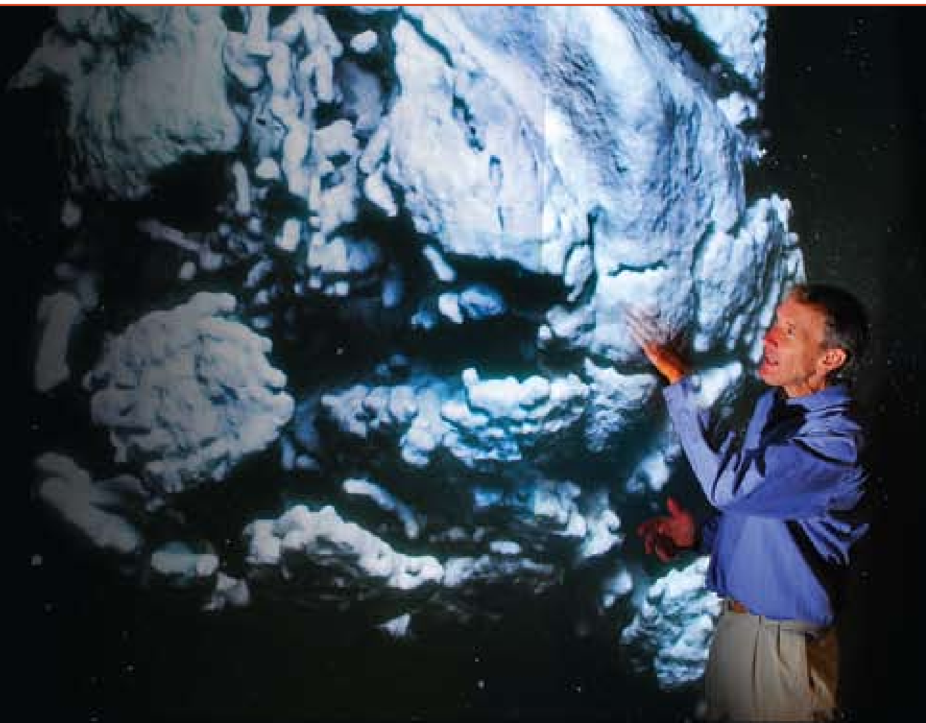
Two-dimensional rendering of a laser "keyhole" weld showing areas where the microstructure of a part's metal is affected by the laser's heat. Laser keyhole welding helps weapons engineers create deep penetrating welds in heat-sensitive components with minimal damage to neighboring materials. This desktop simulation, which resolved a few hundred thousand unknowns, employed Sandia's GOMA multiphysics finite element code, which is unique in its ability to model solids, fluids, and gases as well as phenomena such as capillary forces, melting, and solidification.
Contact: Randy Schunk, prschun@sandia.gov



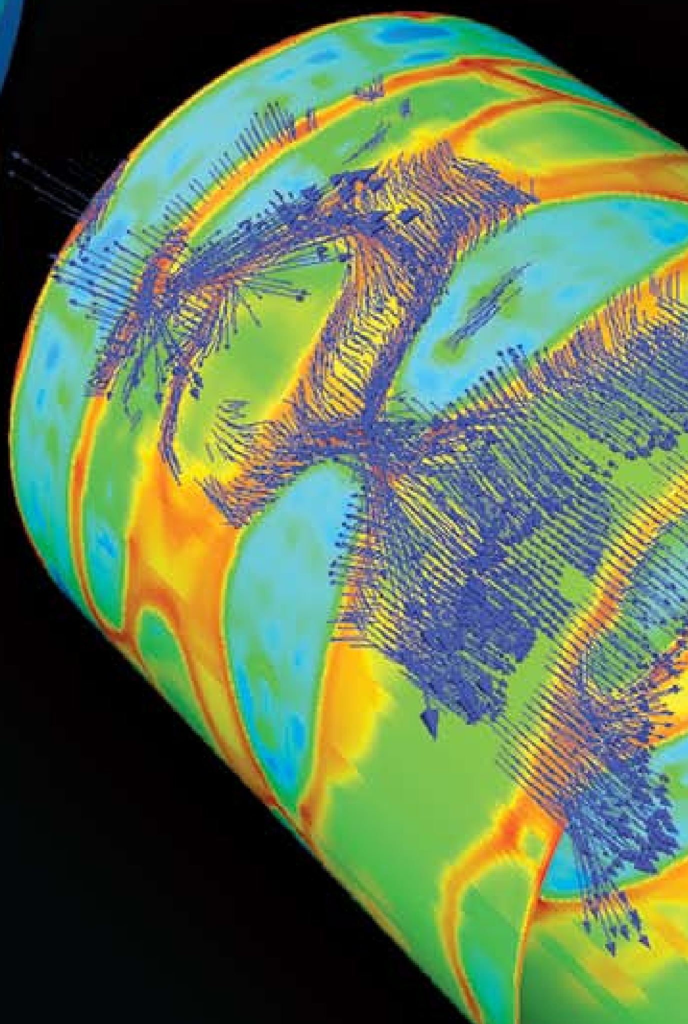
Turbulent hydrogen-air flame from a simulation created by a research team at Sandia's Combustion Research Facility. The 3-D rendering shows (in gold) areas where ideal proportions of fuel and oxygen are present and (in colors) areas where autoignition is taking place. The Sandia group, led by Jackie Chen, recently was awarded six million hours of supercomputing time by DOE's Office of Science to simulate flame stabilization, extinction, ignition, soot formation, and other processes in turbulent flames. Data produced in the project are being used to develop and validate predictive models that could help engineers design future fuel-efficient combustion engines for vehicles and lean power generators. The simulation, with one billion grid points and detailed hydrogen-air chemistry requiring 2.5 million processor hours on the Cray XT3 supercomputer at Oak Ridge National Lab, is the world's largest combustion simulation. The volume rendering was performed by researchers at DOE's Science Discovery through Advanced Computing (SciDAC) Institute for Ultrascale Visualization.
Contact: Jackie Chen, jhchen@sandia.gov



Infrared test photo (above) and cross-section view of three-dimensional fluid dynamics simulation of an ignited hydrogen jet striking a barrier wall (left). Sandia is conducting a combined experimental and modeling program, funded by DOE's Hydrogen Fuel Cells and Infrastructure Technology Program, to characterize and predict the consequences of accidental leaks at high pressure hydrogen-vehicle refueling stations. The rendering is from a FUEGO simulation validated using test data. The FUEGO code was developed as part of DOE's Advanced Scientific Computing program to characterize fire environments for weapons safety. An improved understanding of flame behavior in a variety of leak scenarios is helping determine setback distances and barrier designs for future hydrogen filling stations.
Contact: Chris Moen, cmoen@sandia.gov



Physicist Mark Boslough describes the simulated destruction of asteroid Golevka, a half-kilometer-diameter body discovered in 1991 and studied by radar from various observatories. The simulation models a hypothetical 10 megaton explosive detonation at the asteroid's center. Built from topographical radar data, the model renders one billion computational cells and required 14 hours on 7,200 computational nodes on Sandia's Red Storm supercomputer to process. Building and testing the model helped Sandia refine high-energy shock physics codes used in nuclear weapons work. In addition, says Boslough, it explored options for near-Earth asteroid deflection.
Contact: Mark Boslough, mbboslo@sandia.gov *(Photo by Randy Montoya)*



Modeling and simulation has played a major role in the design of Sandia's Z machine. Here a simulated tungsten Z-pinch wire array under magnetic pressure becomes a plasma and implodes towards Z's center. Colors superimposed on the cylindrical surface represent degrees of plasma density. Dark blue arrows are current-density vectors showing current flowing around areas of low density (light blue). The simulation, which is helping researchers better understand Z's performance, used Sandia's ALEGRA radiation-magnetohydrodynamic code. It was run for six days on 512 processors on Red Storm.
Contact: Tom Mehlhorn, tamehlh@sandia.gov

Less shock, more awe

When designers working on a new high-caliber cannon system for the U.S. Army encountered a problem during testing, Sandia researchers proposed an adjustment that helped preserve in the cannon's design a unique laser ignition system.

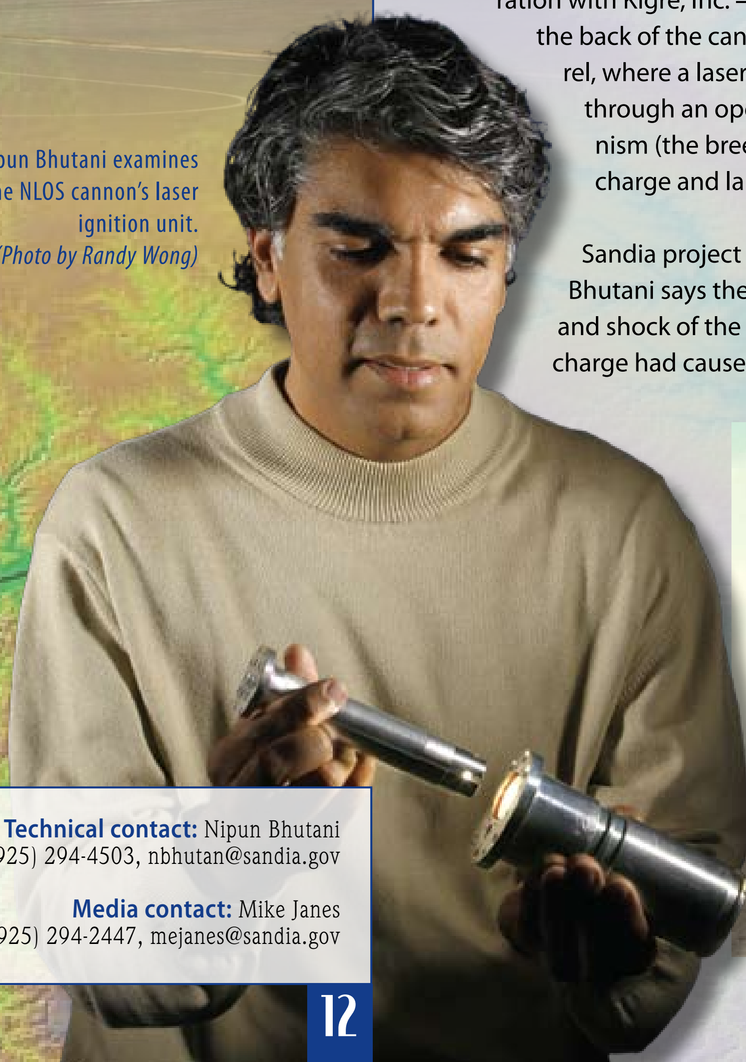
The weapon system, known as the Non-Line-of-Sight Cannon (NLOS cannon), is part of Future Combat Systems (FCS), a key Army modernization program. The completed artillery system will be self-propelled, fully automated, capable of firing six rounds per minute, and lightweight and compact enough so three of the vehicles can be carried aboard a C-17 cargo plane.

Its laser ignition unit — developed by the Army's Armament Research, Development, and Engineering Center (ARDEC) in collaboration with Kigre, Inc. — is mounted on the back of the cannon's gun barrel, where a laser beam is fired through an opening mechanism (the breech) to ignite a charge and launch a shell.

Sandia project manager Nipun Bhutani says the recoil force and shock of the artillery discharge had caused an increase in observed failures during early prototype testing. Instead of abandoning the laser ignition concept in favor of a traditional mechanical ignition system, the Army called in Sandia experts in shock effects on critical components.

To absorb the force of the discharge, Sandia proposed a new vibration isolation system between the laser and the breech that results in much lower shock levels to the ignition system. Lab researchers also applied the Labs' modeling and experimental capabilities to harden the laser igniter. This involved modeling the physics associated with the gun loads and other dynamics inside the ignition system as the cannon is fired. The modeling required the use of dozens of computing nodes for 24 to 36 hours at a time on Sandia's Shasta, Liberty, and Spirit clusters.

BAE Systems is developing the NLOS system as part of an FCS program led by Boeing and SAIC. Sandia, in collaboration with BAE Systems and ARDEC, is developing the vibration isolation system.



Nipun Bhutani examines the NLOS cannon's laser ignition unit. *(Photo by Randy Wong)*

The NLOS Cannon, developed by BAE Systems, will fire six rounds per minute. *(BAE Systems image)*

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Biochemist Joanne Volponi prepares enzyme samples for assaying. *(Photo by Randy Wong)*

Biofuels on tap

Story by Mike Janes

Biofuels such as ethanol could help blunt future crude oil shortages, especially if scientists can, with the help of computers, make enzymes capable of breaking down plant material and converting it to liquid fuel very efficiently.

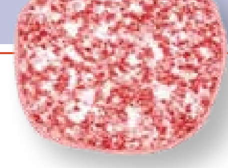
Buried beneath a sulfurous cauldron in European seas lies a class of microbes known as extremophiles, so named because of the extreme environment in which they live and thrive. In the hot, acidic neighborhoods of undersea volcanic vents, some of the world's most unusual forms of life make their homes.

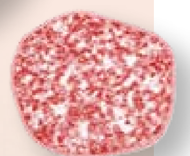
Rajat Sapra examines assays for the screening of engineered enzymes that show increased activity and stability at acidic conditions and high temperatures. *(Photo by Randy Wong)*

Not surprisingly, such hardscrabble organisms possess enzymes — the chemical workhorses of cells — with similarly unique and useful abilities: They break down cellulose into sugars with remarkable efficiency.

Such enzymes are interesting to researchers studying ways to make biofuels from plant materials — called lignocellulosic ethanol — cheaply. If the enzymes can be enlisted to do much of the chemical deconstruction work, they might unlock a new transportation economy based on ethanol derived from candidate plants other than corn.*

A Sandia group led by Blake Simmons is among a handful of U.S. research teams studying extreme enzymes' utility for ethanol production. Sponsored by Sandia's LDRD program, the project will demonstrate computational modeling tools and enzyme engineering methods that could lead to more efficient biofuel processing techniques. The effort is in its second year.





Sulfolobus solfataricus microbes
(Courtesy of Kenneth Stedman, Portland State University)

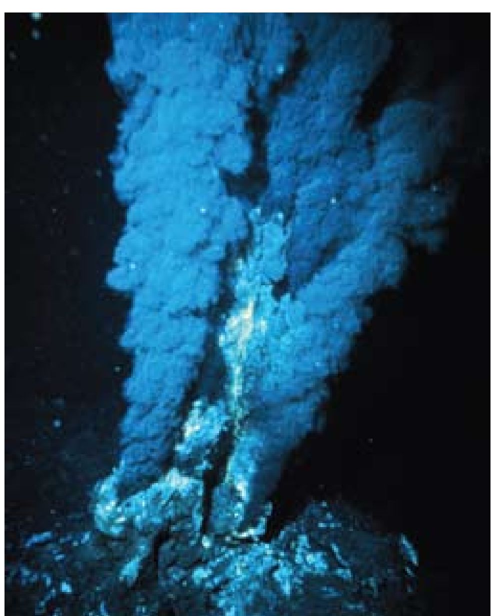
Waste as fuel

Lignocellulose, one of the most abundant renewable organic materials on Earth, is a mix of complex sugars and lignin that gives strength and structure to plant cell walls. To produce fuel ethanol, lignocellulose is, with the help of enzymes or acids, broken down and converted to glucose, or sugar. The glucose is then fermented to produce ethanol and carbon dioxide.**

Because of their chemical simplicity, starchy plants such as corn are the easiest to convert to biofuel. Corn, however, is an important source of food and agricultural feed, so large-scale production of ethanol from corn is not seen as a long-term solution to the world's burgeoning fuel demands.***

Ideally other sources of lignocellulose, such as the billion-plus tons of biomass created annually as byproducts of the timber and agricultural industries, could be converted to fuel instead. This could alleviate the economic pressure on the corn industry (and perhaps lower corn and meat prices) imposed by the growing demand for corn-derived fuel ethanol.

The primary hurdle preventing plant-derived ethanol from becoming a viable transportation fuel is not the availability of biomass, but rather its efficient and cost-effective processing, says Simmons.



Deep-sea hydrothermal vent
(Courtesy of U.S. National Oceanic and Atmospheric Administration)

"Unfortunately, you can't just take a tree trunk, stick it into an enzymatic reactor, and ferment the sugar produced into ethanol with any kind of efficiency," he says. "The process of turning certain lignocellulosic materials into ethanol is very difficult and costly."

That process typically involves several pretreatment steps that break up the initial lignocellulosic material into easily converted biopolymers, such as cellulose, for eventual fermentation.

Quirky microbes

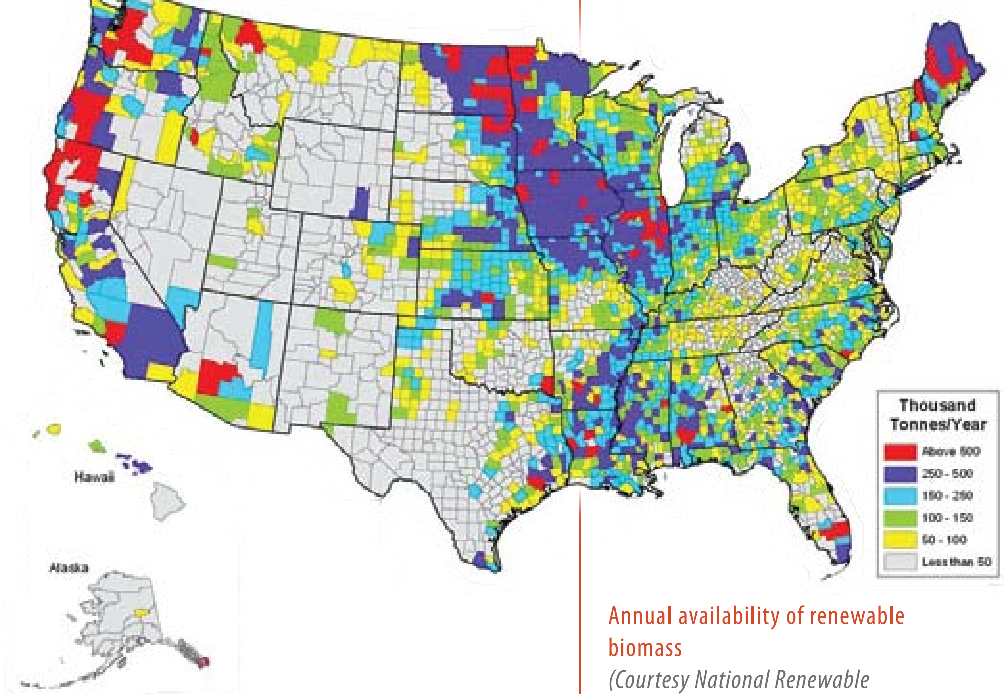
Enzymes isolated from extremophiles might help solve this processing problem. Such microbes — from an ancient branch of microbial life, the archaea, discovered by scientists in 1977 — can be found in a variety of places, including hot springs, deep-sea heat vents, gold mines, and within the rust found under a leaking hot water heater. Some can live without sunlight or carbon as food, and instead survive on sulfur, hydrogen, and other materials that normal organisms can't metabolize.

While other researchers are examining common biomass sources and attempting to express their enzymes at higher temperatures and lowered pH, Sandia has, in effect, taken the opposite approach.

"Instead of trying to create an extremozyme from sources that live in rather benign environmental conditions, why not just manipulate a real one isolated from its natural state?" asks Simmons.

Sandia's current microbe of interest is *Sulfolobus solfataricus*, an organism that prospers in high temperature sulfuric acid environments and expresses enzymes that efficiently break down cellulose into sugars.

Using samples of the DNA that produces these extreme enzymes, the researchers are modifying the enzymes' genetic sequence with the goal of improving performance.



Annual availability of renewable biomass
(Courtesy National Renewable Energy Laboratory)

Candidate mutations are identified through computational modeling performed at Sandia that compares the structure and sequence of the extremozymes with their more benign counterparts to identify key genetic patterns.

The computational modeling has helped the researchers focus on those predicted changes to the genetic sequence that, if a matching enzyme was created in the lab, would have the best chances of improving performance.

"The ultimate dream — and it's only a dream right now — would be to take a poplar tree, put it into a tank, let it sit for three days, then come back and watch as the ethanol comes pouring out of the spigot," says Simmons. "Though we're probably decades away from that, this project aims to consolidate the pretreatment steps and get us one step closer to realizing that vision."

Realistic goal

While various researchers are investigating new technologies and facilities that will allow for processing cellulosic biomass into ethanol, Simmons and his team are hopeful that their method can be efficiently and cheaply integrated with current and future pretreatment steps.

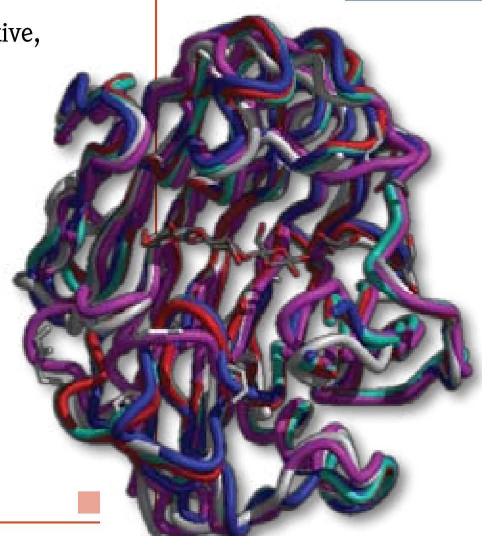
"We believe the use of enzyme engineering to enable the next generation of ethanol bio-refineries, with a focus on improving enzymes isolated from extremophiles, is a realistic and achievable goal," he says.

The project is a component of the Joint BioEnergy Institute (JBEI), a partnership of three national laboratories (including Sandia/California) and three research universities in the San Francisco Bay Area, funded by the U.S. Department of Energy's Office of Science.

JBEI researchers will tackle key scientific problems that hinder the cost-effective conversion of lignocellulose into biofuels and other important chemicals. They also will develop the tools and infrastructure to accelerate future biofuel research and production efforts, and help move new technologies into the commercial sector.

Sandia's JBEI focus will be cost-effective, biologically based renewable energy sources to reduce U.S. dependence on fossil fuels. The Lab's capabilities in enzyme engineering, systems biology, membrane transport, protein expression, and hyperspectral imaging are expected to contribute to the JBEI mission.

For more information about JBEI, visit www.jbei.org.



Modeling is helping researchers identify beneficial changes to an enzyme's genetic sequence.

* In 2006, 13.5 billion gallons of ethanol was used worldwide, with nearly two-thirds of that produced from Brazilian sugar cane or U.S. corn crops.

** Much of the gasoline dispensed in the U.S. is a blend of petroleum and ethanol. Half of Brazilian automobiles are able to run on pure ethanol.

*** A July 2007 report by the National Petroleum Council, "Facing the Hard Truths About Energy," concludes that crude oil supplies won't keep up with global demand for transportation fuel in the next 25 years, and other fuels, including ethanol, will be needed to close the gap.

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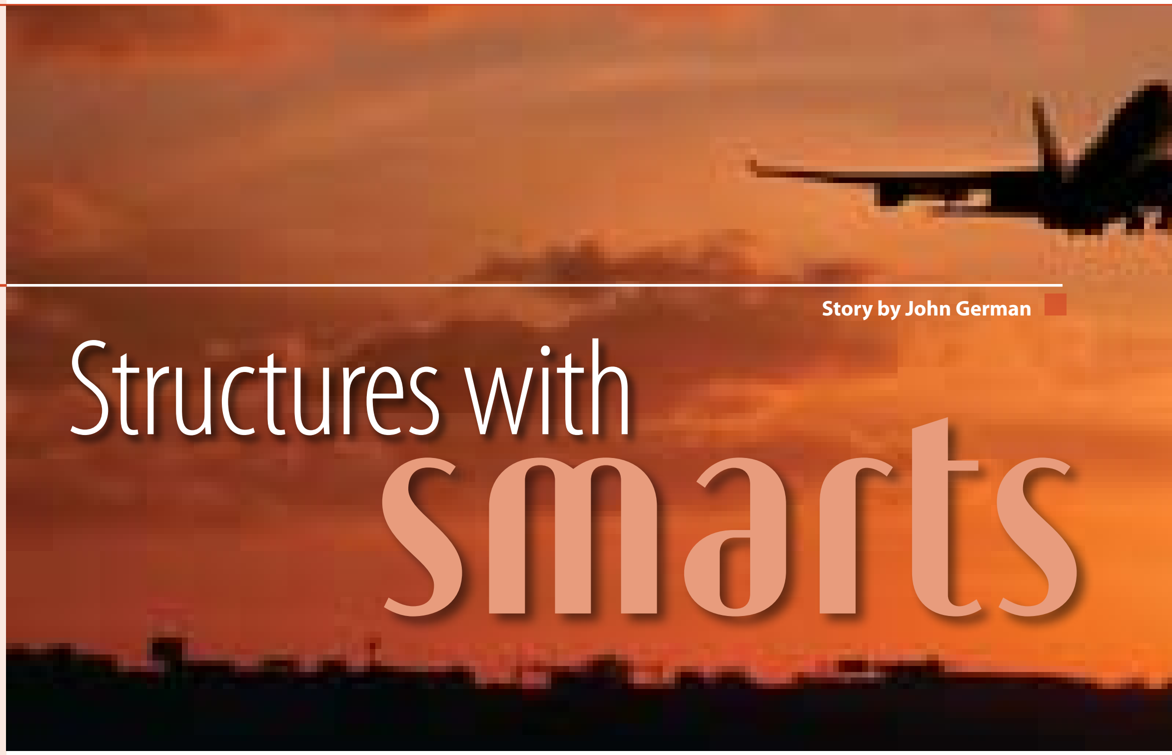


Story by John German

Structures with smarts

The airliner of tomorrow, laden with sensors, might check itself for the effects of aging and notify ground crews at the first sign of wear and tear. Full-time monitoring would improve safety and, perhaps, lower the cost of air travel. It also might head off failure of other metal structures.

Takeoffs and landings, cabin pressurizations, rapid temperature changes, moisture, and turbulence all take a toll on the skin and structure of a commercial aircraft. Over time these repeated stresses can cause tiny cracks and other flaws to form that can, if not remedied, grow into more serious defects.

To find and repair flaws in their earliest formative stages, the airlines schedule inspections at maintenance facilities, where human inspectors aided by high-tech scanners go over each aircraft inch by inch looking for the consequences of aging.

Future commercial jets might be fitted with networks of sensors that watch continuously for the initial signs that defects are forming. Like nerve endings in a human body, these in situ, or permanently installed, sensors offer levels of vigilance and sensitivity to problems that periodic checkups cannot.

Such full-time monitoring could supplement, reduce, or even eliminate scheduled structural inspections, says Dennis Roach, who leads a Sandia team that is evaluating some of the first sensors for structural health monitoring, or SHM, for aircraft and other safety-critical equipment.

"With sensors continually checking for the first signs of wear and tear, you can restrict your maintenance efforts to when you need human intervention," he says.

Rising costs

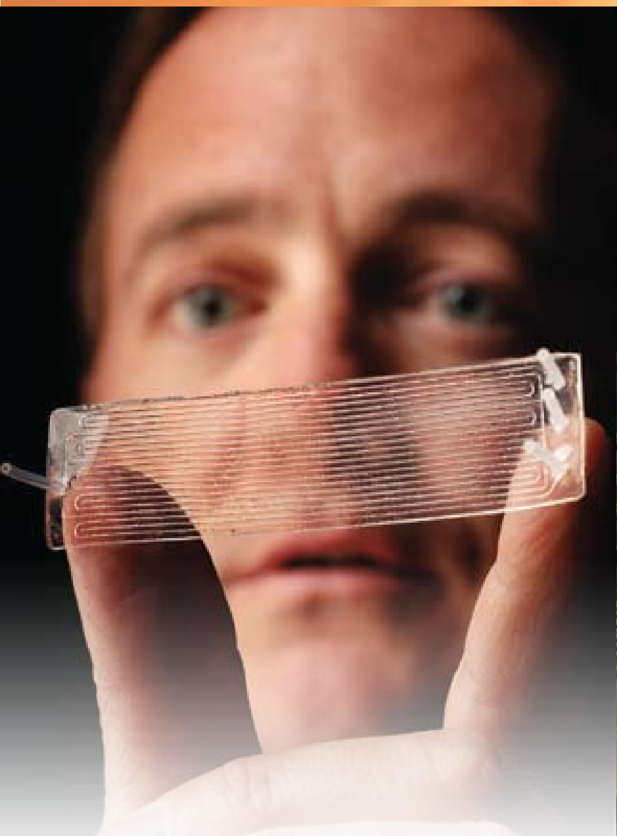
Cracks are just one form of airframe defect. Using nondestructive inspection (NDI) tools that help them locate defects in hard-to-reach places without dismantling the aircraft, inspectors also encounter metal-to-metal adhesive failures, material erosion, impact damage, and corrosion, to name a few.

Sandia's Airworthiness Assurance Program for years has focused on development and evaluation of NDI technologies for defect detection in aging aircraft.

Every day a commercial aircraft isn't flying costs the company tens of thousands of dollars, costs that are eventually passed on to the air traveler.

Aircraft maintenance and repairs now represent about a quarter of the U.S. commercial airline fleet's operating costs, and those costs are rising as aircraft in the fleet age, many well beyond their design lifetimes, he says.

Sensors could monitor the health of a number of safety-critical structures.



Dennis Roach with a Comparative Vacuum Monitoring sensor showing galleries etched into the sensor's underside. *(Photo by Randy Montoya)*

"Airline passengers want safe and reliable transportation at a reasonable price," says Roach. "The aviation industry is continually seeking technologies and processes that enhance aircraft safety and reduce costs."

In a retired jet at Sandia, Dennis Roach and Ciji Nelson prepare SHM sensors. *(Photo by Randy Montoya)*

First acceptance

Initially, full-time monitoring sensors are envisioned for hot spots where flaws are expected to form. Eventually the work could lead to "smart structures" with many sensors that would self-diagnose and signal an operator when repairs are needed.

The Sandia team already has developed or evaluated several types of inexpensive, reliable sensors that can be retro-fitted into aircraft structures for SHM.

One promising candidate, called a Comparative Vacuum Monitoring (CVM) sensor, is a self-adhesive rubber patch, ranging from dime- to credit-card-sized. The rubber's underside is laser-etched with rows of tiny, interconnected channels or galleries to which an air pressure is applied. Any propagating crack in the material under the sensor breaches the galleries and the resulting change in pressure is monitored.

The sensors, made by Structural Monitoring Systems, Inc. (SMS) of Australia, are inexpensive, reliable, durable, and easy to apply, says Roach. They also provide equal or better sensitivity than is achievable with conventional inspection methods, he says.

Boeing recently included CVM technology in the Boeing Common Methods NDI Manual, which allows airlines to work with Boeing and

In situ sensors can be mounted on an aircraft structure.

Full-time monitoring would improve aircraft safety.
(NTSB photo)

the FAA to seek certification of the sensors for specific applications on specific aircraft.

Growing demand

Boeing's acceptance was the culmination of a comprehensive, two-year validation program by Sandia in cooperation with the FAA, SMS, a number of U.S. airlines, and the University of Arizona. Work on additional applications for Southwest, Northwest, and Delta Airlines is under way.

To help address the growing demand for standardized SHM procedures and certification requirements, Sandia helped form the Aerospace Industry Steering Committee for Structural Health Monitoring in November 2006. The international group includes manufacturers, regulators, government agencies, the military, and universities.

The Sandia team also continues to seek acceptance for SHM outside the aerospace industry. Besides aircraft, SHM techniques could monitor the structural well-being of spacecraft, weapons, rail cars, bridges, oil recovery equipment, buildings, armored vehicles, ships, wind turbines, nuclear power plants, and fuel tanks in hydrogen vehicles.

A technician inspects the belly of a Boeing 737.

Kirk Rackow looks for cracks on the tail section of a retired helicopter using a nondestructive inspection device called an eddy current sensor.
(Photo by Randy Montoya)

"Any structure that operates in a fatigue environment with cyclical stresses or other structurally-degrading environment could benefit from frequent sensor monitoring rather than relying only on scheduled inspections," Roach says.

Smart structures

In the future, members of a ground crew might plug a diagnostic system or laptop into a port on the aircraft and download structural health data collected during flight. Ultimately an integrated network of sensors could monitor not only structural materials but also the health of electronics, hydraulics, avionics, and other systems.

The Sandia researchers already are using computerized prognostic and health management software to help them recognize the first signs of fatigue in large metal structures, says Roger Hartman, manager of Sandia's Infrastructure Assurance and NDI Department.

"You begin to evolve a systems approach to making important infrastructure elements safer and more reliable," Hartman says.

"When we set out to do NDI, in the back of our minds we knew that eventually we wanted to create smart structures that 'phone home' when repairs are needed or when the remaining fatigue life drops below acceptable levels," adds Roach. "This is a huge step in the evolution of NDI."

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Stronger than steel

Underneath a New Mexico highway overpass, on either side of an I-beam that supports the bridge, are two composite-fiber patches, each about the size of a car's license plate, installed by Sandia engineers.

The patches represent a successful repair job on a small crack that had formed in the steel beam. Sandia installed the repair on the bridge earlier this year.

The demonstration is an outgrowth of Sandia's decades of work, sponsored by the Federal Aviation Administration, to develop and evaluate technologies that extend the service lives of aging aircraft. The repair demonstration was funded by the LDRD program.

The stronger-than-steel composite repair technique is performing well, says Sandia project lead Dennis Roach, whose team is monitoring the repair over time using embedded sensors that watch for signs that the crack is growing.

The patches — a fast, inexpensive alternative to steel plates or more extensive repairs — are made of flexible, fiber-reinforced composite material adhered to the steel's surface. Produced as a thin tape, the material comprises strong, parallel boron fibers enmeshed in epoxy.

Layers of the tape are successively applied with an adhesive, forming a multilayer laminate. The finished repair is a fraction of an inch thick and much stronger than a typical riveted steel patch of comparable thickness.

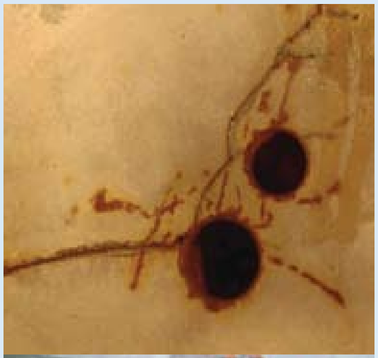
Composite doublers are corrosion resistant and lightweight and can be readily formed into complex shapes without machining.

Bonding composite patches to a metal structure, rather than bolting on a traditional steel patch, also eliminates the need to drill fastener holes that decrease the structure's strength and can act as new crack-initiation sites, says Roach.

Composite patches have gained acceptance in the commercial aviation sector as strong, flexible, lightweight repairs for commercial aircraft. More recently, the Sandia team has been evaluating and testing similar techniques for a variety of other safety-critical structures.

"This project took a technology developed for aircraft repair and applied it to massive steel structures where safety is of utmost concern," says Roach. "While lower-strength fiberglass has been used to repair concrete, this is the first application on a steel superstructure."

Crack in a bridge's I-beam



Bridge repair

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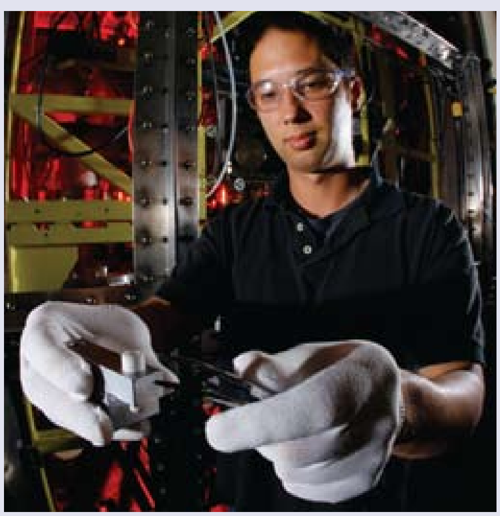
NEWS NOTE

Dan Dedrick handles a complex metal hydride being considered for storage of hydrogen. *(Photo by Randy Wong)*

Filling up with hydrogen

If hydrogen is to be the future fuel of choice for automobiles, researchers must first answer a number of questions associated with its handling and storage.

As part of a three-year, $2 million Department of Energy-funded project, Sandia is developing computational models to better predict the behavior of materials that would be used to store hydrogen in automotive fuel tank systems.



Aaron Highley prepares a metal hydride sample for analysis. *(Photo by Randy Wong)*

Advanced metal hydrides and other chemicals being considered for hydrogen storage absorb and hold hydrogen within their molecular structures and release it when subjected to heat. But hydrides can react when exposed to air and moisture, says principal investigator Dan Dedrick.

The researchers want to know under what conditions, exactly, metal hydrides will react with air and water. They are asking how the materials will perform under normal and accident conditions, as well as after the materials age. And they need to predict the materials' behaviors during manufacturing.

As part of the effort, Sandia will conduct experiments to understand reaction processes. Data gathered in the experiments will be used to build computer models. Through experiments and modeling, the team expects to develop validated computational tools that can predict the behaviors of advanced metal hydrides in a variety of scenarios.

Sandia was one of six institutions that in August received DOE funding for applied hydrogen storage research. In related projects, Sandia is examining ways to lessen the consequences of a leak at a hydrogen filling station (see images on pages 10-11) and reduce the time it would take to fill a metal hydride-based hydrogen fuel tank, among other work.

Sandia leads the DOE Metal Hydrides Center of Excellence and, since 2003, has worked with General Motors in a four-year, $10 million project to develop and test tanks that store hydrogen in a metal hydride medium.

For more information:
www.ca.sandia.gov/hydrogen

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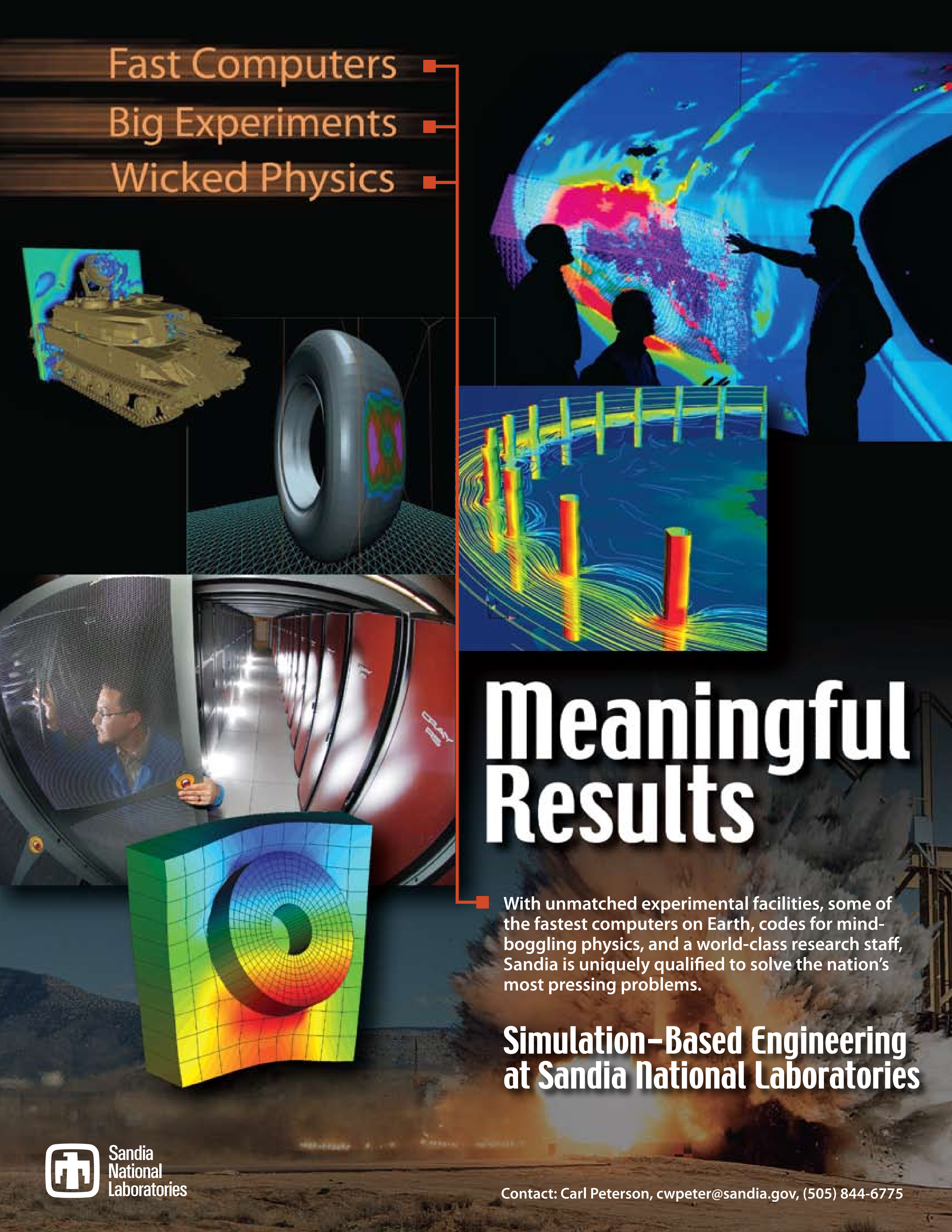
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"Modeling and computer simulations offer their greatest potential when accompanied by experimental validation or when motivated by experimental observation."

Hanchen Huang

Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute

Sandia National Laboratories

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