

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

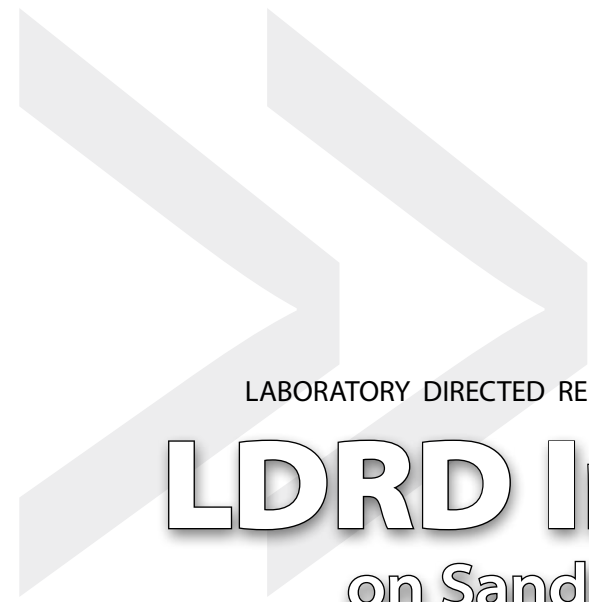
LDRD Impacts

on Sandia and the Nation





ABOUT THE COVER:
Images from some of the case studies in this brochure: a near-UV light-emitting diode (LED), a cell membrane, a NISAC model, synthetic aperture radar (SAR) image of Washington, D.C.



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Sandia National Laboratories' Laboratory Directed Research and Development (LDRD) Program: Value to the Nation

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**Vice President of Science, Technology, and Engineering,
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Inherent to Sandia National Laboratories' Laboratory Directed Research and Development (LDRD) program are the two strategic goals of nurturing our workforce's core science and technology (S&T) expertise and supporting Sandia's national security missions. In these contexts, LDRD investments often provide the stimulus, sometimes the blueprints, and occasionally even the explicit methodologies for the innovative technical solutions that shape our nation's defense, security, and economic well-being. As Sandia's sole discretionary research and development (R&D) program, LDRD is foundational to the future of the Laboratories' ability to provide "exceptional service in the national interest."¹ Sustaining exceptional service implies ongoing, uninterrupted discovery and innovation against the backdrop of a world whose only certainty is change.

The impact of LDRD R&D on Sandia's missions and its contribution to the nation's security is multidimensional, taking forms as varied as the projects themselves. For example, recent LDRD investments in biosciences have enabled Sandia to bring applicable R&D skills to biomedical research, investments that may lead to the development of capabilities for very early diagnosis of illness — presymptomatic diagnosis, a notion that was barely conceivable 30 years ago. In the area of high performance computing (HPC), LDRD has long supported the development of novel modeling and simulation tools that have won multiple R&D 100 awards for innovation and utilization by the broader HPC community. Transfer of these technologies allows end users, engineers and manufacturers to predict the performance of their products with minimal expenditures in actual field testing. LDRD activities

also promote workforce development by providing the opportunity for technical staff, whether existing or new hires, to engage in cutting-edge R&D in response to the ever-challenging world of change that offers context for their work. For example, groundbreaking research efforts in the fields of optoelectronics, materials science, and microelectronics have led to new scientific discoveries and strategic partnerships with DOE, DHS, DOD, EPA. Finally, LDRD is the incubator for many innovative technical solutions for some of our most pressing national security problems. Research in sophisticated detection technologies, such as advanced radars, chemical detectors and microelectromechanical systems, have — subsequent to their genesis in LDRD projects — been incorporated into direct program activities and refined for specific mission applications.

Driving all LDRD-directed research is, above all, a vision for a more-secure, more-prosperous future. While national security innovations cannot be planned nor legislated,² the flexibility and forward-looking nature of the LDRD program enables the Labs to accomplish long-range, innovative research that direct program funding is simply unwilling or unable to pursue. LDRD anticipates solutions to future mission needs by validating the fundamental hypotheses and creating the core technologies from which such innovations can arise. LDRD activities produce major scientific achievements and new S&T capabilities, lead to the creation of new programs, develop new strategic partnerships, and accelerate technology transfer. The case histories in this publication amply illustrate both these contributions and the great service that LDRD-funded research provides to the nation. ★

¹Letter from President Harry S. Truman (1949) to AT&T president offering the company an "opportunity to render an exceptional service in the national interest" by managing Sandia National Laboratories.

²"None of the most important weapons transforming warfare in the 20th century - the airplane, tank, radar, jet engine, helicopter, computer, not even the atomic bomb - owed its initial development to a doctrinal requirement or request of the military." John Chambers, ed., *The Oxford Companion to American Military History*

Introduction

The Laboratory Directed Research & Development (LDRD) program was the vision of a long list of federal government agencies who felt that, at its core, scientific innovation and creativity most commonly emanated from researchers themselves, and that competitive funding of such activities lay at the heart of cutting-edge science and technology. To demonstrate the impact of that research upon both Sandia National Laboratories and the Nation, we have proffered twelve case studies of LDRD programs, showing their evolution from concept to initial technical results and to current theoretical and practical capabilities.

From the days of da Vinci, Galileo, and Newton, science has been an independent activity, freely performed by patrician scientists or funded by their benefactors, both parties driven by incredible curiosity to study problems and reveal mechanisms operational in the natural world. Scientists often labored alone, supported by the few writings that Greek and Arab sages had left them. Universities encouraged this style of work, independent, sometimes in small groups, studying questions that humans had been asking for ages. The result was a pattern of work leading from scientific ideas birthed by the few to research performed by the many, the foundation of the scientific method.

In 1954 the newly formed Atomic Energy Commission (AEC) was tasked to provide "a program . . . fostering research and development in order to encourage maximum scientific and industrial progress." In 1974 the AEC was reorganized, and three years later, the Energy Research Act was passed with a little-noticed paragraph advocating a new approach to research. PL 95-39 stated that "Any Government-owned contractor-operated laboratory . . . may . . . use a reasonable amount of its operating budget for the funding of employee-suggested research projects up to the pilot stage of development." After thirty years of government-sponsored research, this legislation rekindled the age-old approach that ideas springing from the researchers themselves needed to be a part of the R&D mix in national laboratories.

The formal incarnation of the LDRD program occurred in 1991 under the National Defense Authorization Act. Section 3132 explicitly authorized laboratory-directed research and development at all DOE GOCO labs and devised funding to derive from up to 6% (equivalent 8%, loaded) of all lab-targeted DOE national security dollars. While that percentage has varied and despite limitations, the program stands today quite the same as it was originally conceived.

The value and impact of a government or industrial R&D program manifests in a multitude of ways. New solutions bring the national laboratories different skills and capabilities that both solve existing problems and address problems heretofore believed insoluble. They thus result in operational changes in our national security systems and in new programs and program funding. The face of warfare changes from intelligence gained on the field to images sent back from Unattended Aerial Vehicles. Communications move from delicate desktop electronics to radiation hardened CPUs on earth-orbiting satellites. Chemical sensors evolve from bulky bench-top devices to hand-held, 1-minute-analysis chem labs on a chip, sniffing out toxic terrorist-delivered vapors.

Impacts also take the form of increased patent activity, R&D100 Awards, and a growth in the number of publications and citations. Lastly, LDRD provides early career employees the opportunity to prove themselves in the arena of competitive proposal funding, to remain intellectually invigorated, and to leave behind a legacy of innovation.

Not all LDRD projects were as successful as those herein, but that process of weeding-out successes and failures is integral to high-quality science, in which we learn as much from the hypothesis disproved as from the hypothesis confirmed. These projects and programs are the paradigm for R&D investments. They exhibit the means by which research takes risks in extrapolating prior results and in intuiting new problem-solving directions. We at Sandia hope they demonstrate the nucleus of an idea generated by one person, communicated to others, and performed by multidisciplinary teams, by which we may grow as a community and thrive as a nation. ★

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Fine-sculpting the Details on a Classic

Synthetic Aperture Radars

Imagine waves of Nazi bombers flying across the English Channel, undetected, leaving the British with no means to prepare themselves for the defense of their homeland during World War II. Gratefully, however, during the mid-1930s, Robert Watson-Watt of the British Radio Research Station had first demonstrated the capabilities of radar for aircraft detection. This led to the famed Chain Home pulsed radar established along England’s southern and eastern coasts to search for incoming aircraft. It is conceivable that the Battle of Britain might have turned in favor of the Nazis, changed the course of history, had it not been for the ability of the British military to adapt the theoretical basis for radar into functional radar — detectors alerting them to implement defenses against the Nazi bombings — and assisting the citizens of England to take timely measures to withstand those attacks.

During the post-war 1950s timeframe, a key radar development occurred at the Goodyear Aircraft Co. in the form of Synthetic Aperture Radar (SAR). SAR quickly became an alternate imaging modality to airborne photography, able to see through clouds and operate during inclement weather. By the 1980s, SAR’s initial resolution in the 10s of meters had been improved to a remarkable 30 cm (approximately capable of distinguishing two objects only about one foot apart). The development of maneuvering re-entry vehicles with long flight times and targeting scenarios requiring higher precision than possible from inertial navigation were being explored, demanding full radar imaging for guidance and course correction. This issue and other factors concerning a requirement for greater targeting precision than possible with inertial

navigation comprised one set of SAR drivers. SAR’s additional importance to large-area image formation and terrain profiling ensured its sponsorship. This combination of factors drew Sandia scientists and engineers into the SAR arena by the early 1980s.

Sandia’s 25-plus-year role in SAR includes contributions in antennas, miniature electronics, precision navigation, guidance, and digital signal processing. In turn, LDRD’s impact on SAR has taken many forms, but in most cases has served as enabler of new technologies, permitting drastic improvements in resolution, size and weight, image quality, and processing speed. As early as 1983, Sandia was investing in an improved SAR-based directional altimeter, with improvements in terrain mapping, strip image mapping, and real-time processing following shortly thereafter. SAR systems take advantage of the long-range propagation characteristics of radar signals and the information processing capability of modern digital electronics to provide high-resolution imagery, in real time, with minimal constraints on time-of-day and atmospheric conditions — SAR can see through clouds and smoke — and leveraging the unique responses of terrain and cultural targets to radar frequencies.

Most commonly implemented by an aircraft, SAR transmits a wide-bandwidth radar signal and then receives a radar echo (returned signal) from an array of objects scattered along the ground, below. Each ground point returns a radar signal over a large angular sector, and the airplane acts as an extended antenna by continuously collecting data along its flight line, albeit at slightly different times.



An MQ-1 predator, Unmanned Aerial Vehicle (UAV), exemplifying the type of carrier that might be utilized for current iterations of Sandia’s miniSAR radar package.

This effectively produces a receiving radar aperture that may be hundreds of meters long or more — the synthetic aperture. By analogy, imagine holding the shutter open on the lens of your digital camera, pointed out the passenger-side window as your friend’s car moves along a road. Image after successive image would register on the camera’s chip, each superimposed on the prior images. Your lens has become super-wide-angle, taking-in much more territory than it otherwise could, but the photographic information on the chip is a tangled mass of images — which could be untangled, if the camera “knew” exactly at what instant of time each image was captured. In the same sense, for the successively collected radar echoes in SAR, reconstruction algorithms must piece together the reflections from the many points on the ground, recovered over an airplane’s flight line,

and produce full 2D and 3D images in nearly-real-time.

In addition to resolution and operational speed, it was physical size that explicitly began to drive SAR modifications. During 1986-1991 the US Army sponsored development of STARLOS, a real-time SAR with image-formation and automatic target recognition of multiple and simultaneous targets. At 500 lb, this system was a significant improvement over the prior 2000-lb SAR, which did not offer real-time processing of SAR imagery. But power requirements were high, and antenna gimbals had relatively short lifetimes. In 1996, General Atomics Inc. (GA) initiated the Lynx program to reduce system size and weight, even further in order to accommodate the small unmanned aerial vehicles (UAVs) entering common use. Sandia delivered the first prototype compact



A Sandia staff member mounts a miniSAR package on an unmanned aerial vehicle.

SAR to GA in 1999. The sensor offered one-to ten-foot resolution stripmap capability and spotlight (higher-resolution, single-area imaging) resolutions as high as four inches, with a maximum range of 25 to 85 kilometers. Lynx[®] was packaged in two subassemblies, eventually weighing less than 85 lb. Sandia's relationship with GA and the Lynx radar continues to this day.

As regular sponsors worked to build more-effective operational SAR systems, LDRD began to fund many improvements, which further reduced package weight, and also, added multiple new imaging capabilities. With the advent of UAV-mounted SAR came both further size reduction and the ability to image moving targets, creating true radar videography. In FY 2000, a three-year LDRD project aimed at improving system efficiency and reducing size and weight was accompanied by a supplementary LDRD to fabricate a new compact digital receiver, a miniaturized waveform synthesis prototype, and an advanced application-specific integrated circuit. To complete size reduction and enhance on-line processing, an FY2004-2006 LDRD developed a highly modular software architecture and advanced image formation algorithms for lower-resolution images. Together, these efforts enabled the first demonstration of the Sandia MiniSAR, a fully

functional radar with a total weight of less than 30 lb, which first flew in 2005.

MiniSAR required several more steps to truly demonstrate its value. During FY2004–2006, an LDRD drove down processing time and continued to reduce size. It developed new image-formation algorithms and implemented miniaturized field programmable arrays to speed image reconstruction. Smaller electronics along with enhanced autofocus algorithms further reduced size. MiniSAR exhibited unequalled image quality and resolution, achieving four-to five-fold reductions in size, weight, and cost, while providing the nation with a SAR offering stunning new applications for tactical warfare systems.

LDRD has also pursued real-time scene imaging — the ability to provide continuous imaging, a video, of moving targets on the ground. An FY2001–2002 project focused on speeding data acquisition so that images could be processed and reconstructed at video rates. The project team was able to demonstrate the capability for collecting VideoSAR data in several modes and automatically processing these images to any azimuth resolution and pixel spacing. However, VideoSAR images contained so much information that radar operators and ground stations were unable to absorb them in real time. In response, new graphical user interfaces were developed to visually queue users to moving targets by way of tracking algorithms able to display the direction, speed, and size of a moving target. Developers expect to incorporate the capabilities generated under this project in most future SAR systems.

The most recent LDRD projects have concentrated on developing better moving-target imaging and improved image resolution. For example, “Enhanced Inverse SAR” (ISAR) seeks to coherently process a set of radar-pulse echo data to image a target object whose



SAR Image of the riparian ecosystem (“Bosque”) and farmlands bordering the Rio Grande River. Both front and rear covers of this publication show SAR images of Washington, DC.

motion is unknown, data-driven algorithms compensating for the relative motion between radar and target. Another recent LDRD is attempting to lower the spectral noise floor and sustain the exceptionally high dynamic range expected in SAR systems, perhaps ultimately permitting the clear discrimination of images of small targets in an urban environment or other cluttered landscape.

The LDRD program has helped to drive the maturation of Synthetic Aperture Radar at Sandia from the physically massive system of the past to the miniature system of the present, while maintaining extraordinary image quality, enabling the Laboratories to offer the nation capabilities that were otherwise unexpected, by combining small size with a UAV platform.

LDRD projects have reduced size and cost while concomitantly increasing performance, adding video capabilities to extraordinary resolution. Against an operational platform provided by agency sponsors, LDRD's complementary offering became the ingenuity to both technically innovate and to spotlight new applications.

From the early radars of the Battle of Britain to today's remarkable technology, MiniSAR systems, often flying on UAVs, are now crucial to the war against global terrorism, including the security of US borders. Future applications, such as search-and-rescue, ensure that Sandia's investment in SAR will both continue operationally and will continue to pay dividends to the nation. ★

Securing Our Infrastructures

NISAC

Microeconomics, energy supply availability, border security, and most importantly, communication infrastructure as it interconnects all other critical US infrastructures: these are but a few of the national-security areas impacted by the modeling efforts of National Infrastructure Simulation and Analysis Center (NISAC). Established by Sandia and Los Alamos National Laboratories in 2000, and currently funded by the Department of Homeland Security's (DHS) Office of Infrastructure Protection, the center's roots were nourished by ingenuity and foresight dating back to a spate of LDRD-funded projects in the mid-to late-1990s.

Moreover, LDRD continues to fund leading-edge forays into modeling initiatives that both support NISAC efforts, and — according to manager Lillian Snyder — support the advancement of staff and program capabilities amid a seemingly endless natural disaster–provoked flurry of demands for near-instantaneous event analysis. As evidenced by the mathematical complexity of NISAC's models, each infrastructure represents a complex adaptive system — much like a human body, or an ecological community. As such, these systems are susceptible to remarkable and often counterintuitive and unanticipated evolutionary outcomes, as well as to cascading failures, be they organ failure, biological extinction, influenza epidemics, electrical blackouts, or liquidity loss in

payment systems. One key revelation of late-20th Century Dynamical Systems Theory mathematics is that such systems, natural and man-made alike, can be similarly modeled, yet are fraught with uncertainty, accessible only to probabilistic prediction.

Now occupying its own edifice on the Sandia, New Mexico, campus (the first building funded by DHS), NISAC's roots in LDRD were extensively ramified through a fertile soil of ideation — the realization by Snyder and other Sandia staff of the critical nature of cybersecurity, underpinning all other US infrastructure security. President Clinton had defined eight critical infrastructure areas, but much of that infrastructure was under

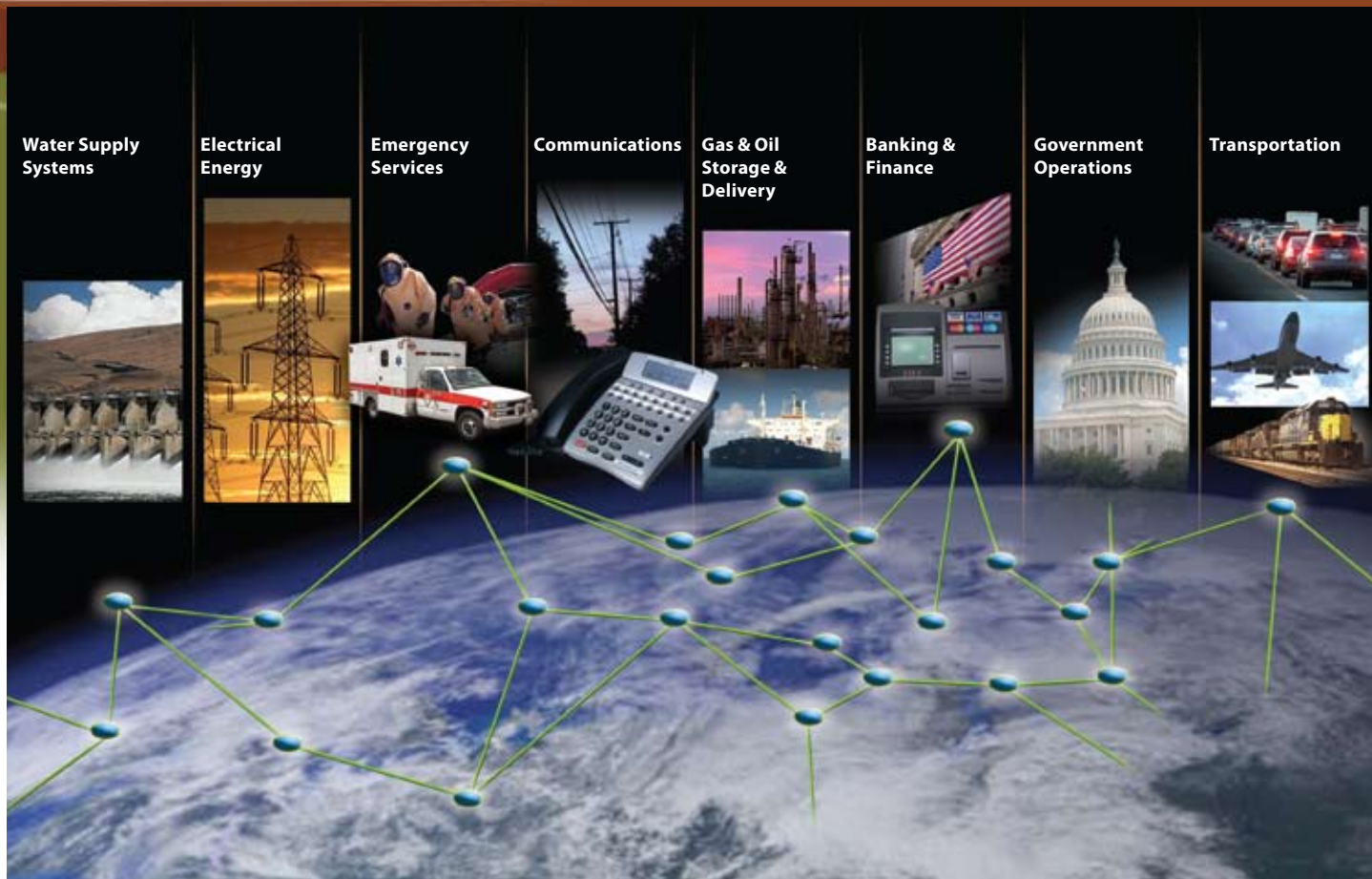


A NISAC model of the interactions among global markets.

private ownership and much of that ownership was narrowly focused on its own slice of the market. By contrast, Sandia staff perceived that the interconnectivity among these physical and economic entities was already large and “growing exponentially,” according to Snyder, and that a national laboratory was well-positioned to see the overview.

Hence LDRD-funded projects in 1996 through 1999, focusing on decision support systems for physical infrastructures and on modeling interdependencies in US infrastructures, resulted in the identification of key modeling approaches such as agent-

based modeling and risk-based characterization of vulnerabilities. For example, a mid-1990s initiative, ASPEN, an agent-based simulation model of the U.S. economy, began to interrogate the strategy of developing quasi-independent software agents. Each such agent possessed built-in reasoning and evolutionary learning-algorithm capabilities representative of decision-makers in a variety of critical infrastructure networks such as the electric grid, fuel-supply, rail transportation, banking and finance infrastructure. This multiple-microeconomic-agent course began to permit researchers to use massively parallel computing resources to simulate the critical



The diversity of infrastructural elements modeled by NISAC in the context of global interconnectivity.

interdependencies that, in the real world, can have devastating domino effects in major crisis situations. The approach represented a significant departure from prevailing macroeconomic modeling. An overarching theme was that the communication infrastructure and its vulnerabilities were a key to interconnecting the other critical infrastructures. Today's preponderance of internet-based communication and the astounding growth of internet-based business transactions are testament to the prescience of these premillennial LDRD-funded projects.

Beyond interdependency, another developing theme became fast-analysis of emergency-response situations. During the California energy crisis of 2000-2001, for example, a fast-analysis infrastructure tool — one that linked up existing predictive tools — was developed and utilized. This prototype of what would become NISAC's Fast Analysis Infrastructures Tool (FAIT) allowed infrastructure owners to submit situational

information and obtain predictive answers, in response.

At its inception, NISAC was funded in the Federal budget by a relatively meager allocation, split between Sandia and Los Alamos. But with the events of 9-11-2001 came DHS and the inclusion of NISAC into the executive order that created the new federal agency. An annual allocation of \$16 to 25M has been written into the DHS budget to support the center's activities since DHS was established. And although ASPEN has continued to evolve and, in its ever-refined versions, finds application to a diversity of modeling initiatives, some LDRD funded, NISAC itself has assembled an impressive variety of modeling and simulation tools for use by both its own staff and by geographically separated decision-makers who must collaborate in crisis management. Frequently, with 17 areas of infrastructure analysis, simulation and response, the center's activities demand an amazingly rapid response based upon predictive tools such as FAIT and the Secure Synchronous

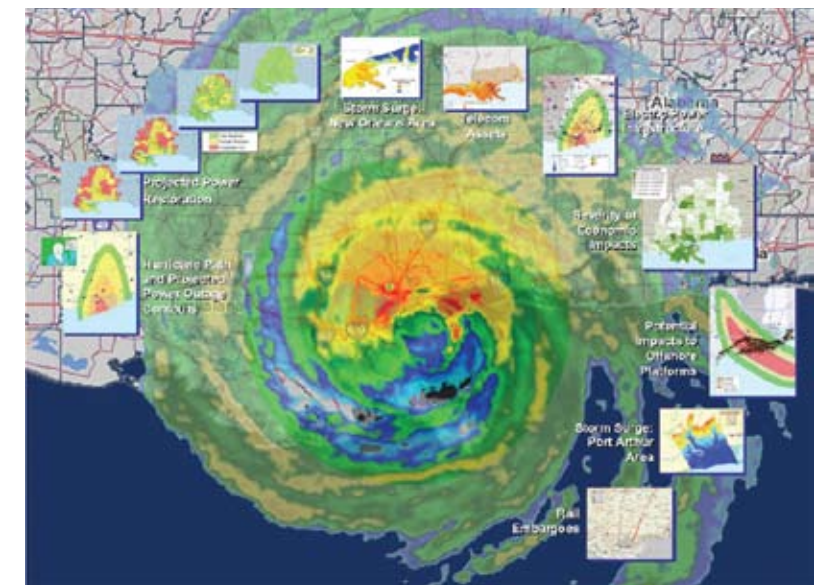
Collaboration framework, part of the agency's mandate to provide real-time assistance to crisis response organizations.

In some sense, this increases the demand for assistance by LDRD-funded projects to help scientists extend the range of possibilities inherent in their modeling toolboxes through developmental research, initiatives that provide resources for policymakers over the longer term. For example, N-ABLE models the economy at the microeconomic level of individual businesses, answering economic policy questions about the effects of infrastructure disruption, while N-SMART focuses specifically on the effects of disruptions in the communications infrastructure.

NISAC's current Port Operations Simulator tool evaluates the short-term effects of shipping container and port security policies on port operations, and together with its Economic Simulator, attempts to uncover potential problems in port-related national security and international trade policies and to unearth viable solutions before problems occur. Developmentally underpinning such current software toolboxes are projects such as the Borders Grand Challenge (2002 through 2004). That LDRD-funded project assembled comprehensive simulation capabilities that took into account an enormous range of positive and negative impacts in allowing modelers to predict the outcomes of possible scenarios — including a diversity of sensor interrogations — for controlling the flow of individuals and goods across US borders by land, sea, and air. Delays, operational costs, altered incentives to suppliers and shippers to utilize such portals all factor into potential impacts, and of course, potential national security outcomes. One can barely imagine the number of possible permutations, making it clear why such models demand such huge investments in computing power. The Grand Challenge was able to develop "high-quality targeted studies" according to project manager Dan Horschel.



NISAC model of banking transactions



Predictive simulation of Gulf-Coast hurricane impacts

What remains is an as yet unrealized need for extension of the research to a nationwide level, where all US ports could be included in predictive simulations of economic and security impacts.

That such massively parallel modeling and simulation efforts are actually effective was evidenced during Hurricane Katrina, when the final 2006 White House report praised NISAC models for their prediction of supply-chain reconfiguration during recovery efforts and called for expanded NISAC presence in such emergencies. Since then, the center has been involved in subsequent hurricanes, and the recent wildfires in California. From scientific inspiration to perception of need through LDRD-funded research to fully realized tools serving the nation, NISAC clearly exemplifies the role of LDRD funding in the process by which Sandia serves the interests of its ultimate stakeholder, the US taxpayer. ★

Miniaturizing Sensors and Mechanisms

Micro-accelerometer Development Supports MEMS

From its beginning, Sandia's LDRD program has supported development of microelectromechanical systems (MEMS) technologies. Each MEMS is a very small, self-contained device integrating electrical and mechanical components in order to detect a change and respond with a micromechanical or micro-electrical control that has consequences in the macroscopic world. For example, imagine that you drop your laptop computer while attempting to place it in its carrying case. Before it hits the ground, it has automatically shut down its hard drive: a MEMS inertial sensor inside your laptop, that detects its acceleration toward the floor has responded with a shut-down control signal so that the read-write heads don't crash down on the hard drive's spinning platters. In addition to this MEMS "accelerometer," (acceleration sensor) other MEMS devices include microscale versions of gyroscopes, robots, engines, locks, transmissions, mirrors, actuators, optical scanners, fluid pumps, transducers, and chemical, pressure, and flow sensors.

Applications continue to emerge as existing and newly developed MEMS are applied to the miniaturization and integration of devices that traditionally have been built on more conventional scales. To accomplish such feats, MEMS extend the fabrication techniques originally developed for the integrated circuit (microchip) industry to add mechanical elements such as beams, gears, diaphragms, and springs. Such devices sense, control, and activate mechanical processes on the

microscale, functioning individually or in arrays to generate their observed effects in our everyday world.

Using the outputs of accelerometers, inertial navigation systems are self-contained units that can automatically determine the position, velocity, and attitude (angular orientation in space) of a moving vehicle or other object; for example, an accelerometer system determines whether the negative acceleration of your auto during impact is sufficient to warrant deployment of the airbags, and the newest computer gaming systems that feature virtual reality sports require multiple MEMS accelerometers. But beyond personal transportation and computer gaming, development of MEMS-based inertial-sensor systems supporting space missions, robotics, and weapons deployment have been the subject of many LDRD projects, and these have been a core contributor to the Laboratories' development of MEMS products, processes, capabilities, and expertise. This has often been true even when projects have not achieved every one of their individual technical goals.

Ernie Garcia has been developing MEMS at Sandia since the 1980s. Over that timespan, Garcia's team has participated in several LDRD projects, including a three-year effort that began in FY1997. Leveraging Sandia's experience in inertial sensor and subsystem development and strong capability in surface-micromachine structures and circuitry, the team's ultimate vision was to develop a low-



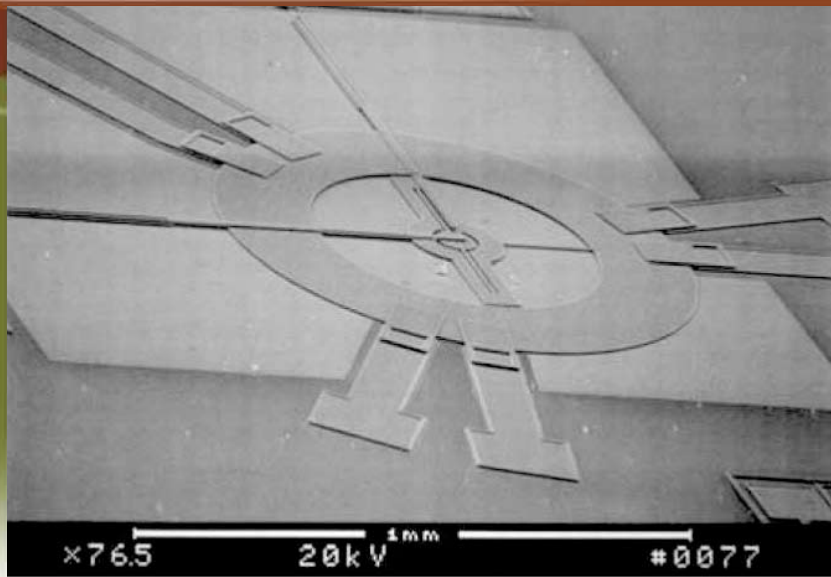
Sandia developed mini-robot, occupying 1/4 in³ and weighing less than an ounce — possibly the smallest untethered robot ever created; MEMS inertial guidance offers the potential of fully autonomous operation.

cost "inertial guidance system on a chip" that could provide attitude, velocity, and position for short-term tactical missile or robotic guidance applications. The project plan included the design, development, and testing of an accelerometer and a gyroscope (spatial orientation sensor), that would be fabricated using surface-micromachined, monolithic silicon microchip manufacturing technology.

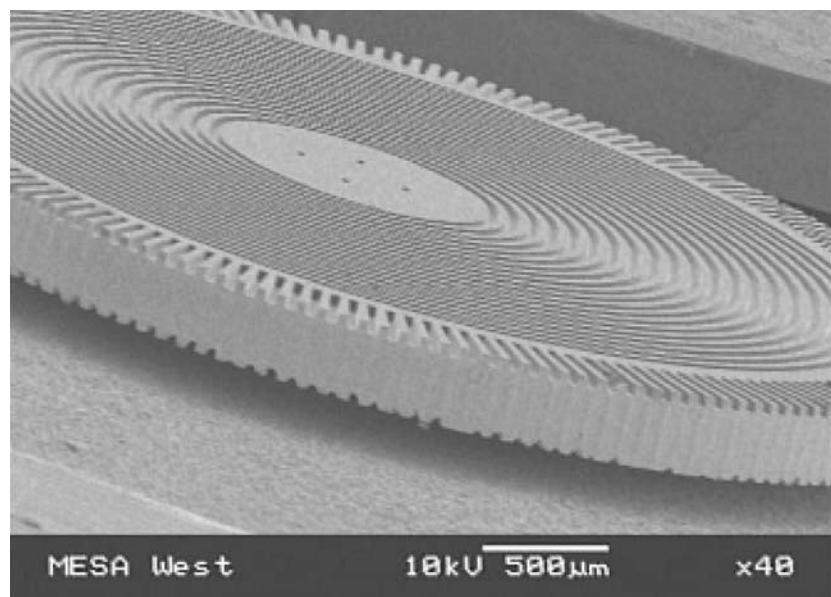
The ultimate goal was fabrication of an integrated sensor, in which accelerometer, gyroscope, and electronics would be incorporated into a single chip. The team identified and evaluated concepts, fabricating prototypes for the mechanical parts of accelerometer and gyroscope while maintaining separation between micromechanical components and electronics chips. Impediments to microscale fabrication of these devices can be daunting — both

accelerometers and gyroscopes require proof (or reference) masses, that is, objects that inertially resist motion in a known fashion. In the case of a micro-gyroscope, the mass must rotate, such that changes in its orientation become a measure of the angular forces acting on it, and therefore of any change in its spatial orientation.

The gyroscope work progressed with relative ease. The team accomplished development, fabrication, and testing of a prototype device that used MEMS micro-engines as drivers for the rotating mass (rotor), and developed a concept for a gas bearing (to reduce friction during rotation). Fabricating an accelerometer with great enough proof mass presented a major materials challenge, and the team chose an engineering technique known as silicon micromolding. Binding of the accelerometer mass to the underlying substrate via stiction



SEM image of micromachined free-rotor microgyro for application in an inertial sensor unit.



SEM image of a prototype grooved proof mass designed and fabricated for testing in a levitated 3-D micro-accelerometer.

(a type of friction) continued to be a problem, however.

The project made excellent technical progress, and the team improved key MEMS fabrication processes as a result, but the accelerometer problems proved insurmountable within the timeframe of the project. Even so, among the project's technical achievements were the first-of-its-kind demonstration of a micromachined rigid body gyroscope — using a Sandian micro-engine

to spin a microsuspended rotor. Palpable contributions thus ensued to development of the Sandia Ultra-planar, Multi-level MEMS Technology (SUMMiT™) fabrication process. SUMMiT V™, the latest level of deployment, is a five-layer polycrystalline silicon surface micromachining process that is among the most advanced approaches to fabrication of MEMS devices.

In another FY 2001–2003 project, Frank Peter and his team envisioned the possibility of using MEMS as the basis for a major improvement in the state-of-the-art of accelerometers for tactical, and possibly navigation grade, inertial guidance applications. Peter's innovation employed a spinning mass (rotor) suspended in either a vacuum or a fluid-filled cavity. The rotor position was sensed capacitatively — changes in position registered as changes in voltage within an electrical circuit — and actuated electrostatically in six degrees of freedom. The electronic measurement and control circuitry used custom electronics chips surface-bonded on the outside of the sensor body.

The project team decided to utilize a hybrid MEMS fabrication approach that would free them from the limitations of any given silicon chip fabrication process, and thereby, expanded the range of design options (e.g., material choice, feature size, and thickness) available to them. Because of this, their final design realized many favorable device attributes, ultimately resulting in increased device sensitivity and reduced mechanical and electrical noise, key attributes for any device of this type.

Successful demonstrations led to the design, fabrication and testing of several prototype accelerometers. However, process integration challenges during fabrication of the prototypes led to several modes of catastrophic failure. And although Peter's team was able to resolve



The setting sun reflects off the glass of the cylindrical training center attached to Sandia's new MicroLab building, the second of three to come online of \$500 M MESA project. (Photo by Bill Doty)

a number of these problems, short circuits that damaged critical electrode assemblies remained unresolved.

Peter remains convinced that the overall design concept is sound, but further work is needed to address the unsolved fabrication and process integration issues on the rotor electrodes. As was the case for Garcia's earlier LDRD effort, the design and fabrication of prototype accelerometer hardware drove successful development and refinement of several entirely new MEMS fabrication processes, many of which have commercial value and represent important enablers for the realization of a wide range of potentially important microdevices.

Based, in large measure, on LDRD-supported advances in specific MEMS devices, such as inertial sensors and accelerometers, and driven by the enabling technologies that these LDRD projects have spawned, Sandia's commitment to and investment in MEMS has continued to grow. Indeed, the Lab's most recent

expression of these values has taken the form of the Microsystems and Engineering Sciences Applications (MESA) project, which was formally dedicated on August 23, 2007. As the largest infrastructure project in Sandia's history, costing \$518 million, the 400,000 square-foot complex is made up of three individual buildings: the Microelectronics Development Laboratory and MicroFab; the Microsystems Laboratory; and the Weapons Integration Facility. R&D activities in MESA support both classified and unclassified work. In addition to fabricating electronic circuits, the MESA facility also makes MEMS for advanced security systems, sensors, guidance systems, and other applications.

Among his comments at the dedication ceremony, Sandia Director Tom Hunter noted, "... [MESA] will allow this Laboratory to develop little things that you cannot see that do things you cannot imagine." Sandia's LDRD program continues to contribute to the development of unique cutting-edge MEMS technologies that make those little things possible. ★

The Oil of the 21st Century

Global Water-security Initiatives

Safety, security, and sustainability: the thematic triad that serves as an organizing focus for Sandia’s current array of activities in water resource management defines an enormous range of R&D, much of which has its roots in LDRD-funded projects. From simulating watershed dynamics to modeling and assessing infrastructures, to developing water-purification methodologies, Sandia scientists have springboarded LDRD projects into a diverse array of programs and partnerships answering the challenge of a global crisis that promises to be to the 21st century what oil was to the 20th.

Although the late 1990s provided the discussion hotbed ignited by Sandia’s realization of the magnitude of forthcoming domestic and global water issues, it was FY 2001 before the embers of that hotbed fueled the initial group of LDRD projects. Since then, those first endeavors have reduplicated and grown to engage the resources of 17 Laboratory centers at one time or another, according to Senior Manager, John Merson. A comprehensive strategic planning effort led to a portfolio of themes — “a well-integrated strategy was our intent from the very beginning,” recalls former Geosciences and Environment Center Director, Peter Davies. That portfolio began with infrastructure physical security risk assessment, whose obvious necessity was revalidated by 9-11-2001. Geopolitical destabilization with concomitant permissive growth of terrorism made water-scarcity issues an urgent matter for a national security laboratory. With mid-latitude river basins stressed throughout the world, water-management projects, although initially carried-out in the US, were globally relevant



A riparian (river) ecosystem — the Rio Grande — in the midst of surrounding desert carries precious water for irrigation, ranching, and domestic use.

to the extent that they provided a test bed for other locales potentially harboring sources of international terrorism.

Prompted by 9-11, the EPA requested that Sandia assess the water security of major US cities. Initially possible only on a limited basis, Sandia’s longer-term response was to prototype training methodologies and risk-assessment tools that self-proliferated, such that in addition to assessment of seven major municipal systems, ultimately, approximately 90% of US cities with greater than 100,000 connections in their water systems were analyzed. The EPA’s National Homeland Security Center in Cincinnati has been a major partner and source of funding in this national effort.

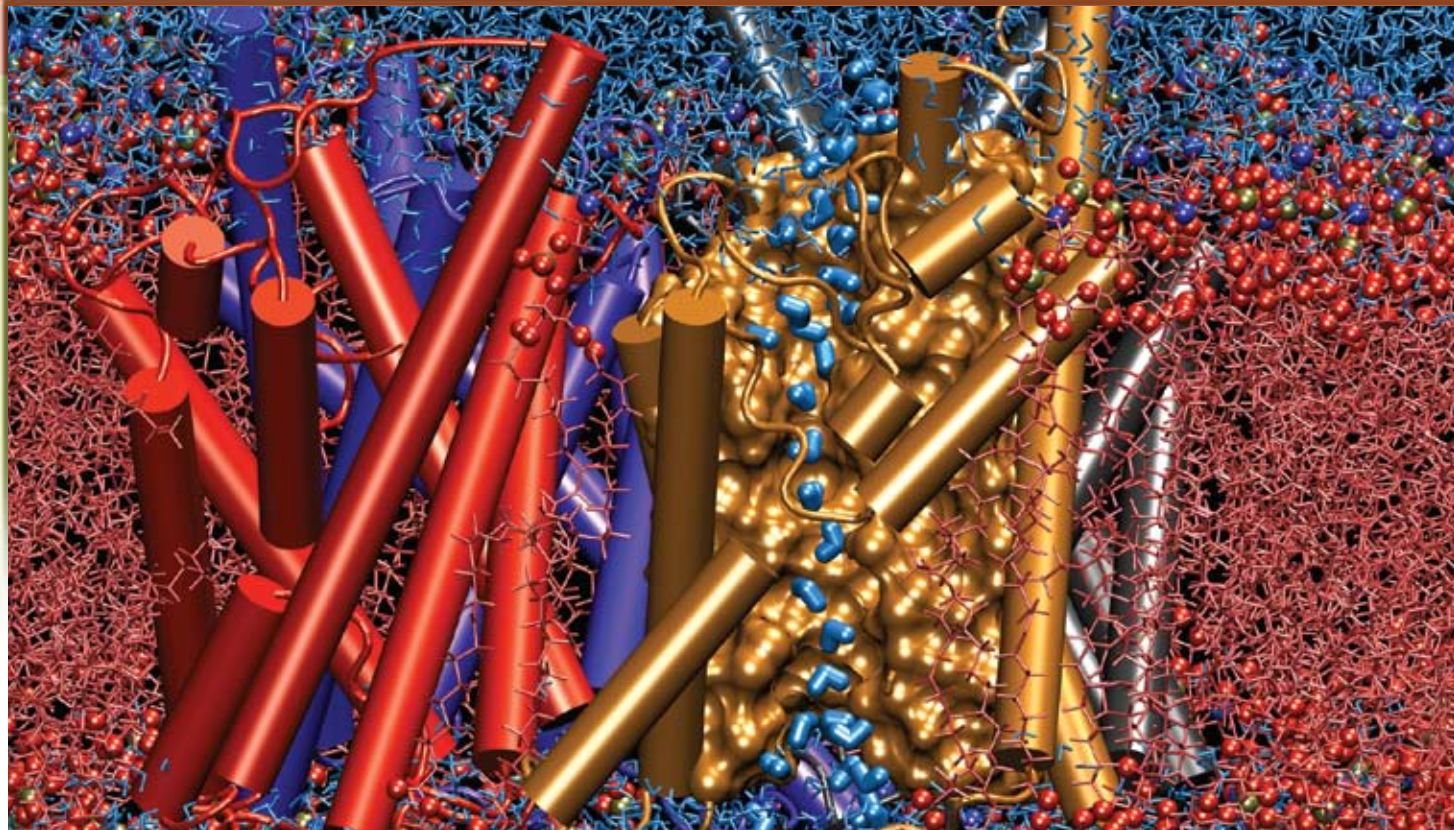
FY 2001–2003 LDRD-funded initiatives ranged from dynamic simulation modeling of watersheds to providing regional water managers with policy and management options, to sensor initiatives for monitoring EPA-regulated compounds such as arsenic.

The 2001 change in EPA’s arsenic regulation —from 50 ppb to 10 ppb allowable — was rightly perceived as having huge financial and technological impact, particularly on small to medium-sized water-management regions. With follow-on funding from DOE and AwwaRF (American Water Works Association Research Foundation), a partnership of Sandia, AwwaRF, and New Mexico State University/WERC evaluated designs for arsenic removal. Sandia’s long history with understanding fate and transport of materials flowing through porous media provided a solid foundation for performing calculations and engineering materials.

“The roots of the modeling and water management initiatives are clearly in LDRD,” asserts Davies. As part of the initiative, several community-based projects were initiated, using

a Sandia-developed resource-planning toolbox to assist managers, water professionals, and the public to examine alternative solutions to regional issues (collaboration with the Utton Center of UNM School of Law). A Middle Rio Grande Project engaged several north-central NM counties, then, later, extended into Mexico, and indeed, these tools were later used as far away as the Middle East. Modeling initiatives have since spread to other partnerships in Europe and Asia.

In FY 2002, desalination initiatives became part of the LDRD investment in foundational capabilities, and they vividly highlight the foresight of LDRD in spurring crucially vital science and technology. With 97% of the world’s water either saline or brackish, a key realization was that tapping those resources would require new technological approaches.



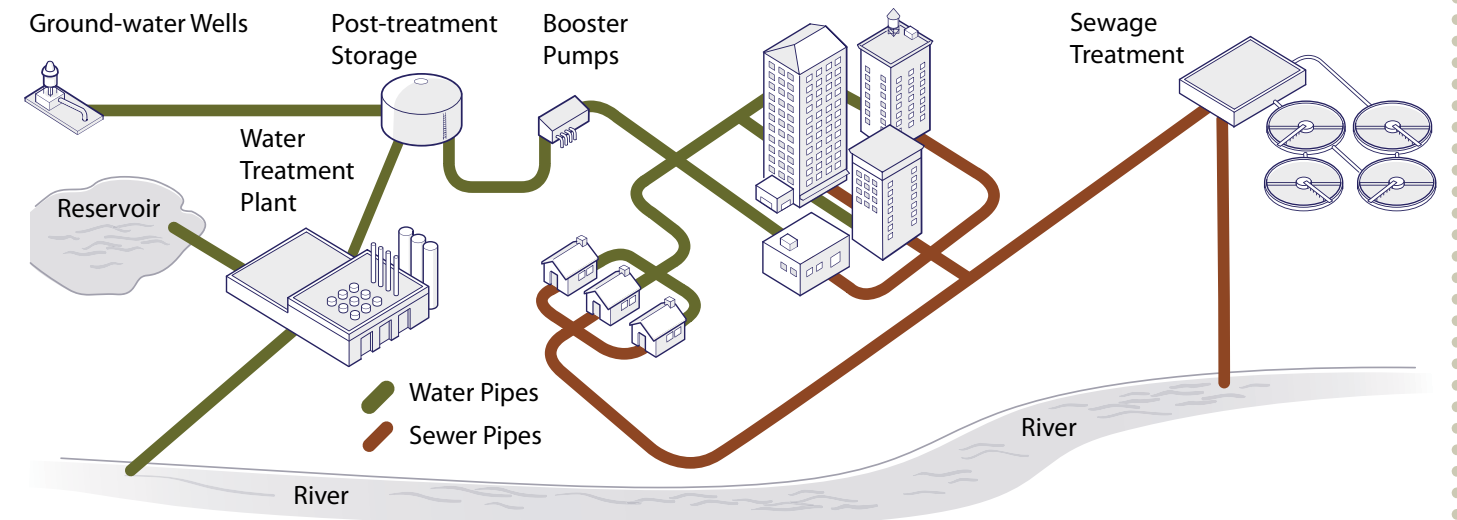
Computer model of a cell membrane showing an aquaporin protein (gold) with water molecules (blue boomerang shapes) in single-file transit through its transmembrane channel. Salts are excluded, only water allowed to transit — exactly the desired properties of desalination membranes. (Image courtesy of Emad Tajkhorshid, University of Illinois, Urbana-Champaign).

Currently employed reverse osmosis (RO) desalination technologies had originated in a burst of federal funding during the 1960s and 1970s, and that funding stream had subsequently dwindled to barely a trickle. Therefore, while the scientific initiative moved forward, a parallel collaborative interaction with the Bureau of Reclamation produced the 2003 Desalination Roadmap, a critically important document. National Academy of Sciences review of this early roadmap reinforced the importance of future desalination technical challenges and suggested that additional work remained in fully framing the depth of associated scientific challenges.

This 2003 roadmap and the national dialogue it created served as a catalyst, putting desalination back on the map in the US. Congressional support for desalination research through both the Bureau of Reclamation and Department of Energy led to the formation of the National Desalination Task force, a partnership among Sandia,

the Federal Bureau of Reclamation (BOR), AwwaRF, and the WaterReuse Foundation. In addition to the approximately \$10M of federal funding over the period 2004 –2007, the Water Resources Department of the State of California also granted task force partners \$1M for a study in that state, with the task force itself matching that grant.

The significance of the partnership between Sandia and the Bureau of Reclamation cannot be overemphasized. The National Desalination Research facility in Alamogordo, NM is now poised to investigate both cutting-edge desalination methodologies and measures for the disposition (and hopefully even the reclamation) of the concentrated brine byproduct of desalination. With the assistance of Senators Domenici and Bingaman, the facility's recent grand opening signals the ongoing forward motion of Sandia's water initiative. And the external funding from the BOR, and DOE (through NETL, the National Energy Technology



The elements of a generic urban water system.

Laboratory) is one example of the return on investment from LDRD funding.

And while the nation anticipates the impending publication of the follow-on Water Purification Roadmap, LDRD resources have been laying foundation in other arenas. Life science now occupies a good deal of LDRD attention. For cells utilize protein water-channels (aquaporins) that can likely teach membrane developers a thing or two about desalination. On the flip-side, contaminating drinking water with disease vectors like *V. cholera* is a lingering threat, and the fouling of desalination membranes by microorganismal growth is one of several technological challenges facing developers.

In light of these daunting challenges, Sandia has engaged in several international partnerships, even to the inclusion of the Middle East, where, for example, Turkish dam-construction projects near the headwaters of the Tigris River have frequently produced tension with its downstream neighbors, Syria and Iraq. The necessity for such research and the need to continue to secure follow-on funding is clearly illustrated by two facts that transcend water issues' high-profile status: First, 40% of the cost of desalination is energy — one can no more readily separate energy and water than one can disjoin photosynthesis and sunlight. Second, desalination produces a concentrated brine as a byproduct. So although

a recently opened El Paso, TX desalination facility yields 30 million gallons of drinking water per day, it also produces 3- to 6-million gallons of brine per day that must be reutilized or disposed of.

Looking to the future, a key remaining question is where Sandia should invest its resources to build the capabilities that enable it to remain on the cutting edge? Sandia has built a very strong working relationships with EPA, and is a key R&D player in this arena. Partnerships with the Bureau of Reclamation and the National Desalination Task force offer other examples. As Sandia develops these partnerships, the Laboratories must also continue their work to anticipate the future — the technical challenges that will emerge as pressure continues to mount on water as a strategic resource. Clearly, bringing the cost of desalination into the range of current water-treatment is one area for ongoing investment. Current Sandia research initiatives — such as its participation in NSF Science and Technology Center for the Sustainability of semi-Arid Hydrology and Riparian Areas (SAHRA) — suggest that the ongoing refinement of modeling toolboxes for local decision-makers is another activity imperative to the preservation of domestic and global water security. Undoubtedly, as it has before, LDRD will support whatever is the next great science or technology in this ever more crucial arena. ★

Shielding Delicate Electronics

Radiation-hardened Electronics and LDRD Adaptation

Since the advent of both atomic weapons and orbiting satellites, electronics designers have had to face the issue of how to sustain operation in the presence of damaging radiation to delicate, miniature electrical components. As an example, on September 6, 1976, Viktor Belenko, a Russian pilot, defected to Japan in his Soviet MiG-25 jet, permitting Western governments their first look at this fast, maneuverable technology. To the surprise of Belenko's interrogators, they found that most on-board avionics in this advanced aircraft utilized vacuum tube technology, not solid-state electronics. Beyond ruggedness and easy replaceability, such vacuum components were highly radiation hard. That is, they could continue to operate properly even in a high-intensity radiation environment.

Whether passive resistors, capacitors, and coils, or today's fully integrated circuits, the issue of radiation-hardness is key to both US national security and our space program. A nuclear blast could send a pulse of radiation (in the form of gamma rays and neutrons) large distances from the explosion. Additionally, satellites in orbit inevitably accumulate a large dose of gammas, neutrons, and charged particles from the sun over the years of their operating lifetime. Since the mid-60s Sandia researchers have worked to reduce the sensitivity of control systems, communications systems, firing sets, and sensors, to such damaging radiation impacts, thus preserving the integrity of such control systems under these extreme conditions.

While LDRDs have only impacted this program since 1991, radiation hardening of electronics was actively pursued at Sandia, largely under wraps, during the 1960s and 1970s and continues today. The US military was the Laboratories' primary customer, working closely with Sandia and several commercial vendors to find new materials and to understand radiation damage physics. The problems were intimidating. Passive components could change their electronic values or simply short out. Active components, like transistors, could switch from off to on or reverse, ceasing proper circuit operation. Integrated circuits consisting of millions of transistors could cease communicating internally and externally.

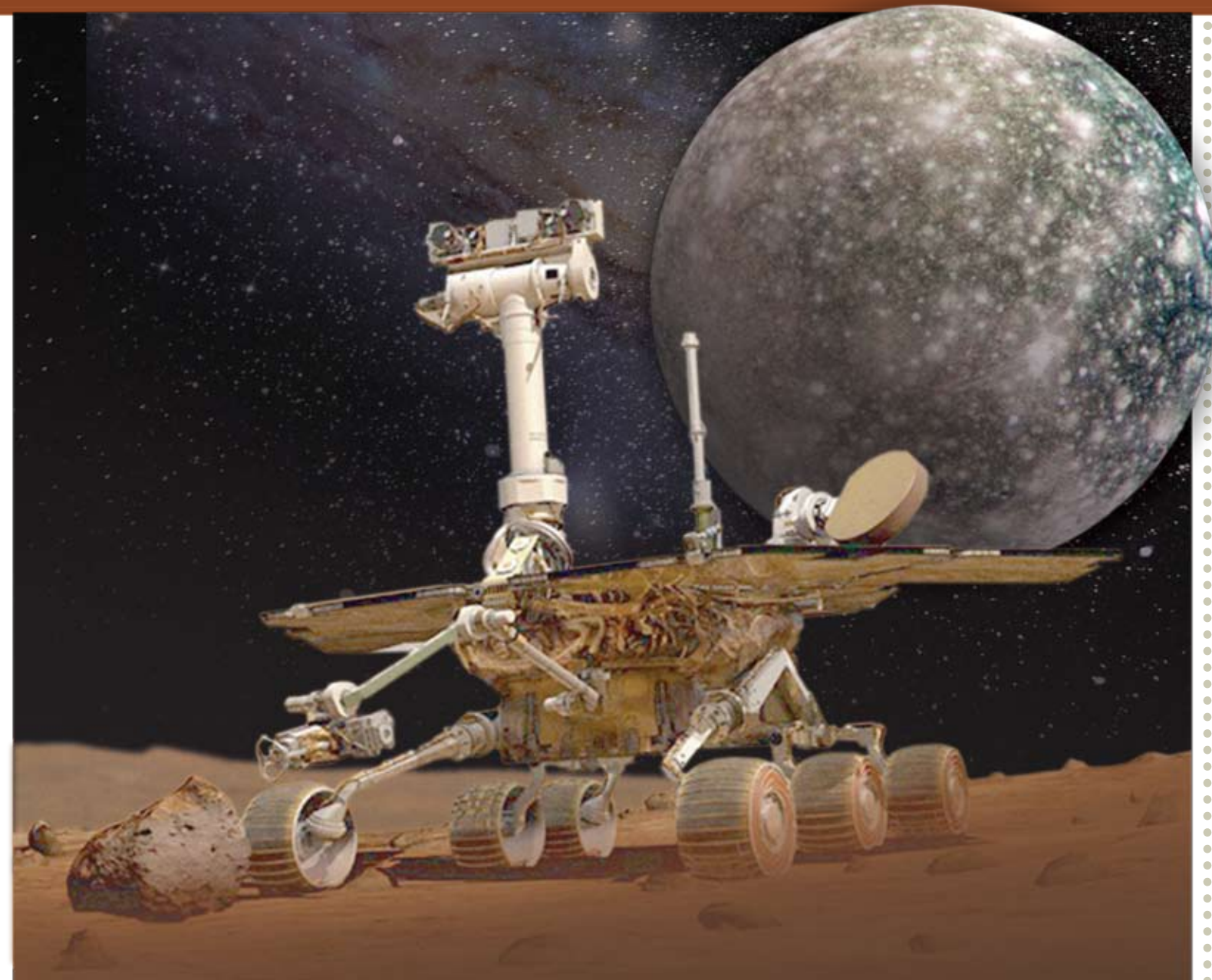
Gamma rays, neutrons, and charged particles have the nasty habit of kicking out free electrons and creating sinks for other charges, wherever they are halted by the atoms of an absorbing material. If they stop in an electronic material, they leave behind a path or collection of electrons that can switch on a transistor, open an electronic gate, change a resistor's value, add an unexpected "bit" to a computer calculation, destroy the solid-state memory, or short out a capacitor. To thwart this, researchers at Sandia have used LDRDs to study different materials such as silicon-on-oxides, gallium arsenide, germanium, chalcogenide, and others, which restrict the flow of such induced free charges and limit the damage

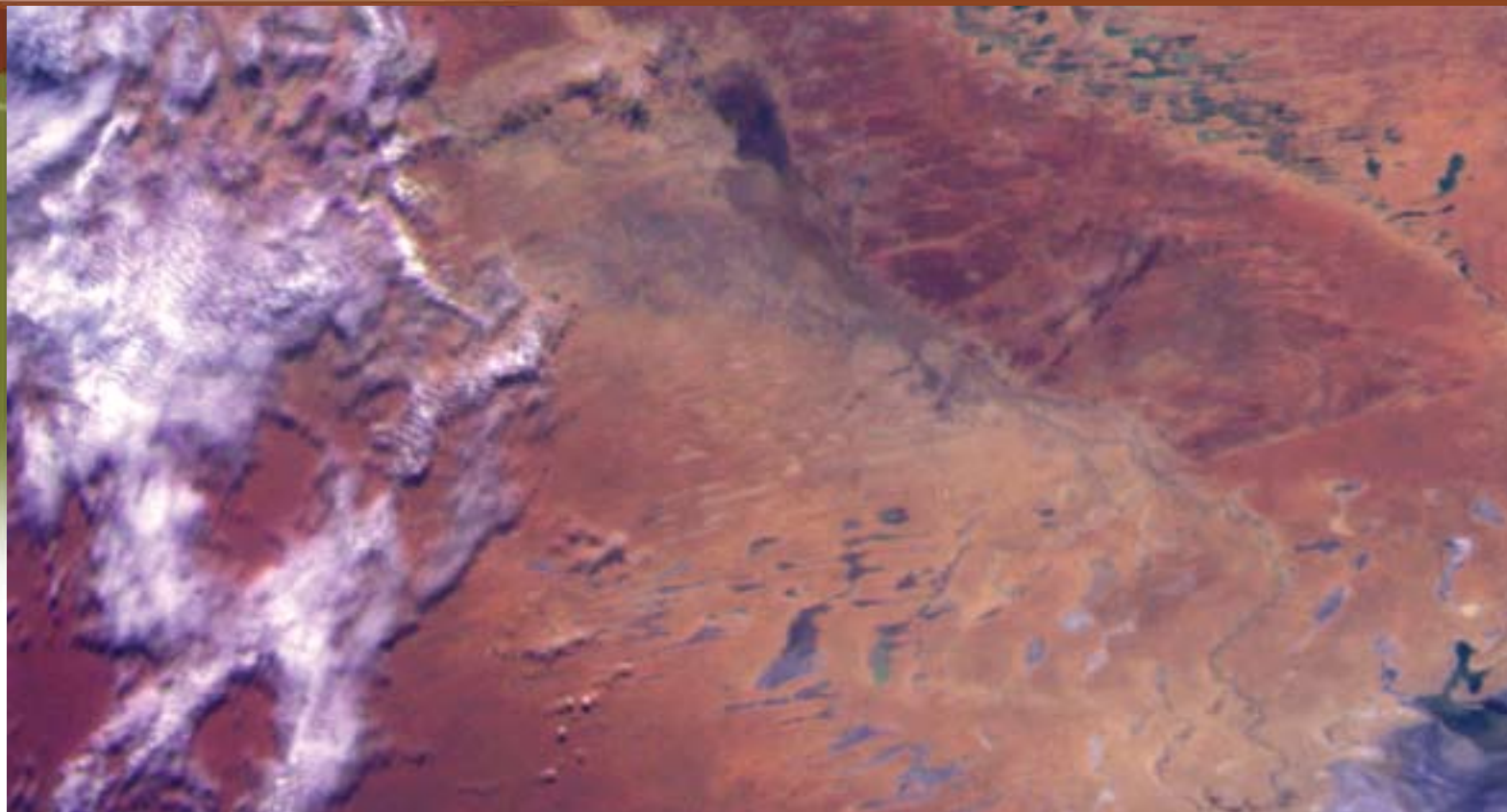
when compared to silicon. Some materials, like the chalcogenides (sulfur, selenium, and tellurium exemplify chalcogen elements) use physical phase changes rather than charge storage for memory retention. Others use optical interconnects to maintain intra-circuit communications.

In the 1960s, the market for electronics in the US was in the \$100-200 M range. The DoD was the largest customer and the simplest approach to hardening was to pre-irradiate electronics to attempt to saturate the damage level, that is to "pre-damage" the material while retaining functionality. Such treatment reduced circuit gains, but it also precluded or severely limited further

A drawing of the Mars Rover is backdropped by a colorized Galileo-generated photo of Callisto, one of Jupiter's four largest moons and its orbitally most remote. NASA technologies like Galileo and the rovers require radiation-hardened components, enabling them to functionally persevere in the high-radiation environment of space.

damage. Since most commercial electronics manufacturers were selling to the military, they closely worked with Sandia to radiation harden ("rad-harden") their products. However, by the mid-1970s, as very large scale integration circuitry was taking off, the consumer electronics market exploded to a \$150B industry. By the early 1980s, commercial vendors had almost completely





The Simpson Desert, Australia, a colorized image produced by the spacecraft Galileo before it departed earth en route to Jupiter.

turned away from the military market, which was now only a bit player.

Today, only Sandia and Honeywell remain contributors to the radiation hardened electronics manufacturing market, developing new solutions to reducing component size and increasing capability in the high-dose and pulsed-radiation environments. Sandia supplies rad-hardened components to customers, such as NNSA, NASA, the Navy, and the Air Force for aerospace and weapons applications. The Laboratories will purchase commercial parts or buy electronics to drawings, and build electrical simulations of these circuits. Beyond these commercial, off-the-shelf components, Sandia designs and fabricates radiation-hardened, application-specific integrated circuits for the customer's end use.

A significant contribution to the NASA space program is exemplified by the spacecraft, Galileo, which carried out an investigation of the planet Jupiter and its moons during the 1990s. Sandia designed,

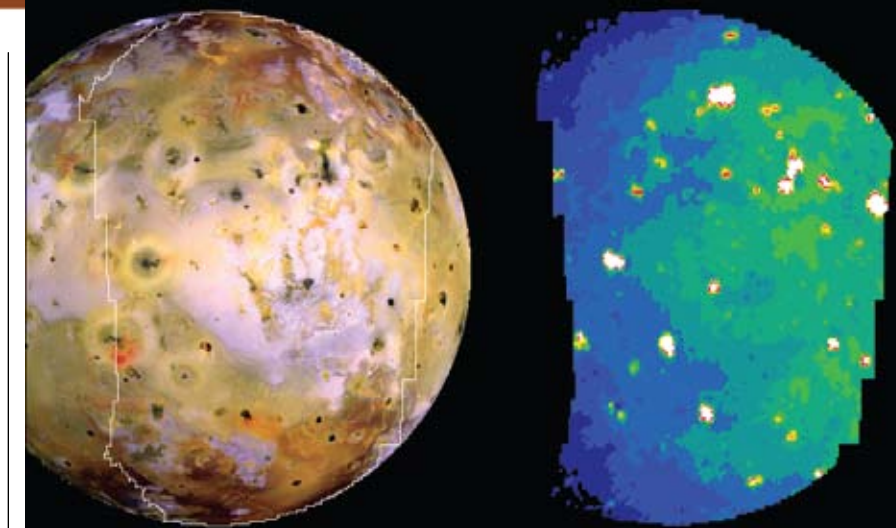
fabricated, and tested the radiation-hardened integrated circuits on the spacecraft, which returned enormous quantities of data from highly challenging radiation-filled environments such as that of the Jovian moon, Io, to which Galileo passed in rather close proximity.

LDRD has contributed to the development of new concepts for rad-hardened computer memories, sensors, interconnects, and capacitors, primarily, although not exclusively applied to nuclear weapons and avionics. A 1996 project addressed processing techniques for silicon-on-insulator memories that were based on the presence of defects to reduce the transport of radiation-induced charges. Today, such memories are commercial off-the-shelf products. During 2003-2004, a new concept was examined to produce highly radiation hardened memories using materials called chalcogenides, for example, mixtures of germanium, antimony, and tellurium. These devices based memory upon phase changes, which immensely increased local electrical

resistance, to create a computational "bit" of stored memory. The polycrystalline state (low resistance) provided the "zero" and the amorphous state (~1000-times greater resistance) provided the "one." These devices were coprocessed with BAE Systems for Sandia and the Air Force Research Laboratory, and today the C-RAM (chalcogenide random access memory) is another off-the-shelf product, http://www.baesystems.com/ProductsServices/bae_prod_eis_cram.html.

One of the simplest, yet highly radiation sensitive electrical components of today's integrated circuits is the capacitor used for storing charge. Conceptually no more than two conducting plates separated by an insulator, the capacitor can be readily discharged by a gamma ray, a fast charged particle, or a high flux of energetic neutrons. To increase radiation hardness, a recent LDRD worked to develop a new insulator, which would permit high stand-off voltages while having extremely limited electrical current flow when exposed to radiation sources. Mylar is a common insulator, but radiation induced currents prevent its use at high voltages. However, by doping the mylar with certain large molecules, the resistance to radiation dramatically rises, and the capacitor can handle extremely high currents, discharge rates, and support high energy density.

The Mylar was loaded with trinitrofluorenone (TNF), which had been previously used to produce coatings on auto windows for sunroofs. However, during the project, TNF received classification as an explosive and was no longer readily available. In order to produce TNF-like capacitors in-house, the LDRD team turned to a couple of young polymer chemical engineers to devise novel synthesis techniques. Within the three years of this project they were able to not only snatch this project from the jaws of defeat, but were able to demonstrate the significant improvement attainable by using



A colorized image and corresponding "hotspot" map of Jupiter's moon, Io, together with a closeup of a portion of its topography. Io's extreme radiation environment provided an ample test of the durability of the Sandia-developed radiation-hardened components on the Galileo spacecraft.

such a doped Mylar film from which to build capacitors.

The Rad Hard LDRD program provided both an opportunity for researchers to directly contribute to the nuclear weapons area, defense systems and assessments area, and science, technology and engineering areas, but also to re-vitalize the laboratory by finding and employing young scientists with creative new ideas. Few examples of LDRD impact are so convincing or so complete. ★

Slashing CO₂ Emissions by Rocketing Efficiency

Solid State Lighting

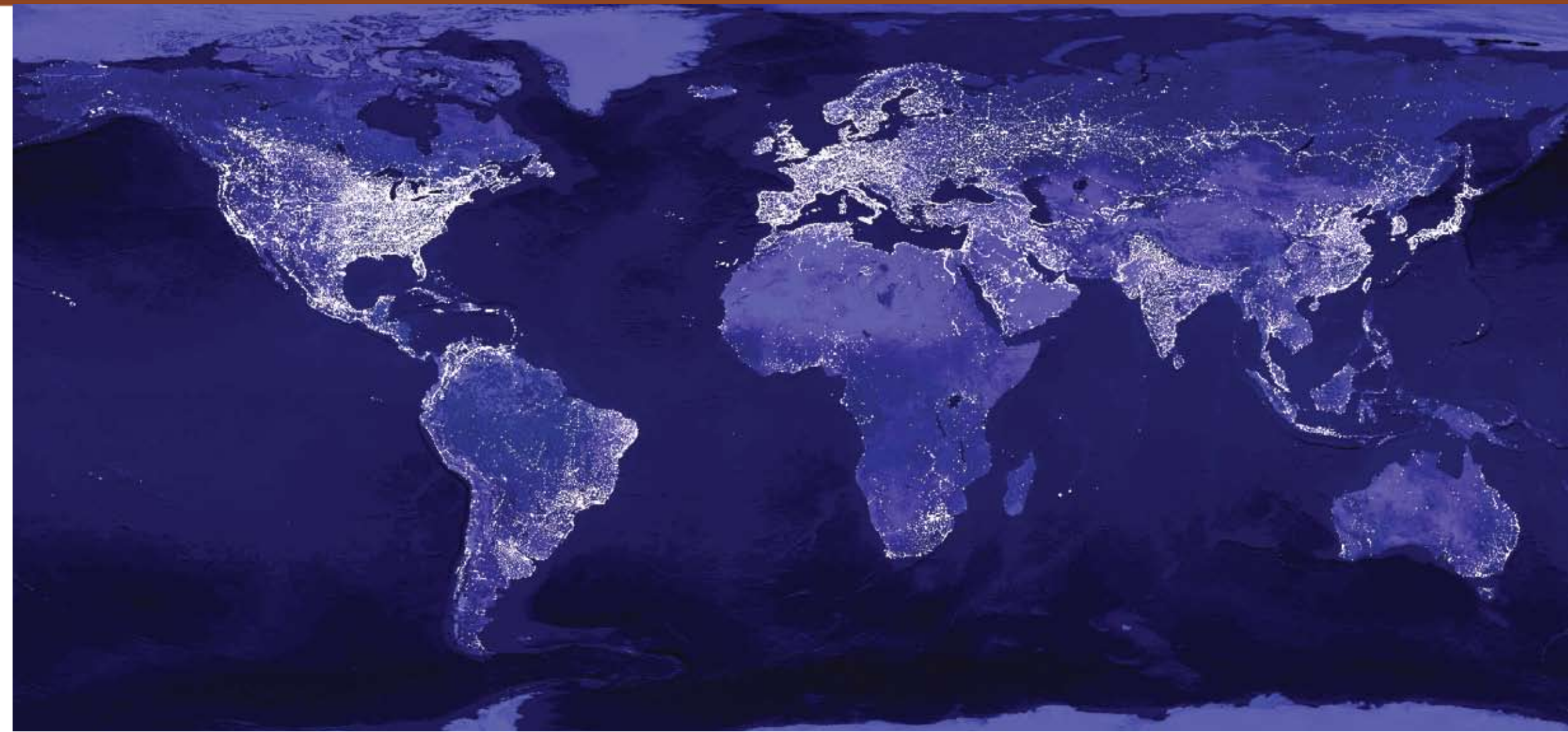
Recent issues surrounding CO₂ emissions and energy-consumption efficiency are closely tied to the arena of home and business lighting, which account for about 20% of global electricity use, or about 7% of global energy use. With standard incandescent lighting, we have, for over a century, been generating much more heat than light — for every watt of electricity consumed, incandescents use only 5% of that energy to produce light. While, in contrast, fluorescent lighting reaches 25% efficiency, Sandia scientists fully subscribe to the possibility of at least doubling that efficiency, to 50%, with solid state lighting (SSL).

Our common experience of such LEDs (light-emitting diodes) occurs in the red lights on cell phones, and mp3 players, where they sip energy from the devices' battery. There are also several types of diode lasers, as well — these can be thought of as super-LEDs, where the semiconductor's light energy is optically or electrically amplified. In the public sector, SSL is best exemplified by red-LED traffic lights, the savings in electricity and dollars to municipalities significant.

Unfortunately, while red and infrared LEDs have been relatively easy to optimize, some other spectral colors have proven more difficult. A phenomenon known as nonradiative recombination severely constrains green-wavelength emission, diminishing the number of lumens per Watt (and hence, the efficiency) obtained. And since combining green, red and blue LEDs is one

efficient route to white LED lighting (and thus, everyday home and business illumination), this issue is crucial.

Hence, based on 1990s Sandia research — much of it LDRD-funded — into optoelectronics, the science of producing and extracting light from electronically excited materials, the LDRD program funded a Solid State Lighting Grand Challenge from FY 2001 through FY 2003 to the approximately \$7 million (total) level. From its inception, the scope was quite broad, ranging from fundamental materials physics problems to assembly of these materials into the layered p-doped/n-doped structures comprising LEDs, to methodologies for enhancing light extraction, and even into related issues such as practical applications for LEDs in areas other than lighting (for example in biothreat detection).



Composite satellite image illustrating worldwide use of electric lighting (courtesy, NASA).

And from the beginning, there were interested corporate partners, such as the Silicon Valley lighting company, Lumileds.

Significantly, it was also during the grand challenge period when DOE recognized the great need for a roadmap. Combined private/public arousal marked a recognition of the enormous market and global impact potential for LED technology. Given that, in addition to markedly increasing efficiency, LEDs can bring lighting to regions where candles and oil lamps still form the primary lighting mechanisms, these developments presaged a transition of inherently inexorable momentum. From the standpoints of peak oil and global climate change, there may possibly be no more important single transition than LED lighting (symbolized by LED lighting of the entire swimming venue at the 2008 Chinese Olympic

games). In response, DOE initiated a series of Technology Roadmap Workshops and Reports, with Sandia chosen as a major contributor and Roadmap Reports editor. Sandia has since organized numerous workshops evidencing unparalleled pre- and post-grand challenge leadership in the underpinning science and engineering. With technical support from Sandia, DOE then worked to establish an SSL R&D program and concomitant product development program, collectively known as the Next Generation Lighting Initiative. In 2007, Sandia was chosen as the lead lab of the National Center for Solid State Lighting R&D.

“We worked hard . . . the center didn't just fall into our laps,” emphasizes senior manager Jerry Simmons. With the center came FY 2007-2008 funding of \$5M, \$3.2M for several Sandia projects; but despite a strong



TOP: LEDs light the exterior of the Lumileds building (courtesy, Lumileds).

BOTTOM: NASDAQ display, a composite of 18-million LEDs, overlooking NYC's Times Square.

backing from Senator Bingaman's office, it has been unclear whether additional center funding will be forthcoming; Bingaman had earlier played a key role in SSL funding authorization that appeared in the 2005 Energy Bill. Regrettably, the Lumileds partnership has since failed to develop in a completely meaningful fashion, although the connection with Sandia is sustained on an intellectual level, according to project staff. Lumileds became a wholly owned Philips Inc. subsidiary in 2006, and in a \$40B annual market, part of the block to collaboration is legal, tracing back to a change in Federal law (specific to the *Next Generation Lighting* initiative) defining the means whereby small companies, DOE Labs, and universities may retain control of intellectual property developed through federally funded research.



Incandescent, fluorescent, or LED, the basic physics is straightforward, but the nuances can be excruciatingly challenging. Add electrical energy to matter, and that extra energy can serve to raise electrons to higher energy levels. As certain of these electrons drop back to lower energy states, some of the energy difference is liberated as emitted light (some as heat). Depending on the exact nature of the energetic transitions (governed by quantum mechanics), that light can be infrared, visible of various energies (colors), ultraviolet (UV) or beyond.

From the tungsten filament of an incandescent lightbulb or the phosphor coating of a

fluorescent tube or compact fluorescent bulb, the light can easily escape to the surroundings. But owing to their solid, layered, microchip-like structure, LEDs tend to trap their emitted light, and part of the issue is to design micro and nanostructures that strategically improve light emission (extraction). With gallium nitride-based materials at the center of LED nanoneering, indium gallium nitride has become a central research material for green LEDs and aluminum gallium nitride for UV-emitting LEDs. These research areas are synergistic in terms of the basic physics, and the DARPA SUVOS program, (2002–2005) and DARPA's current SAIL program have funded the UV work, particularly in its applicability to bioagent and other threat detection. In addition to DARPA and the National Center for SSL funding, the LDRD program has continued to fund basic physics, materials research, and light-extraction technologies.

Key among the current LDRD-supported projects are nanofabrication and characterization of various types of photonic crystals. These crystals are essentially periodic arrangements designed to improve the emission of photons and their escape to the surroundings as useful illumination. This latter research area is every bit as critical as that of light generation. Understanding how to improve light extraction and better appreciating the sources and mechanisms of energy loss are both critical to improving efficiency, the name of the game for making SSL competitive. A related piece to the materials puzzle is cost-competitive fabrication using the most-favorable materials and chip-manufacturing technologies, and LDRD-funded initiatives are also addressing this challenge.

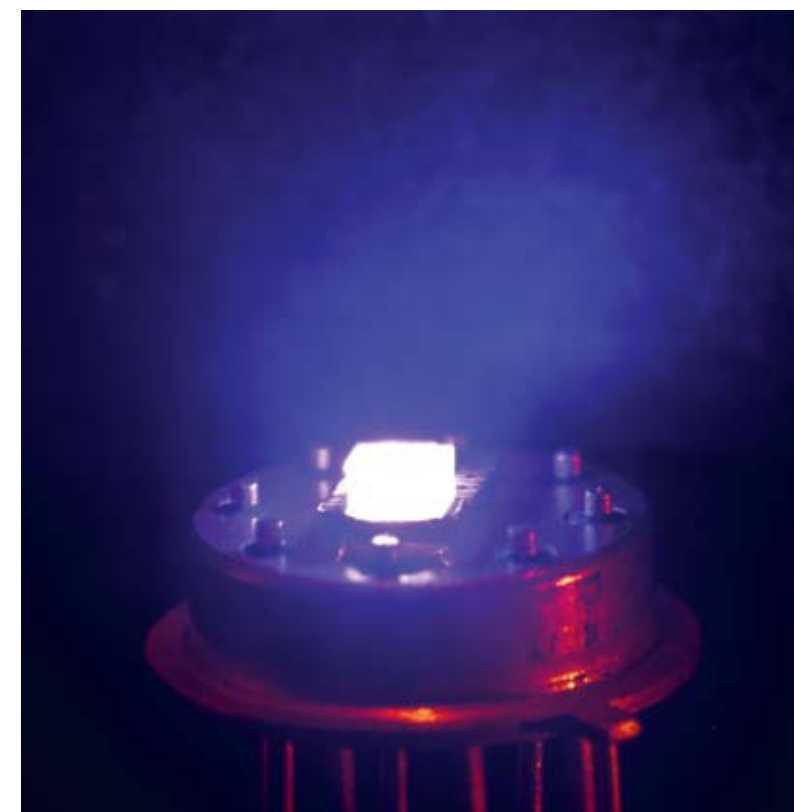
Along the way, ingenious LDRD-funded developments — such as the tungsten photonic lattice — have shown promise. Yet, their ultimate contribution remains to be realized, although commercial ventures based on Sandia nanoengineering have arisen and are now reputedly poised to contribute product solutions.

It is also important to note that although refinements involving infrared-emitting solid-state devices do not always contribute to solutions for visible lighting, IR remains the light-encoded medium of choice for a huge number of applications, used in electronics of all types — remote-controls for TVs and other electronics exemplifying a small slice of that market.

Although Sandia project managers express hope that funding for ongoing initiatives may be forthcoming from DOE's Office of Basic Energy Sciences (BES) and also from the State of New Mexico's economic development initiatives in nanotechnology, another key development from the Sandia standpoint is the 2006 formation of the Sandia-led National Institute for Nano-Engineering (NINE). NINE members include many corporations, such as Intel, IBM, and Lockheed Martin, as well as numerous prominent universities. Perhaps, SSL may ultimately receive some attention as the "flip-side" of photovoltaic technology: in the former, electrons drop to lower-energy states accompanied by light emission; in the latter, sunlight absorption raises electrons to higher-energy states, thereby generating electrical currents (the fundamental energy transformation in green-plant photosynthesis). A current LDRD in partnership with Rensselaer Polytechnic Institute (RPI) exemplifies the basic materials science effort to understand the path toward high-efficiency green LEDs in the context of the more-fundamental physics and nanoengineering issues whose solution should eventually turn the planet toward an economically feasible display of solid-state lighting; a globally extended version of the 18-million LEDs currently populating the NASDAQ display perennially blazing above New York's Times Square. ★



LEDs illuminate the text encircling the statue of Thomas Jefferson, in the Jefferson Memorial, Washington, DC.



A near-ultraviolet (390 nm) LED in the laboratory.

Enabling Ever More-sensitive Chemical Detectives

Chemical Preconcentrators



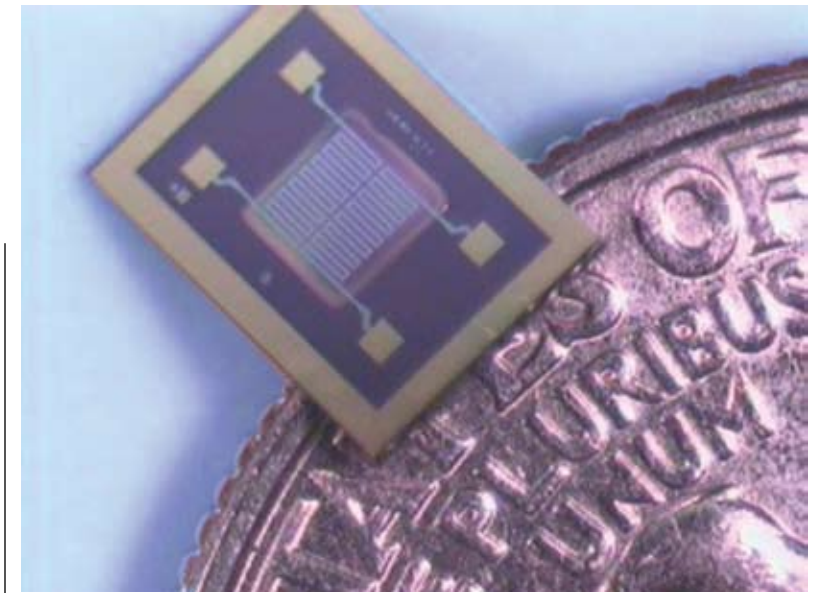
Sandia developed sample collection and preconcentration systems and integrated them with a commercial detector to build the first engineering prototype of this explosives detection personnel portal.

Imagine an apparently pristine lake where residents and vacationers fish, boat, and swim. Suddenly, based on reports of repeated human illness after fish consumption, regional environmental managers suspect that a pocket of organic toxins (the legacy of a now-defunct pesticide manufacturing facility) may be leaching residue into the lake shore. The lake, of course, also contains petrochemicals from boating and other byproducts of human activity, as well as substances of ecological origin. But the problem for investigators is to collect enough of the suspected toxins, without analyzing massive volumes of lake water in which the toxins from the former pesticide plant are likely highly diluted. And while this might appear to be the stuff of a Hollywood film script, it is actually an example of the type of real-life quandary encountered by regulators, safety experts, first responders, law enforcement, and health service providers that could benefit from the application of Sandia-developed preconcentrator technologies.

Chemical preconcentrators (PCs) are devices that efficiently collect substances of specific interest, such as industrial toxins, from large volumes of fluids or air in order to ensure that analytical instruments can efficiently and accurately characterize the chemistry of these substances. Sandia has a long history of developing and applying innovative and advanced preconcentrators for many types of analytes (analyzed substances), including toxic industrial chemicals, narcotics, biological toxins, explosives and other substances. The many different applications include screening materials for industrial

contamination, drug detection at portals, and efficient detection of explosives in various contexts. For example, preconcentration technologies, relying substantially on LDRD support for their development, have been incorporated into portable devices such as the Hound[®] and MicroHound[®]; a remotely operated explosives detection system such as the RoboHound[®]; SnifferStar[®] for deployment on unmanned aerial vehicles; and commercially available explosives detection personnel portals deployed at airports and in buildings. In addition, as detailed in another study in this publication, the MicroChemLab[™] provides self-contained gas and liquid analysis in a hand-held, rapid-result analysis system for a broad range of applications. MicroChemLab[™] employs a preconcentrator as the first of its three separation-and-analysis stages.

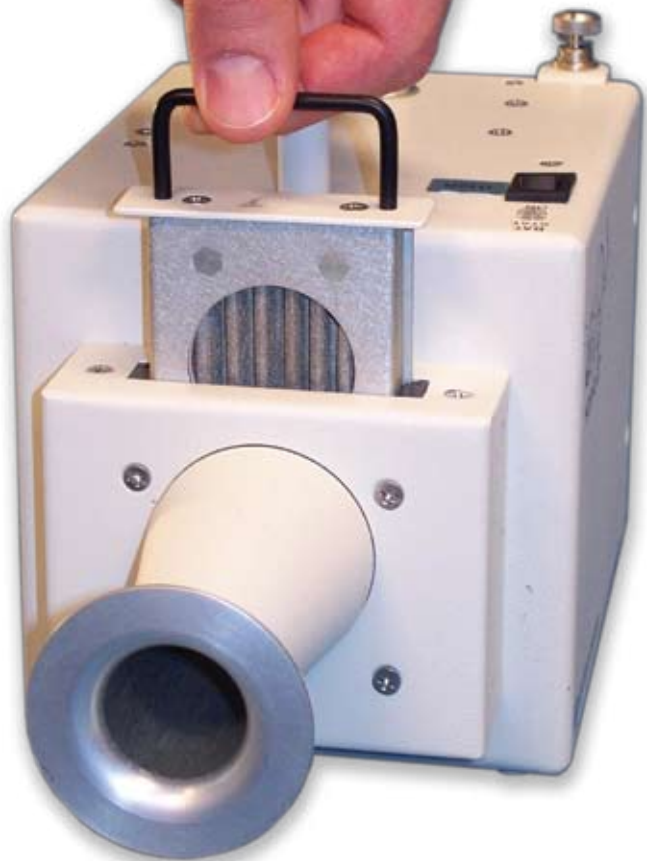
Motivated by a growing need among Sandia customers for trace chemical agent detection in the nano- (one-billionth, 10^{-9}), pico- (one-trillionth, 10^{-12}), and femto (one-quadrillionth, 10^{-15})-gram ranges, Sandia sponsored a 2001–2004 LDRD on the use of coatings for chemical preconcentrators to improve chemical agent collection. Potential customers include DOE, DoD, the National Guard, emergency support teams, law enforcement, and first responders. The engineering solution was a spinoff of a patented screen that successfully preconcentrates explosives, improving the sensitivity of some detectors by a factor of 10,000. Coating the screen mitigated problems connected with poor efficiency of chemical binding (adsorption) and breakdown (decomposition) of the molecular structure



Preconcentrator resting on a dime. The size of the PC is 4.5 mm x 6.5 mm with a heated central area of 2.5 mm.

during unbinding (desorption). For example, the project demonstrated reliable detection in small quantities of 20 nanograms or less of the flame retardant and chemical precursor to sarin nerve gas, dimethyl methylphosphonate. Nitroglycerine (an explosive and medication for cardiac patients) was detected reliably on nanoporous carbon-coated screens, with extremely low detection limits.

An ongoing issue in preconcentrator development has been their use in portable detection devices employed in the field by soldiers, law-enforcement officers, or first responders. For example, such situations demand rapid identification of chemicals without the delay inherent in conveying samples to an analytical laboratory. Often, the survival of soldiers/responders and minimizing the danger to the surrounding populace is contingent upon immediate knowledge of an unidentified substance's toxicity with no time for a lengthy analysis,



The Hound® portable explosives detector will benefit from LDRD-developed preconcentrator technology.

and with no immediate access to a laboratory. Even in the case of drug investigations, the health risks of prolonged exposure, such as those to law-enforcement officers with repeated methamphetamine contact are well documented. Such examples emphasize the importance of rapid identification.

Since the original 1997 microfabricated preconcentrator was developed for MicroChemLab, the challenges in this portable, rapid-analysis context have been to improve upon the ability of preconcentrators to adsorb greater quantities of target substances, while retaining the rapid desorption capabilities present in MicroChemLab,

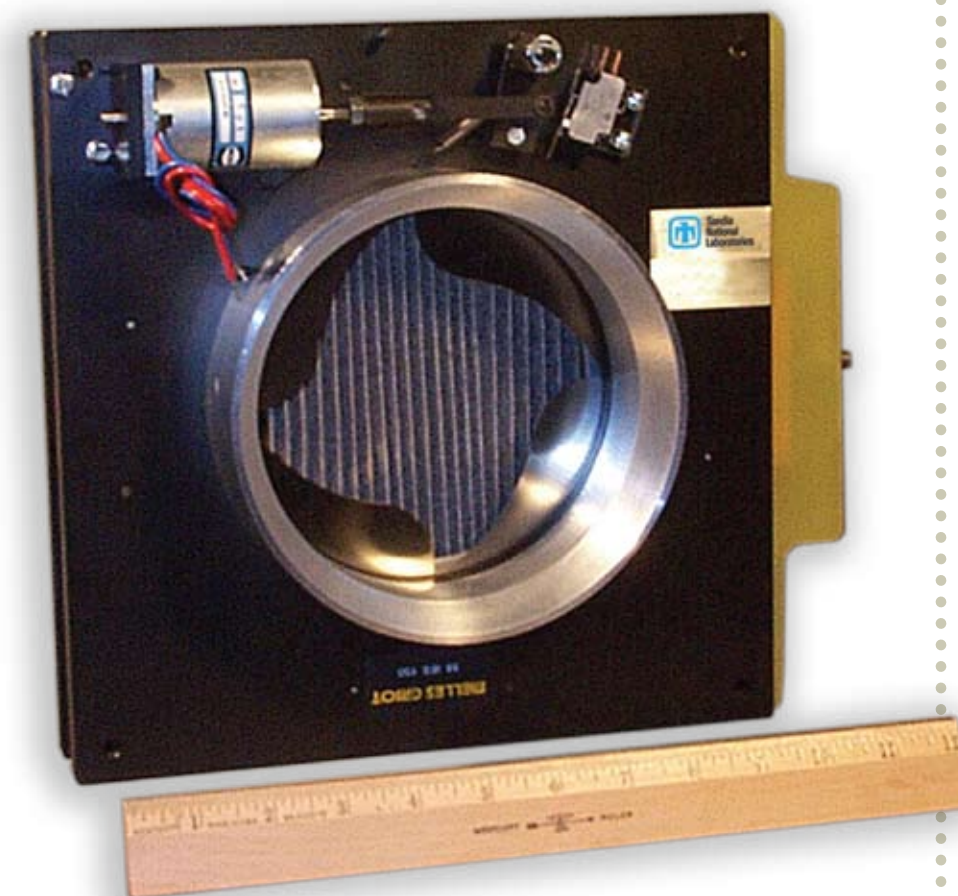
where complete concentration, separation, and analytical identification of samples were accomplished in 1 to 2 minutes. In addition, preconcentrators should bind as broad a range of potential analytes (whether chemical agents, explosives, or drugs) as possible, demonstrating effectiveness with both stable liquid and volatile (tendency to vaporize) substances. The goal was to maximize the surface area of preconcentrators to allow them to bind more molecules of a given analyte substance as a sample flowed through them, then to rapidly release the analyte upon heating, to permit its identification by a variety of downstream methods, depending upon the type of chemical being analyzed. Addressing such considerations would ensure that sufficient analyte would be trapped for analysis by the preconcentrator in a particular instrument such as MicroChemLab. The original preconcentrator was planar, or two-dimensional, and therefore limited in its surface area available for binding analytes. In a 2003 LDRD-funded project, Ron Manginell and his team tested several designs to address these issues.

The team retained the thermally isolating silicon nitride membrane used in the planar preconcentrator, but added a three-dimensional adsorbent coating zone, developing and testing two 3D engineering designs. In the first design, the flow of analyte was maintained perpendicular to the preconcentrator, through microstructures that essentially comprised a set of coated nested cylinders (concentric smaller-diameter silicon tubes within progressively larger-diameter tubes). In the second design, the preconcentrator was designed with microscopic fins that projected from the two-dimensional surface. Directing the flow parallel to the surface and past the protruding coated fins allowed enhanced adsorption of the analytes.

Depending on the targeted analytes, the project team employed a variety of different adsorbents to coat the surfaces of the two enhanced-surface-area designs. For example, thin film sol-gels (colloidal solids with some properties of liquids) were used for trihalomethane compounds; nanoporous carbon was employed for toxic industrial chemicals; in other instances surface-functionalized commercially available adsorbents were optimal. Computational modeling accompanied the engineering design studies, so that the team would be better able to predict faster desorbing designs.

Although a modest increase in power consumption and slower heating was observed for the 3D preconcentrators, there was a 30- to 100-fold increase in adsorbent surface area and collection capacity compared with the planar (2D) design. This increased collection capacity provides benefits for virtually all preconcentrator applications, allowing detection of target chemicals at lower concentrations in the detection systems in which these preconcentrators are used.

“This device can work with different types of microanalytical systems, is small, uses minute amounts of power, is extremely portable, and is inexpensive to produce — all making it very interesting to both industry and the military,” says Manginell. In addition, the collection capacity of the 3D preconcentrator extends the range of applications to include volatile compounds, such as liquid explosives and many liquid



Sandia's patented two-stage preconcentrator collects heavy organic molecules typically found in high explosives from very large, dilute air streams.

explosive components. This bodes well for several future application areas.

In 2006, a foiled terrorist plot to smuggle liquid explosive components aboard airliners provided ample evidence of the need for such enhanced detection capabilities. “Flexible and accurate new detection technologies provide important additional tools to our security officers,” said Transportation Safety Administration Chief Technology Officer Mike Golden, addressing the agency’s response to the terrorist threats. Advances in deployable preconcentrator technology epitomize the ever-improving suite of new tools to which Sandia engineering, driven by LDRD support, is contributing. ★

Neutralizing National Security Threats

Earth Penetrators and Sensors for Hard and Deeply Buried Targets

Noting that adversarial targets of strategic and tactical importance were moving to underground facilities, the 1995 Counterproliferation Program Review Committee recommended that their defeat should be a top priority. Potential US adversaries have constructed hidden facilities deep below the surface and hardened them with additional concrete to resist penetrator weapons currently in the US conventional arsenal. In order to maintain our national security, designers at Sandia began studying advanced warheads to hold these facilities at risk. Since the mid-nineties, the LDRD program has served as a foundation from which to evaluate approaches to earth penetrators for the defeat of such hard and deeply buried targets (HDBT), disseminating project results into areas of nonproliferation (seismic imaging and compact air-delivered sensors for the Defense Advanced Research Projects Agency [DARPA]) and space exploration (lunar and Mars studies for NASA).

Several salient challenges loomed ahead for this program, each simultaneously representing both scientific challenge and national-security imperative. The most difficult entailed the development of a methodology for identifying and characterizing the conditions of the ground

cover and/or protective wall design of an HDBT before an attack. A second involved solving the problem of monitoring the high-G acceleration environment encountered as a penetrator broke through the ground, a successful solution poised to provide real-time indications of the condition of the penetrator during its underground flight. And as a final challenge, designers wished to establish pinpoint control of the penetrator's firing set such that it would trigger at the optimal time in its inward penetrating trajectory, thereby maximizing lethal effects of its explosive load.

In 1995, the first HDBT LDRD began developing algorithms to accurately simulate

An earth penetrator approaching its target during a test.



the interaction of a high-mass earth penetrator with various types of cover and concrete. This study began to address the issues of increasing the velocity of impact, keeping the penetrator on target, and characterizing its motion. Sandia staff directly addressed the last of those challenges in a following LDRD that sought to develop small, light, data recorders to measure and report multi-axis accelerations that were expected to exceed 10,000 Gs. The goal of the LDRD projects was to shift the methodology of the penetrator-development program from “build and test” to the far more-efficient “design, build, and test.” Over the succeeding decade, high-G data-recorder developments accomplished the task of characterizing a

penetrator's motion to and through an HDBT. In turn, this knowledge enabled design refinements, facilitating optimal motion after penetration. Building on investments by the Defense Threat Reduction Agency (DTRA) and other external agencies, subsequent LDRD projects birthed refined accelerometer design and improved communication techniques, drawing engineers closer to characterizing the loading environment that the payload must survive during the piercing of a target.

In 1997, scientists and engineers began addressing the issue of site characterization, testing the feasibility of monitoring seismic emissions from deep facilities as a means of



An illustration of the penetrator's potency through a wall of steel-reinforced concrete.

providing long-distance observations. An initial LDRD combined seismic modeling, signal analysis, and experimental tests, followed by a second project that employed enhanced 3D geophysical modeling to optimize potential sensor layout and distribution, assessed the isolation of local soil effects, and exploited advanced signal-processing techniques. To validate these advanced geophysical and signal-processing methods, this team used the novel algorithms to process data previously acquired at the Nevada Test Site. From 2002 through 2007 a series of LDRDs added modeling capability for such areas as rock penetration, fracture and fragmentation modeling, and the penetration of both continuous and fragmented materials.

Stepping up to the daunting challenge of site pre-characterization, Sandia boldly initiated a 2003 Grand Challenge LDRD on the earth penetrator problem, with David Gardner as principal investigator. A multidisciplinary

systems approach, this initiative integrated Sandia expertise in seismic imaging, air-deployed sensors and sensor networks, earth penetrators, and modeling and simulation. Key investigations would center on a sensor system that would help ensure a nuclear-weapon earth penetrator's success through the process of rapid geologic site characterization. The team's goal was to collect penetrability and seismic data using a network of aerially deployed, earth-penetrating sensors and active sources in order to combine penetrability data with a seismic velocity map to determine optimal aim-points.

This project assailed the huge challenge of delivering aerial probes and aerial seismic sensors to a geological site, penetrating the site to assess geology, and effectively communicating this data to a central receiver even in the presence of radio interference and/or dense foliage. The probe employed a novel design, separating, upon impact, into two sections, the forward which penetrated deeply into the earth and transmitted geological data to the aftbody, lodged near the earth's surface. This arrangement was designed to more-effectively relay that geological data back to a central communications receiver. The drop tests of five sensor units and two probes enabled collection of flight characteristics and superior penetration performance data. The probes separated well and transmitted their data clearly, and the sensors lodged at the surface and collected and recorded data for seismic mapping, closing this successful Grand Challenge. Follow-on DARPA funding supported ongoing development of design portions of this concept in preparation for genuine field applications.

Eric Klamerus headed another LDRD focused on improving the challenge of optimizing the moment of detonation by upgrading an earth penetrator's firing set. Postulating that precise firing of the weapon's

fuze could dramatically improve operation, Klamerus's team packaged and demonstrated survival of a prototype fireset and data recorder at an extremely high-speed penetration environment, the broader goal to gain a more-fundamental understanding of the effect of very high speed impacts on penetrator electronics. Ultimately, this knowledge, in part acquired through simulation, is enabling the design of both more robust fuzes and data recorders for both conventional and nuclear applications. More globally, that knowledge is guiding future investments in penetrator joint and case design, guidance and control technology, shock-hardened electronics design, electronics packaging design, and intelligent fuze algorithms development.

The results have been dramatic, showing test firings into simulated structures in which the penetrator was retrieved intact and the fireset fired at just the correct moment. These areas of investigation, in turn, impact such ongoing Sandia activities as the DTRA Hard Target Defeat program, the Department of Defense/DOE Munitions Memorandum of Understanding, and the Fast Tactical Missile System-Penetrator (TACMS-P) program.

As is often the case, such investigations, which are singularly focused by a specific project goal — in this case, securing the nation against constantly evolving HDBT risks — spur the development of algorithms and engineering techniques that broadly impact seemingly unrelated areas. For example, based upon these new capabilities, Sandia has proposed similar technological approaches for NASA missions probing lunar and Martian landscapes in pursuit of improved geological understanding (and a search for water and minerals for potential colonization) of our nearest astronomical neighbors. ★



Post-test condition of a penetrator target, a series of concrete blocks, viewed after several penetrated target blocks were removed



The second stage of the geological site-characterization probe transmits radio signals about geological data back to central communications.

Ultrafast Laboratory-in-miniature

MicroChemLab



A recent version of the hand-held microchemlab portable laboratory.

Those with an ear attuned to the dialogue in the mid-1990s analytical chemistry community, were privy to a “buzz about a Lab on a chip,” according to Sandia Program Manager, Duane Lindner. Spurred by advances in microfabrication and advanced microsystems integration, scientists were intrigued by the possibilities of miniaturizing chemical analysis capabilities so they would be conducted in “laboratories” approximately the size of a credit card. Appropriately, Sandia scientists took the lead in actualizing this vision. The result was not simply a technology, but also a conceptual framework and business model for the Grand Challenge–level project: high-visibility, ultrahigh-risk initiatives propelled through LDRD funding. For the initial years of the millennium, “Grand Challenge” became synonymous with “MicroChemLab” (μ ChemLab™).

Playing off existing strengths in analytical chemistry, microfabrication, and sensor systems, both New Mexico (NM) and California (CA) staff recognized the technical challenge, and developed a vision for actualization. The NM team envisioned a miniaturized gas chromatography (GC)-based analytical tool, while the CA team moved toward a liquid chromatography (LC) platform. Microtechnologies to separate and subsequently identify chemicals would shrink the analytical system from the order of meters to that of millimeters.

Sandia program management assembled a multi-organizational management team, an external advisory board, and a legal team

to oversee patent and technology licensing issues. And according to former project manager, Steve Martin, the insightfulness of the technical staff was matched by the perceptiveness of upper management to champion and adequately fund, from 1997 through 2001, the Grand Challenge LDRD (GC-LDRD) — which funded both the research itself and the hiring of postdoctoral staff. While the emphasis on developing an integrated MicroChemLab prototype was central to the GC-LDRD project, the management team recognized that Sandia also needed to provide some of the fundamental scientific understanding required to enable development of such devices. This part of the project was known as Science on the Microscale and was funded as part of the GC-LDRD.

Within the GC-LDRD, the gas chromatography effort focused on detection of chemical warfare agents, the liquid chromatography team on detection of explosive residues. This work ultimately produced a prototype unitary dual-function device —the MicroChemLab “gold brick.” As the GC-LDRD proceeded, DOE initiated the Chemical and Biological National Security program in 1997. Eventually, this program provided additional funding for MicroChemLab but changed the LC focus toward biotoxin detection. Although a rather large reset, the more-significant realization was the difficulty of incorporating both technologies into a single hand-held device. Each technology was difficult; in the same box, it became “hard-squared,” Lindner recalls. Under DOE sponsorship, the project underwent a transition back to a somewhat separate two-team developmental mode. The key demonstration was that it worked as a



Microchemlab’s analytical data can be quickly downloaded to either a PC, or as shown here, even to a personal digital assistant (PDA).

low (battery)-power, handheld unit, able to separate and identify chemical agents with extremely high sensitivity and ease of use — and within a one-minute timeframe, far faster than traditional chromatography apparatus, which required many hours to perform such separations.

The GC version features three miniaturized processing stages, together with a pump and valve system to control gas flow. In stage one, a sample is reversibly collected and concentrated onto a membrane, which can be coated with a diversity of films, each of which selects an analytical choice-range of chemical compound types for analysis — for example, one such coating might select organic chemical structures related to the chemical toxins Sarin and VX. A heating element then desorbs or frees the chemicals in the vapor phase, the flow system suctions the mixture of gaseous chemicals into stage two, a gas chromatography “column,” a micro-spiral etched into a silicon wafer, that occupies only 1 cm² of space, but is, remarkably, about 1 meter long. By either coating the walls of this spiral or filling it with coated beads, the concentrated gases released from stage one enter and are transiently bound to the column, gas molecules binding and unbinding with



The originally produced Microchemlab proof-of-principle “gold brick,” showing the intricate internal engineering

different strengths and time courses as they “bounce” through the spiral as a function of their exact chemical structures.

Hence, at the exit of the spiral, the original mixture is now separated, molecules exiting at slightly different times contingent upon that binding-unbinding history within the column. This typically requires less than a minute. As the separated chemicals exit, they encounter stage three, a number of surface acoustic wave (SAW) sensors, coated surfaces that vibrate with sound waves. Momentary sticking of the sequentially exiting gas molecules from the spiral changes the vibration the SAWs, in such a way that an electronic circuit can detect the mass of whatever substance has exited the column at a particular time. This combination of preconcentrator coating choice and separation of materials by the column allows identification of substances in the sample after each of the substances exits the column and is reversibly bound by the SAWs.

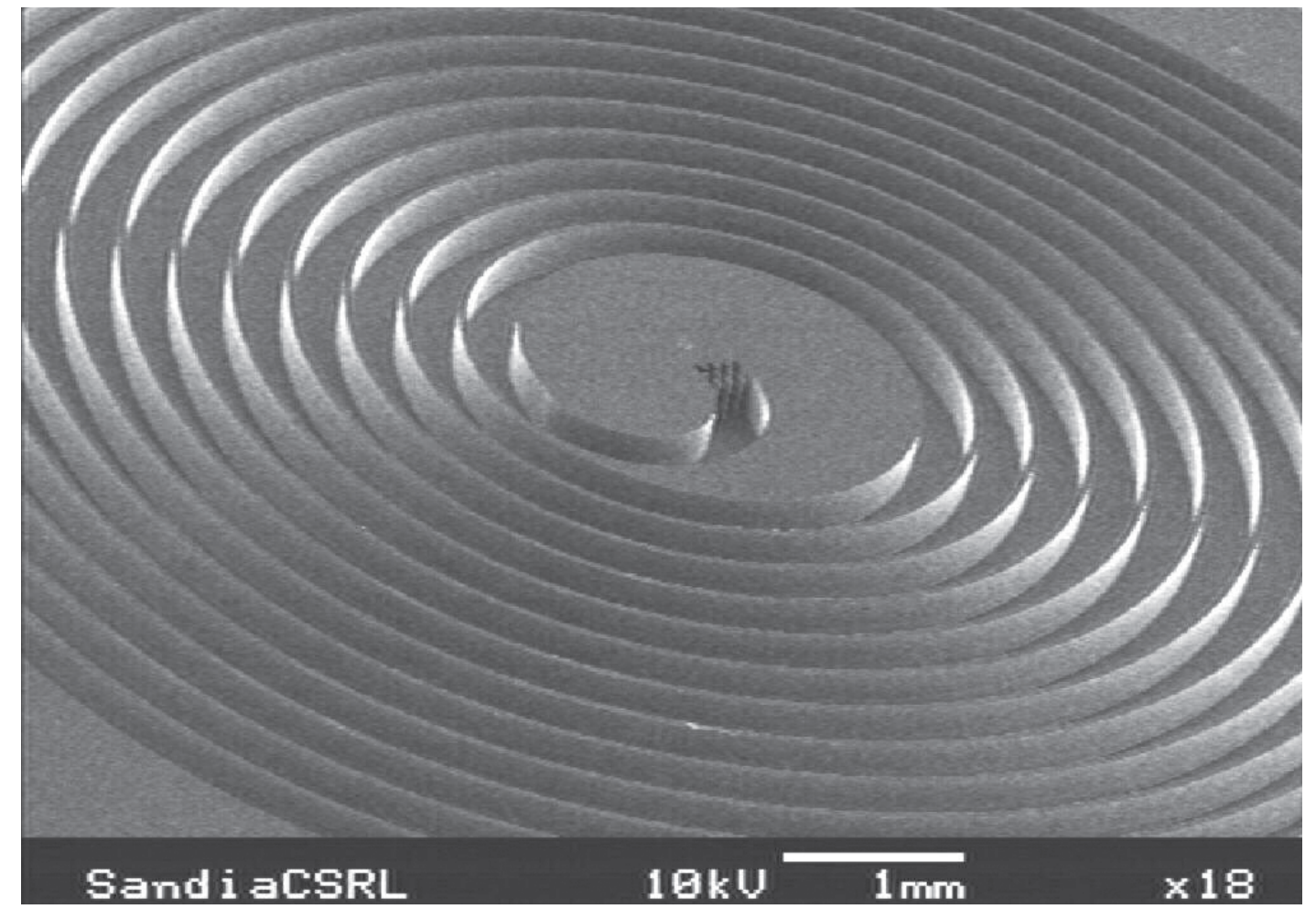
Although the specific techniques differ for liquid mixture separation and detection (notably fluorescence-based optical detection after ultraviolet excitation of separated molecules), the LC version operates on similar overall principles, but relies on Sandia’s ongoing refinement of microfluidics technology

for controlling minute flow volumes. This connection is paralleled by several others provoking the LDRD funding of a number of follow-on projects related in one way or another to the refinement of microtechnologies with global application to other Sandia initiatives: preconcentrator refinement, new optical-detector systems, and broadening detection capabilities from molecules to entire microorganisms (such as viruses).

“LDRD was crucial to set the stage for subsequent investments,” says Martin. Despite a brief funding valley at the end of the grand challenge LDRD, subsequent and current investments by a variety of agencies have been significant. For example, FY 2003 brought investments by DOE, DHS, DoD, DTRA (Defense Threat Reduction Agency) the FAA, General Electric, and Bristol-Myers Squibb, in addition to Lockheed Martin. This illustrates the recognition of the broad applicability of the technology in areas such as chemical weapons, nuclear nonproliferation, natural gas composition, water-quality analysis and pharmaceutical manufacturing.

There has been one minor disappointment in the initiative — despite MicroChemLab’s™ obvious advantages, intellectual property and technology licensing issues have produced delays in establishing a solid corporate base for production of commercial units. For example, a CRADA with the Waters Corporation was direct evidence of the technology’s commercial value, yet, years later, Waters has yet to bring a product to market. On the other hand, the startup venture, Exigent Technologies, has burgeoned from its few Sandian founders to approximately 125 employees in just a few years.

“We tend to do things by hand,” points-out long-term GC team member Pat Lewis, “while industry needs something that’s less of a hybrid, easier to manufacture. It’s frustrating to see the technology languish . . . see the military sending soldiers out with the technology they’re



A recent gas chromatography “column” design, allowing an approximately one-meter-long separation channel to fit within a one square-centimeter area of etched chip.

using now,” he adds. And dissatisfied with Microchemlab’s 1- to 2-minute cycle time, Lewis’ expectations are that the systems can be further miniaturized, cycle times reduced to 30 seconds or less. Moreover, he is confident that by incorporating multiply parallel systems within the same handheld unit, the technology can be expanded to detect 30 to 50 substances per device, significantly more than is currently attainable.

Lewis’ startup, Defiant Technologies is now licensed to produce the GC version, while Exigent holds an LC license. In addition, Labsmith, a manufacturer of fittings and couplers for assay equipment, holds the license for marketing Sandia-developed microfittings essential for microfluidics. And back at Sandia,

LDRD funding drives research into improved separation columns, dielectric-potential-driven micropumps, and the MISL Grand Challenge in the system dynamics of immune responses — as well as an academic affiliation with George Mason University for biomarker identification. And NIH is sponsoring the development of “point of care” medical diagnostic systems, exploiting the huge potential for saliva-based presymptomatic diagnosis of disease. This illustrates how improved analytical capability can drive scientific progress toward unwinding a seemingly intractable knot of complexity, in this instance, the permutations of immune system responses. From detecting chemical weapons to rapidly diagnosing illness at point of care — such is the amazing breadth of the MicroChemLab™ story. ★

Boldly Bridging Diverse National Security Arenas

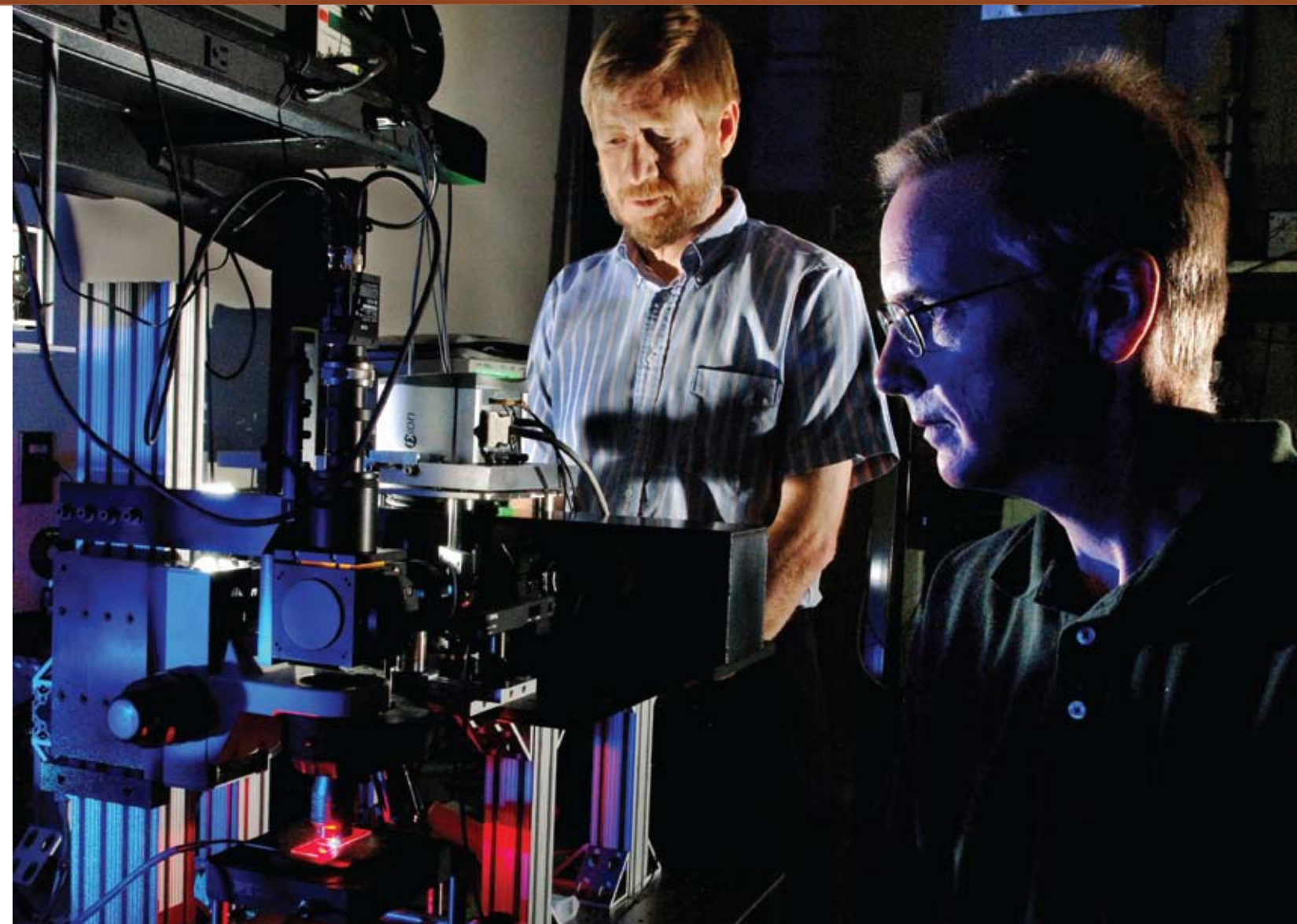
Hyperspectral Signal Extraction

The encoding of information is all around us in everyday life — voice signals encoded as pulses in phone lines, email text encoded as bytes of information routed between computers that ultimately decode it back to text. Often, such signals are encoded by light (as in optical fibers), and sometimes optical encoding can be quite complex, taking the form of complicated spectra, which have long been fundamental tools of scientific research. Such spectral techniques employ light of various wavelengths — infrared (IR), visible, ultraviolet (UV), and x-rays — to interrogate structures. And in response, spectral data are collected as light waves absorbed, reflected or emitted from these interrogated structures, be they inanimate or those of living cells. The returning (spectral) light can be of a variety of wavelengths and can be collected in several spatial dimensions. Encoded in this absorbed, reflected or emitted light can be information about molecular structure, energy transformations, and the dynamic processes of living cells and tissues. When all possibilities for such spectra are considered, the complexity of the encoded information can be overwhelming.

Multivariate data analysis represents a variety of mathematical approaches for extracting qualitative and quantitative chemical information from spectral data collected from a sample. Among these multivariate approaches is multivariate curve resolution (MCR), which allows chemical information to be obtained from hyperspectral

images collected from 2D or 3D objects using light collected at hundreds of different spectral wavelengths. From its first roots in late-1970s Sandia research to the first LDRD-funded projects in the early 1990s, Sandia research teams have doggedly sought new applications of these multivariate spectral analysis approaches. As an example, early applications in multivariate data analysis enabled a Sandia team and collaborators from the University of New Mexico to patent a technique, in 1989, to measure any analyte (analyzed substance) within the human body using infrared light absorbed or reflected from skin or other body tissues. This work led to the commercialization of a noninvasive alcohol monitor that measures blood alcohol by analyzing reflected light from the forearm.

Hyperspectral 2D or 3D spatial images can often include nearly a million spectra, each containing hundreds of spectral wavelengths of light. Applied to these hyperspectral images, MCR can allow researchers to understand the way the spectra from individual chemical components in the sample combine to form each spectrum in the image. The output from this process is a set of individual spectral fingerprints for the material being imaged. These spectral fingerprints reveal the identity of individual components in the material, their quantity, and their spatial location in the sample. Because such spectra and their information about molecules and nano- or microstructures are fundamental to a broad swath of research endeavors at Sandia and



Mike Sinclair and Dave Haaland monitor an experiment on the hyperspectral microscope, an instrument that has contributed to several research areas.

elsewhere, hyperspectral imaging and its subsequent signal extraction by MCR have been of enormous value in a diversity of research areas. Appropriately, researchers* from numerous disciplines within Sandia have contributed to this work, including those from the areas of Microsystems Materials, Materials Characterization, Biomolecular Imaging, Statistics, and the entire Grand Challenge team currently developing the Microscale Immune Studies Laboratory (MISL), a team itself drawing from many different groups within the Laboratories.

In addition to refining the MCR technique, Sandia researchers have participated in the development of several hyperspectral

microscopes, which collect spectral information from thousands to millions of 2D or 3D image pixels from chemical or biological samples. Using these new microscopes and MCR methods, they have solved problems encountered with commercial microscopes that exhibited poor reproducibility and misquantitation due to extraneous light derived from the presence of unexpected impurities. Such initiatives, many funded at least in part by LDRD, have permitted extension of the utility of MCR from 1D spectra of analytes to 2- and 3D hyperspectral images. A team of

*Dave Haaland, Mike Sinclair, Mike Keenan, Dave Melgaard, Chris Stork, Howland Jones, Jeri Timlin, Mark Van Benthem, and Ed Thomas; and the MISL team



Former President Clinton shows an intense interest in a noninvasive blood glucose monitor during a visit to Sandia.

experimentalists, statisticians, and computer scientists has applied the MCR approach to such projects as inferring the quality of aging polymeric and nuclear reactor materials, and recently, to the simultaneous and rapid monitoring of gene expression of thousands of genes from a living organism. This breadth of scientific inquiry indicates the value of MCR at rendering spectral information more accessible, and therefore, more valuable for researchers.

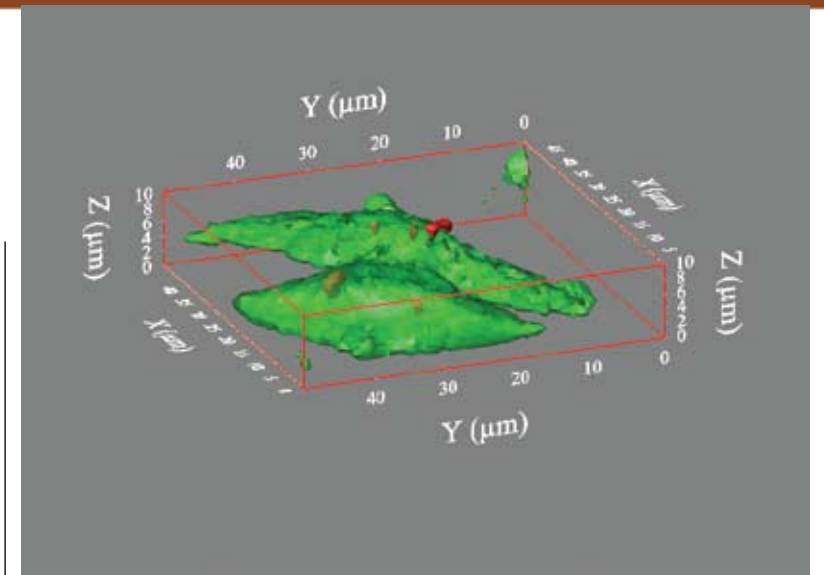
Sandia researchers first attempted to apply multivariate analysis to aging explosives, gaining useful information, but finding that there was an extraordinary amount of data to reduce. A collaboration of chemists, computer scientists, and statisticians, this team worked to accelerate the processing algorithms and thereby extend this work to large-scale quantitative IR spectroscopy. It developed techniques to perform quantitative analysis of chemicals, which resulted in the 1989 patent,

and this, in turn, lead to work on noninvasive techniques to both monitor and identify blood sugars, an initiative obviously benefiting diabetics who must continually use invasive skin pricks to draw blood for glucose testing. In 1993, this work also lead to the formation of a small startup company in Albuquerque, Rio Grande Medical Technologies, which was able to secure more than \$60M in funding from a subsidiary of Johnson and Johnson over a 15-year period. A portion of this money funded a CRADA between Rio Grande Medical Technologies and Sandia for production of a commercial device to noninvasively monitor blood glucose levels in diabetic patients.

LDRD funding has driven a host of new applications for MCR. In the area of material-durability diagnostics, one LDRD developed IR spectroscopic techniques to quickly identify chemical constituents of materials and then make inferences about their aging

characteristics and viability, work directly impacting evaluation of the aging of materials used in airplanes and nuclear reactors. In life science applications, another LDRD funded development of a new hyperspectral microarray scanner for simultaneously comparing the expression levels of thousands of genes from samples placed on a single microscope slide (known as a microarray). The use of MCR techniques to analyze the data for gene expression improved the accuracy of the measurements. In this type of fundamental genetics research, living cells are exposed to a variety of different environmental or chemical situations and their genetic response assayed by fluorescence spectroscopy. Typically, cells respond to an environmental change — a hormone signal, for example — by activating formerly quiescent genes and silencing formerly active genes (intermediate levels of so-called “gene expression” are, of course, also possible).

The same general pattern of changing gene expression also characterizes the activation of cell division in quiescent cells — for example, in wound healing, where cells around the edges of a wound begin to rapidly divide to close the gap in a wounded tissue’s surface. And in certain instances of cancer, cells overexpress or inappropriately express genes associated with growth. Hence, biologists often wish to simultaneously screen for changes in the expression of many genes, over time, with the necessity to screen arrays of thousands of genes (DNA microarrays) via spectroscopy. The development of the hyperspectral microarray scanner and the use of MCR to analyze the generated data helped leverage Sandia collaborations with UNM professors Cheryl Willman and Maggie Werner-Washburne that were funded by the Keck Foundation, NIH, and Sandia’s LDRD program. The Sandia/ UNM collaboration pursued information about changing patterns of gene expression in the cryogenically stored cells of different leukemia patients and in yeast cells emerging from their quiescent stationary (nondividing) state.



Hyperspectral fluorescence image from the MISL Grand Challenge: E. Coli (bacteria) labeled with fluorescent protein (AsRed) invading two elongated macrophages (a type of immune system white blood cell) expressing green fluorescent protein–labeled RelA protein residing mostly in their cytoplasm – thus the two cells appear filled with green, except for the red or reddish-brown pockets of ingested bacteria.

Not satisfied with current capabilities, Sandia MCR researchers have also contributed expertise to the LDRD Grand Challenge, MISL, in which the MCR-driven 3D hyperspectral confocal fluorescence microscope is the keystone instrument for analyzing protein signaling in living cells; to monitor patterns of protein signaling among the cells of the immune system that change almost from moment to moment in an immune response.

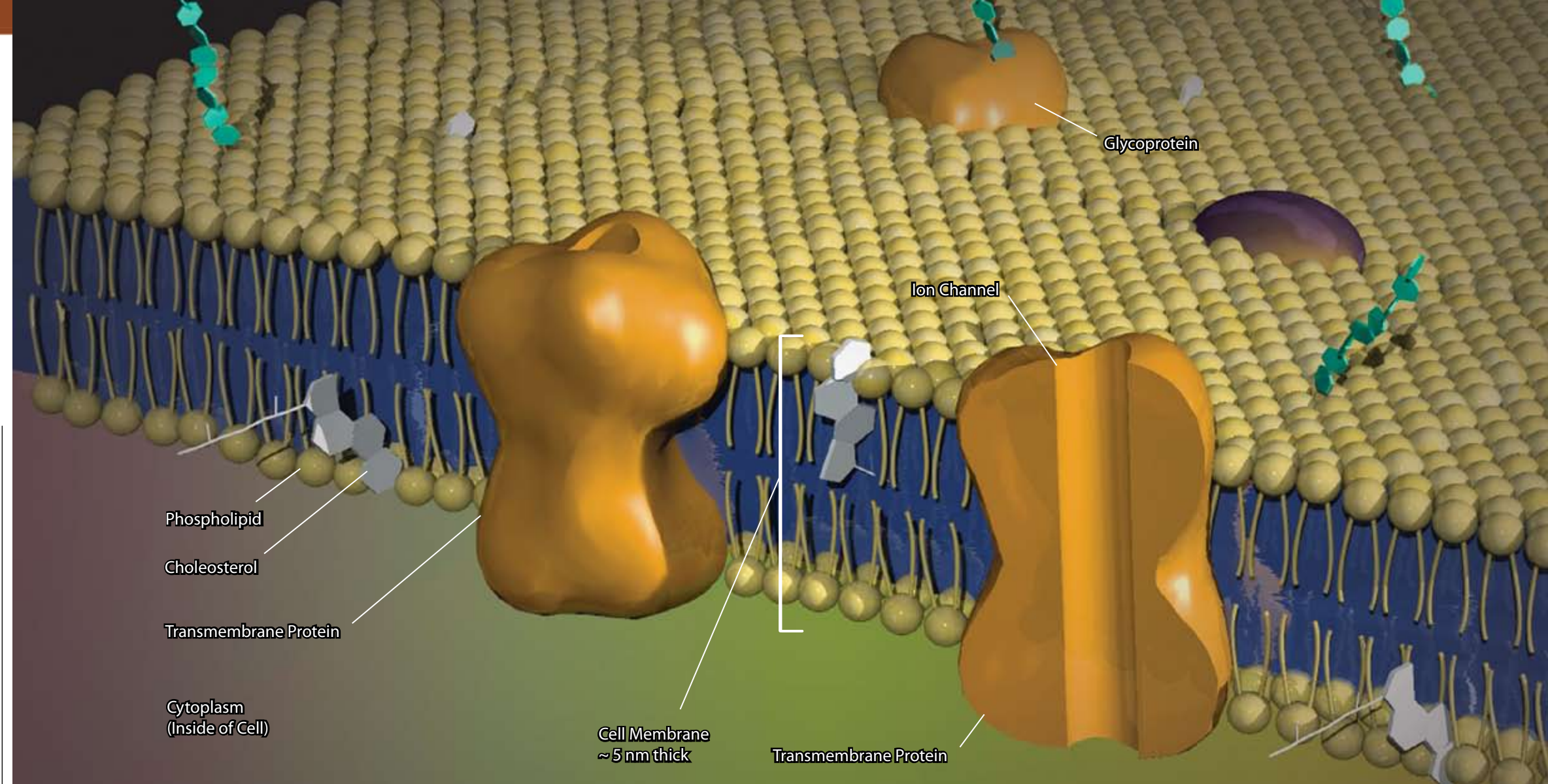
Taken as a whole, this work has elicited funding from the DOE Genomes to Life program, NIH funding for rat brain imaging, gene expression analysis, and microarray scanning, EPA funding of a gene expression program, and a CRADA with Monsanto to develop improved seed-based products for biofuels. And beyond the exemplary research described herein, there are, additionally, several other major hyperspectral research efforts ongoing at Sandia. Quite remarkably, over 30 years after its initial incarnation, a broad diversity of Sandia researchers are still striving to perfect multivariate analysis techniques — all in service to the nation, and in the broader context, for the betterment of mankind. ★

A New Biosciences Capability for Sandia

Interfacial Biosciences Grand Challenge (IBIG)

The anthrax bioterrorism incidents that struck fear into Americans, post-9/11/01; the bioagent experimentation and fatal subway nerve-gas attacks of the Japanese in 1995; bioterrorism alone could easily be construed as adequate reason for Sandia to invest in a larger slice of biosciences research. Biological counterterrorism has become symbolic of our age, and as the ultimate natural representative of nanotechnology, cells and their molecular interactions were a logical fit for a laboratory like Sandia, with such extensive high performance computing and nanotechnology expertise. It was against this backdrop that Sandia management approved LDRD-driven entry into bioscience research with the Interfacial Biosciences Grand Challenge (IBIG), by far the Laboratories' highest-funded bioscience commitment to that point in time.

Funded from FY 2001–2003 at \$7.2 million, IBIG's major thrust would be to tackle key obstacles to achieving a better understanding of the function of the living cell's most important nanoportal, its outer membrane, a thin sheet of (fatty) lipid studded with thousands of different protein molecules. Some of these membrane proteins regulate entry/exit of salts like sodium and calcium, others mechanically assembling cells into tissues and organs, still others receiving hormonal signals. But many membrane proteins can have their normal function subverted by bacterial toxins (such as anthrax) and viruses (like HIV), pathogens that use specific membrane proteins to gain entry into



cells and damage or kill them. Consequently, from both health and bioterrorism perspectives, understanding the cell's outer membrane at a more-fundamental level became a national-security priority for Sandia.

The completion of the human genome project had unfolded many mysteries of the DNA library deep inside a cell's nucleus, and it was time to study genes-in-action, to clarify how gene-encoded proteins choreographed the remarkable molecular dances occurring in and around cells. The outer membrane, the interface between a cell and its environment and its relationship to other cells was clearly key. According to Len Napolitano, IBIG project manager, Sandia was uniquely positioned to do this work. "Based on Sandia's existing capabilities in bioanalytical technology, computer science and surface science, this

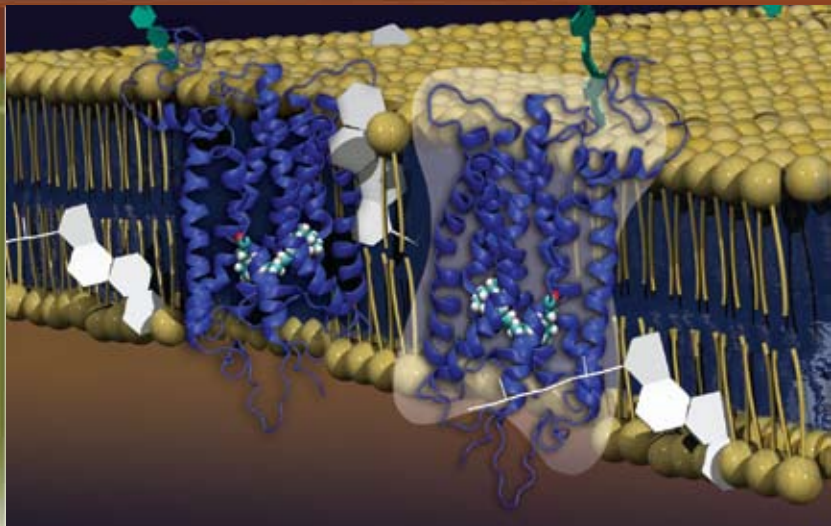
project should catalyze a leap forward, creating a unique niche for Sandia in biotechnology," he observed.

Imagine a plastic bag filled with potassium and phosphates and many specialized nanostructures and immersed in a container of salty (sodium and calcium chloride) water in which are also found very small amounts of hormones. The plastic bag (the cell's outer membrane) is studded with a fantastic array of shapes — barrels, undulating snakes, pockets, channels —each shape a different protein. Such is an oversimplified picture of the cell. Initially the IBIG team was focused on the technical aspects of developing a proof-of-principle for determining the structure of those differently shaped membrane proteins, by working in experimental biology, protein chemistry, and computer modeling and simulation.

Schematic representation of a cell membrane showing representative types of membrane proteins and glycoproteins.

Eventually, the project focus was narrowed toward clarifying the structure and function of rhodopsin, an elegantly shaped protein molecule penetrating through the membrane of the rod photoreceptor cell in the retina of the eye. Struck by photons of light, this protein changes shape to begin a complex process that, nanoseconds later, causes a change in signals passing to the optic nerve, ultimately resulting in visual perception deep in the brain.

IBIG leveraged Sandia's capabilities in bioanalytical technology, computer science, and surface science to enable modeling and measurement of such sophisticated nanomolecular processes as rhodopsin's shape-shifting in vision. A number of



Ribbon model of the protein rhodopsin, a transmembrane, vitamin-A-associated protein (“opsin”), shown in the context of the membrane of the rod photoreceptor cells of the retina. Absorption of even a single photon of visible light induces an amplifying cascade of biochemical signals that ultimately results in a signal from the retina to the visual cortex of the brain.

innovative experimental methods for working with integral cell membrane proteins at the molecular level were developed, and a method for establishing the structure and function of membrane proteins was tested. The challenge was to integrate a core of technologies that could provide structural and function information about the cell’s membrane at the molecular level. Such technologies include mass spectrometry, a suite of novel scanning probe microscopes, and state of the art membrane simulation capabilities using massively parallel computers.

But the initiative was actually much broader in impact. The consistent view is that IBIG gave the Laboratory entrée as a “player” in biology R&D, establishing a bioscience capability and the Labs as credible in the biotechnology world. It created new facilities and hired new people. “Before IBIG, Sandia was not a player in experimental bioscience,” opined Joe Schoeniger, IBIG principal investigator.

Certainly, bioscience is grander in scope than simply a cell’s genes and its membrane, encompassing the crucial concept of complex systems dynamics — the mathematical physics

that describe how trillions of cells, combined into tissues and complex organs like the kidney are choreographed by only about 30,000 genes and perhaps 100,000 different proteins. With IBIG, Sandia had merely scratched the surface, demonstrating a capability to do high-quality work in a few focused areas of research, with the potential to do much more. Nonetheless, there is little doubt that without IBIG, along with the earlier Molecular Integrated Microsystems (MIMS) Grand Challenge, Sandia would not have been positioned to participate in the dramatically expanded biologically based programs of DOE, DoD, and more recently, DHS.

Significantly, given Sandia’s commitment to establish a role in biodefense, IBIG also positioned Sandia to compete for bioscience funding from NIH, for example, a recently completed project in collaboration with the University of Michigan Dental School, the project’s purpose to develop and demonstrate the Integrated Microfluidic System for Oral Diagnostics. Funded by the National Institute of Dental and Craniofacial Research, the initiative represented Sandia’s first ever NIH-funded project. Earlier this year, the National Institute of Allergy and Infectious Diseases announced funding for a portable microfluidic platform for rapid detection of biotoxins, this five-year project, a Sandia collaboration with the University of Massachusetts (Dartmouth) and Bio-Rad Laboratories. These initiatives demonstrate that Sandia’s unique skills in nano- and microtechnology — in this instance, microfluidic platforms — were simply awaiting the Laboratories’ entry into cell and molecular biology as providing the proper conditions for the myriad possibilities now developing for biological investigation.

Inherent in these possibilities are medical-intervention technologies, particularly in

bioterrorism-related incidents. Anup Singh, Sandia principal investigator on both NIH projects, says a lightweight, portable device for measuring exposure to toxins would allow on-site emergency personnel to draw blood samples and make a rapid determination of the degree of exposure. Individuals requiring follow-up treatment could then be monitored, and appropriate treatment initiated.

Acknowledging the ongoing Sandia commitment, in January 2005, the BioScience Research Foundation (RF) was created to establish a more focused bioscience and technology capability at the Labs. The primary thrusts of this new RF are biodefense and emerging infectious diseases (EID) and biofuels. And as it did at IBIG’s inception, LDRD continues to drive the creativity forward. The Microscale Immune Studies Laboratory (MISL) is an LDRD-funded Grand Challenge focused on normal and abnormal patterns of cell signaling occurring in response to infection — with signaling proteins (cytokines) and their protein-receptors in the membranes of other cells taking center-stage in inflammation and immune defenses. MISL is the flagship project in the BioScience RF’s biodefense and EID thrust. Meanwhile, in the biofuels arena, Sandia’s participation in the Joint BioEnergy Institute (JBEI) a partnership of three national laboratories and three San Francisco Area research institutions, forms a major initial commitment.

Given the US current preoccupation with renewable energy, JBEI has recently been chosen to host one of three bioenergy research centers funded by DOE through the DOE Genomes to Life (GTL) Program and is a major DOE effort within the Biological and Environmental Research (BER) Program. This new center is expected to receive \$125 million in DOE funding over five years. According to



Partnership of three national laboratories— including Sandia — and three Bay Area research universities is hosting the Joint BioEnergy Institute (JBEI), its logo superimposed on switchgrass, one proposed source of biomass for biofuels production.

DOE Undersecretary for Science Raymond Orbach, “this early infusion of funds will enable JBEI to get underway immediately on the urgent quest for the transformation breakthroughs our nation needs to usher in a new biofuels economy.”

Bioterrorism, biofuels, or simply the elucidation of the molecular interactions underpinning cell membrane proteins — bioscience is now and will presumably remain a central component of Sandia’s national-security mission, its competence ever evolving to address national priorities. The benefits of the IBIG LDRD investment permeate research initiatives Laboratory wide as the capabilities seeded by this effort, and the lessons gleaned from Sandia’s study of biological systems, engender new approaches to other problems in material science and nanotechnology, all of which ultimately serve the nation’s interest. ★

Maintaining Razor-sharp Simulation Accuracy

DAKOTA

In the world of nuclear weapons and other environments where “failure is not an option,” designers and engineers need tools to confidently support high-consequence, risk-informed decision-making. Sandia’s DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) enables these staff members to answer, with greater certainty, important questions such as, “what is the best design?”, “how much better is it than similar alternatives?”, “how safe is my design?”, and “how certain am I about the answer?”

Virtual prototypes — fabricated through computational simulation — can be important tools in the engineering sciences for understanding and optimizing complex systems and reducing design cycle times and development costs. Early in 1994, Sandia recruited Mike Eldred as a postdoctoral research associate because of his background in computational design and process optimization at a time when there was an urgent need to develop a more consistent and sustained effort in this area, to better support the DOE’s stockpile stewardship mission. But little did Eldred suspect that his first project would continue to be a central theme in his career at the Laboratories.

Eldred served as one of three co-Principal Investigators in an LDRD project entitled, “Optimization Strategies for Computationally Challenging Problems in Engineering,” eventually serving as the project’s sole PI in FY1996 and 1997. The vision and overarching

goal for the project was to develop a systematic, rapid method of determining optimal solutions to complex engineering problems using computer simulations. The project’s expectation was that improved designs and enhanced system performances across numerous real-world domains would lead to reduced dependence on physical prototypes and testing, in turn, shortening design cycles and reducing development costs.

The team’s research focused on increasing the robustness and efficiency of its optimization algorithms. Analyzing various optimization strategies led to development of new approaches validated on selected test problems. Iterating this process produced algorithms and heuristics with the highest potential impact. Ultimately, the project developed application-specific techniques, fundamental optimization algorithms, multilevel hybrid and sequential approximate optimization strategies, parallel processing approaches, and automatic differentiation and adjoint sensitivity methods. By 1998, the project launched the DAKOTA general purpose toolkit for the integration of commercial and Sandia analysis capabilities. DAKOTA has continued to grow and evolve to support a range of new and exciting applications. DAKOTA 4.1 was released late in 2007.

A fundamental issue in simulation and virtual prototyping is the need for verification, validation, and uncertainty quantification to establish the credibility of the simulation-



Lockheed Martin engineers coupled their high-fidelity computational fluid dynamics software with Sandia’s DAKOTA software to perform shape optimization of the F-35 fuel tank shape.

software packages and computational models. Verification ensures that the model accurately represents a physical process; validation determines, quantitatively, the degree of agreement between experimental data and simulation data; and uncertainty quantification is a key element of validation, encompassing a broad range of mathematical and statistical analysis methods.

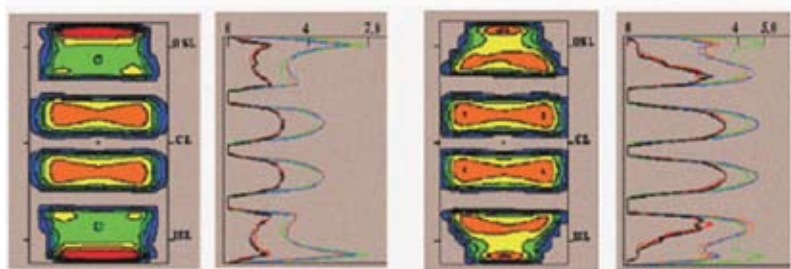
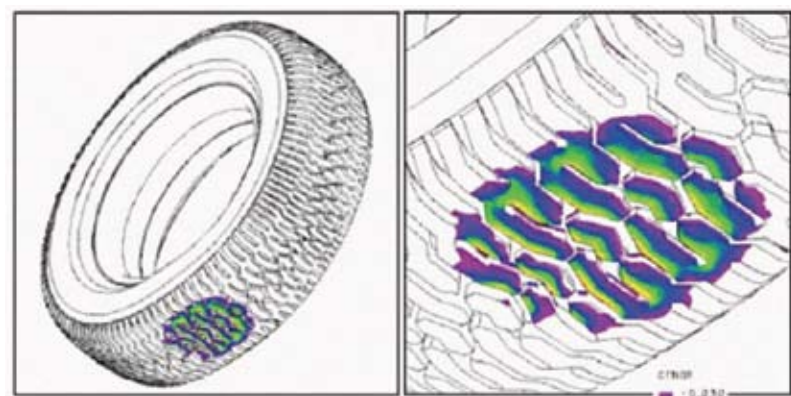
Eldred believes that one of the keys to DAKOTA’s adoption and its continued success is an ongoing commitment to the need for production software, focused on applications, with a real understanding of a given customer’s issues in deployment of the toolkit. After the LDRD project ended, the team continued to support DAKOTA with such application emphasis. The ability to deploy and apply the software so soon after its development was a unique advantage not shared by most other LDRD projects.

Interfaces between DAKOTA and user simulation codes can be developed rapidly; and it can be used both on massively parallel computing platforms (thousands to tens of

thousands of processors) as well as on a single workstation or a network of workstations. Applications of the software toolkit have moved well beyond simply supporting Sandia’s nuclear weapons mission. To date, there are more than 4,000 registered external user sites around the world. Successfully ported to most common UNIX-based workstations including Sun, SGI, DEC, IBM, and Linux-based PCs, much of DAKOTA’s applications growth has been in the private sector, well outside of Sandia’s NW mission space.

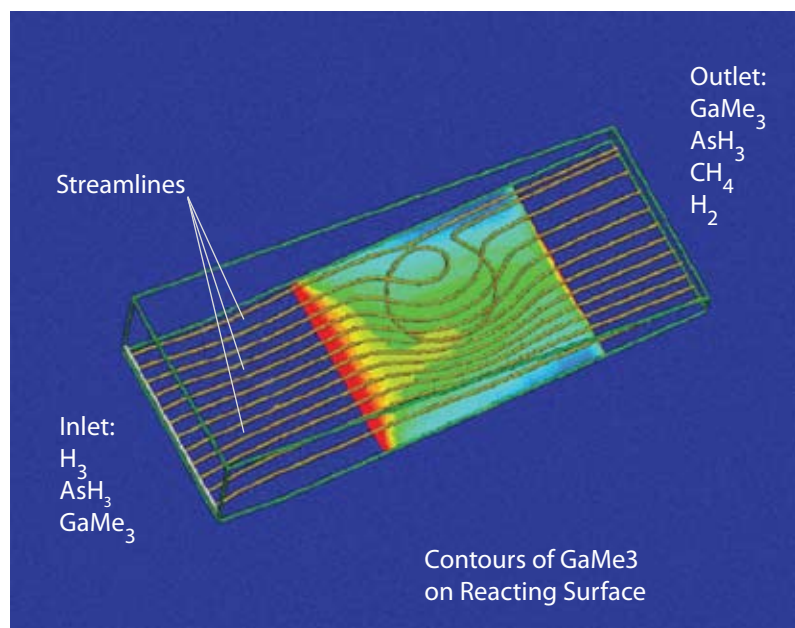
Exemplifying a non-nuclear weapons application is DAKOTA’s use in the design of the external fuel tanks for Lockheed Martin’s F-35 Joint Strike Fighter. Lockheed Martin engineers coupled their high-fidelity computational fluid dynamics software with DAKOTA parametric analysis and optimization software to create an optimal F-35 fuel tank shape. Wind tunnel tests subsequently validated the aerodynamic performance of the optimized tank.

In another transportation application, improved tire design is a salient outcome of



Original Optimized

A joint effort between Sandia and the Goodyear Tire & Rubber Company to more accurately simulate tire performance has provided Goodyear with improved design capabilities, including numerical optimization of tire design to maximize tire-wear performance through footprint indicators.



Visualization of 3D optimization model for chemical vapor deposition of silicon using a horizontal rotating disk reactor showing the large effect of disk rotation on streamlines and deposition rate. Light blue and green are relatively high concentrations; red the lowest.

a joint effort between Sandia and Goodyear Tire & Rubber Company to more accurately simulate tire performance. A more robust and reliable capability for numerical optimization of tire design maximizes tire-wear performance through footprint indicators; the result, improved operational efficiency, reduced development and testing costs, and increased profitability.

Today the DOE Advanced Strategic Computing (ASC™) Program funds the core DAKOTA effort. As such, DAKOTA represents a key asset for ensuring the predictive capability essential to stockpile stewardship in the context of a moratorium on nuclear testing. Established in 1995, ASC™ supports the US Defense Programs’ shift in emphasis from test-based confidence to simulation-based confidence in the performance, safety, and reliability of nuclear weapons.

For Sandia, the key anticipated outcome of the LDRD project was simply a more-unified treatment of certain classes of optimization problems to support the Labs’ nuclear weapons program, and this outcome is entirely evident in DAKOTA’s current set of reusable tools. Unexpected was the continued growth of DAKOTA, which now represents an entire line of growing Sandia business; DAKOTA continues to grow, with applications for DOE and other federal agencies, including DoD and NASA.

Now Sandia’s DAKOTA Project Lead, Eldred anticipates exciting future directions for DAKOTA. “Today, the optimization algorithm operates as the ‘outer loop’ in the process with the simulation code forming an ‘inner loop,’” he says. “In this case, the optimization simply accepts the simulation code and the results of its computations. In the future, we may reinvent what DAKOTA looks like to more fully integrate the optimization and simulation codes.” As an important corollary to this look forward is a glance over Eldred’s shoulder. “Without LDRD support, DAKOTA simply wouldn’t have happened,” he opines. ★



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