SANDIA NATIONAL LABORATORIES

LDRD

Laboratory Directed Research and Development
2008 Highlights

Sandia National Laboratories

From the Chief Technology Officer

The Laboratory Directed Research and Development (LDRD) program is the sole discretionary research and development (R&D) investment program at Sandia. LDRD provides the opportunity for our technical staff to contribute to our Nation's future, to our collective ability to address and find solutions to a range of often daunting scientific and technological challenges. The outcomes of their efforts will help shape the remainder of the Twenty-first Century and beyond.

From renewable energy to nanotechnology and materials science to cyber-chemo- and biodefense — all supported and facilitated by Sandia's remarkable computational capabilities — LDRD projects support Sandia's missions, and hence, address the nation's pressing challenges. This brochure offers an overview of 45 Sandia LDRD projects that were ongoing in FY 08, and also highlights seven recent projects that were deemed worthy of an LDRD Award for Excellence. This award clearly implies both scientific excellence and large potential for actual mission impact on the part of the respective project teams. This brochure highlights only a small sampling of the LDRD program, providing a window into the program's S&T advances and its potential for impact on National imperatives.

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About LDRD

Maintaining Sandia's world-class science, technology, and engineering capabilities and anticipating their evolution in response to future challenges are absolutely essential to the Laboratories' ability to address national security needs. Authorized by Congress in 1991, the Laboratory Directed Research and Development (LDRD) Program reflects precisely that congressional intent — to encourage and sustain preeminent science and technology by investing in high-risk, potentially high-payoff research and development. The program is designed to proactively anticipate the breadth and depth of research and technological development that oncoming challenges will require.

LDRD projects seek innovative technical solutions to our nation's most-significant challenges, often in collaboration with corporate and academic partners. LDRD allows Sandia to recruit and retain outstanding scientific and engineering talent in service to the Laboratories' five primary strategic business areas: nuclear weapons; energy resources and nonproliferation; defense systems and assessments; homeland security and defense; and science, technology, and engineering foundations.

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2008 LDRD Award for Excellence Winners:
8, 9, 13, 17, 24, 30, 31

Cover Image:
Solar thermal collection dishes at Sandia, a part of the LDRD initiative to employ solar energy in the production of transportation fuels from carbon dioxide.

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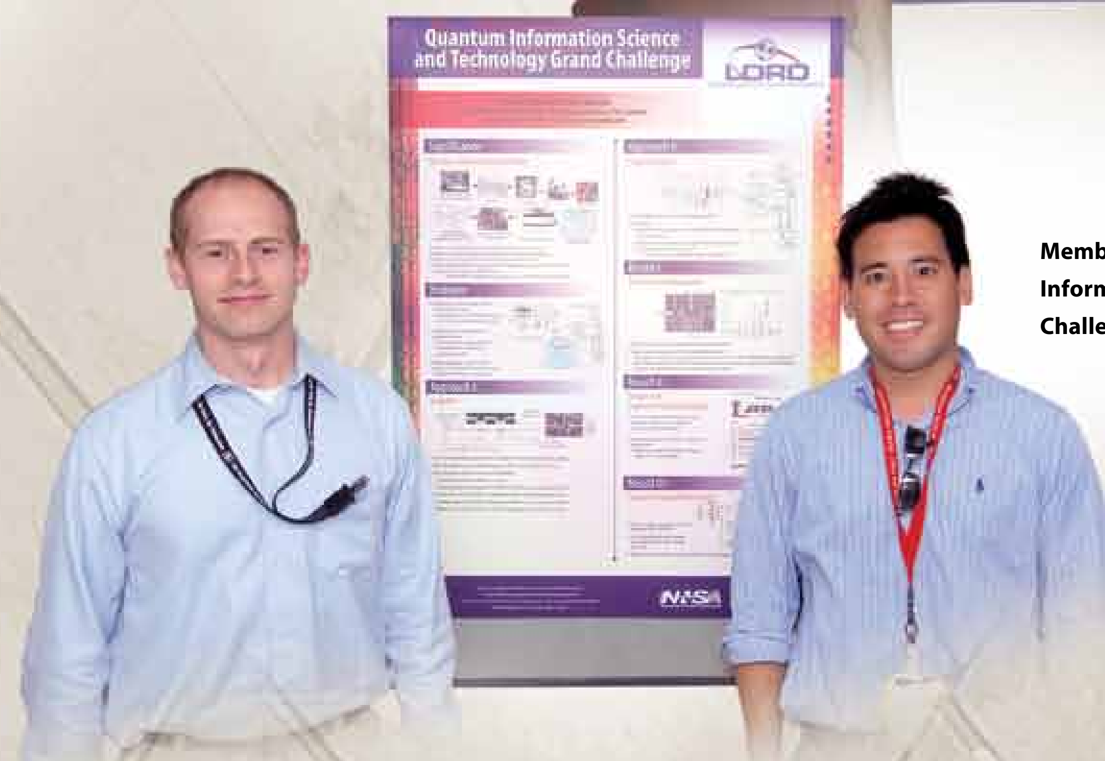
The LDRD Program at Sandia:

Mandated by US Congress in 1992, the LDRD Program functions on a fixed percentage of Sandia's annual DOE/NNSA budget. From that budget base, the LDRD program allocates research funding to meritorious projects that both serve the Laboratory's national-security mission and propose leading-edge, high-risk activities, with high potential impact on both the Laboratory and the scientific community at large. Project selection is highly competitive and only one in ten project ideas are funded. On an approximately 6.7% budgetary investment, tangible impacts include over 25% of Laboratory refereed publications, almost half of its patents, and about 60% of its R&D100 awards.

Vice-president and Chief Technology Officer, Rick Stulen overviews the LDRD Day Agenda.

Oral presentations were given by (left-to-right), Kevin Strecker, Anup Singh, Hung (Jacques) Loui, David Gardner, and Lisa Mondy.

Members of the award-winning Metal Organic Frameworks team with their poster.



Members of the Quantum Information Sciences Grand Challenge Team with their poster.

Award for Excellence recipients with CTO Rick Stulen.
Left-to right: Randy Cygan, Mark Allendorf, George Vizkelethy, CTO Stulen, John Ganter, Karen Waldrip, Chris Apblett, and Igal Brener.

S&T Research Supported by LDRD and their Groupings in this Brochure

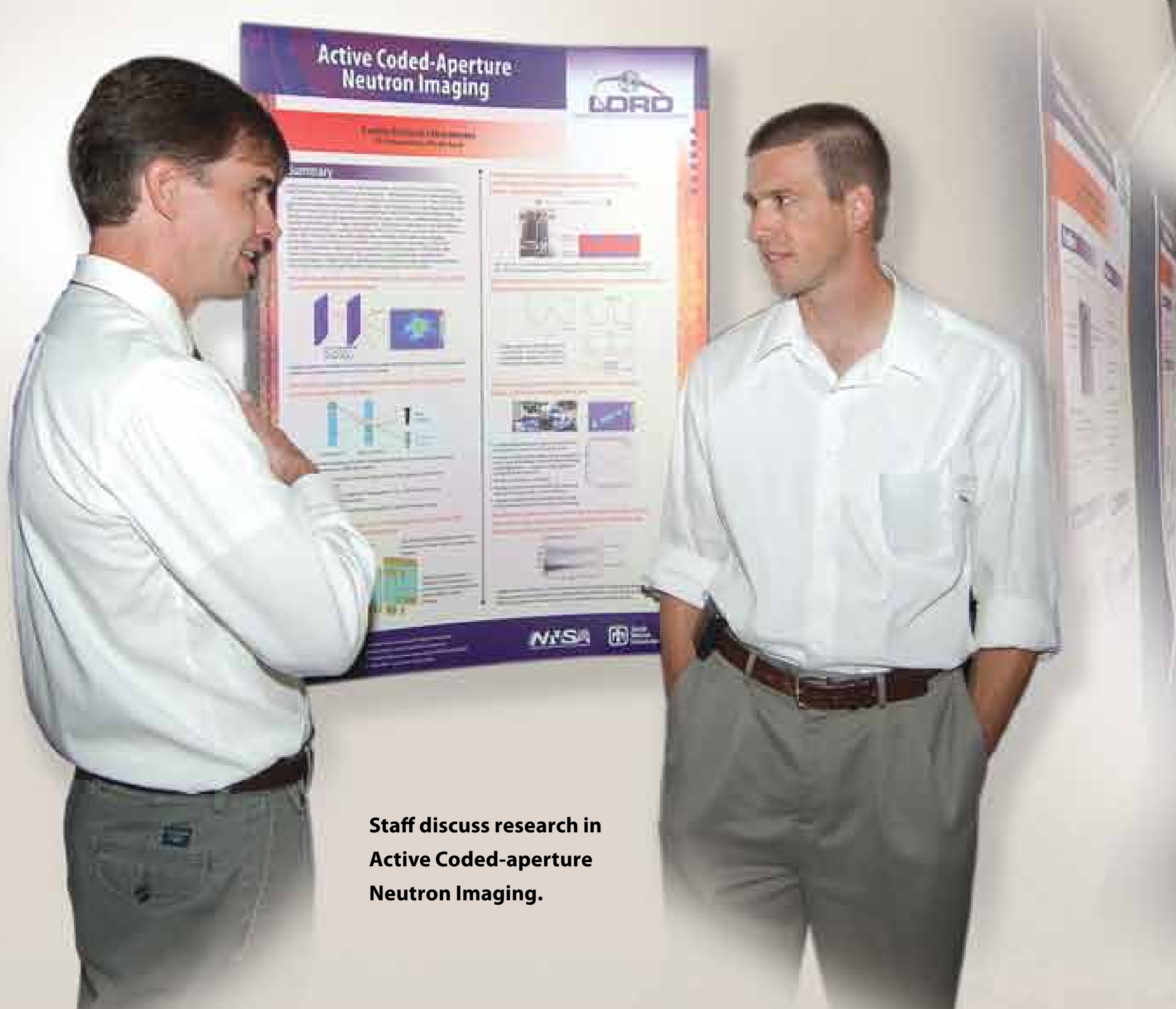
LDRD funding is formally disbursed into nine investment areas as follows: Nanoscience-to Microsystems, Defense Systems and Assessments, Nuclear Weapons, Grand Challenges, Seniors, New Directions, Enable Predictive Simulation, Strategic Partnerships, and Energy, Resources, and Nonproliferation. This brochure covers a small subset of LDRD research for FY 2008, and while the prior categorization is useful as an internal Sandia tool to better allocate its project funding streams, to other audiences, those groupings can be confusing. Therefore, for the purposes of this brochure, we have somewhat artificially condensed this investment area categorization into five groupings: Nanoscience, Materials and Microsystem Engineering, Computation and Simulation, National Security Applications, and Life and Cognitive Sciences. This artificial sub-categorization is especially apparent when one considers that, to be funded, all projects must demonstrate service to Sandia's national-security mission, hence, in reality, all projects could be placed in that National Security Applications category.

In addition to these groupings, this brochure also describes the work of seven projects — in different S&T arenas, but all serving Sandia's national security mission— honored with an 2008 LDRD Award for Excellence.

Mike Wanke presents his Terahertz Microelectronics Transceiver poster.

Jim Miller presents his poster on work comprising a portion of the Sunshine-to-Petrol initiative.

Tina Nenoff discusses her work on radiolytic formation of superalloy nanoparticles.

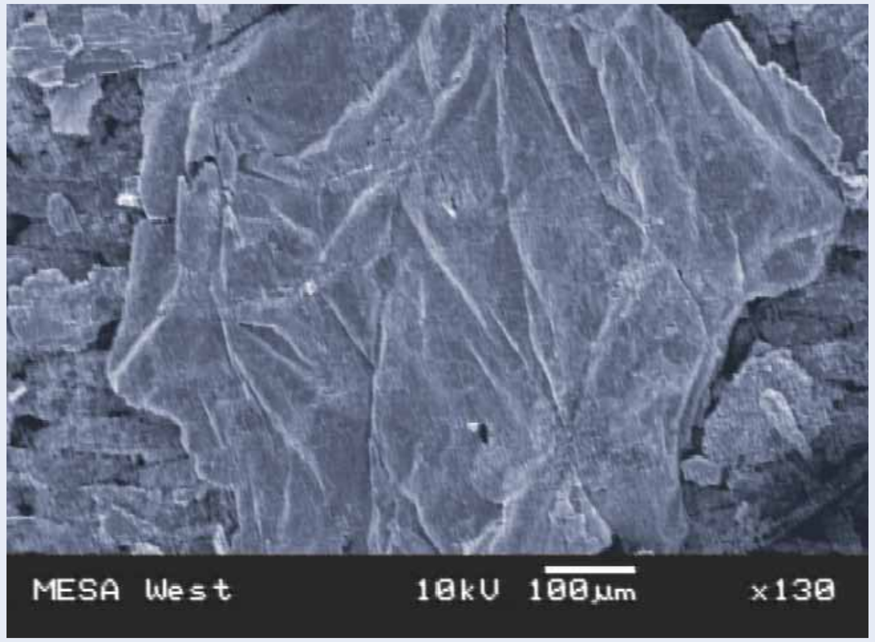


Staff discuss research in Active Coded-aperture Neutron Imaging.

The afternoon poster session was well-attended with vigorous and engaged discussion.

Molten Salt-Based Growth of Bulk GaN and InN

Karen Waldrip



Micrograph of a nitride crystal grown by the molten salt technique.

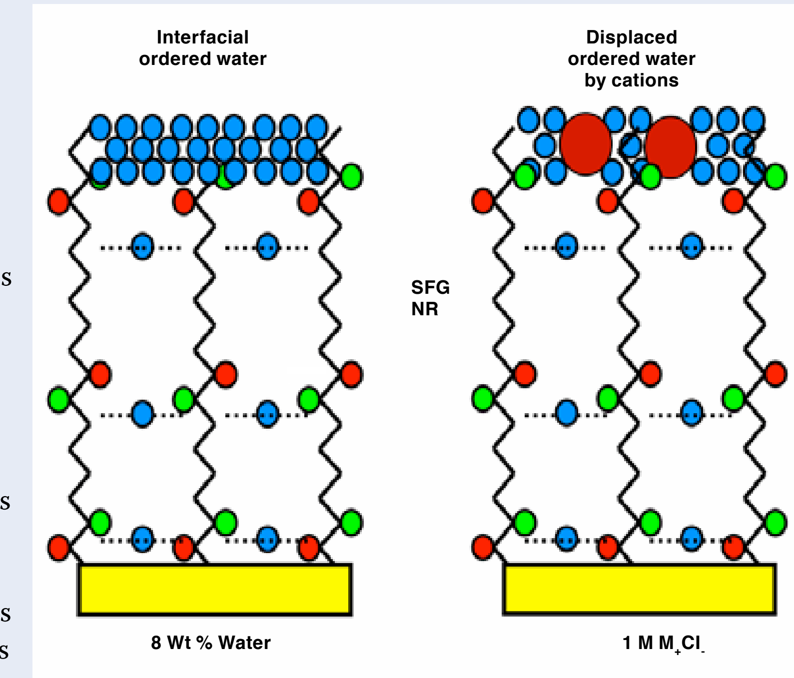
The low-cost manufacture of solid-state-lighting LEDs (light-emitting diodes) for both home and business lighting, consumer electronics, and chemical/biological detection for homeland security applications, has been and continues to be a daunting materials challenge. And that challenge is a critical subcomponent of the evolution of US and global energy policy, given that LEDs can be even more efficient than fluorescent light bulbs for transforming electrical energy to light (by a factor of 2 or more). A limiting factor in this challenge continues to be the production of the materials that compose most LEDs —gallium, indium, and aluminum nitrides, and alloys of these materials. This project approached the generation of these materials in a fashion quite different from traditional methods.

Normally, crystals of these materials are grown on a substrate (for example, sapphire), whose precise crystal structure (in terms of atomic spacing within the crystal) may be different enough from the growing nitride layer to induce the formation of defects known as dislocations. Hence, processes have been pursued for growing bulk nitrides on extant native substrates of the same composition; but the chemical conditions required for this material growth include extremely high processing pressures, and growth kinetics are slow. Hence, although they may generate higher-quality materials for LEDs and other electronics, these processes appear to be too slow and too costly to ultimately make the market for these energy-efficient products sufficiently competitive.

This project has developed an electrochemical method for the growth of gallium nitride and the other nitrides, by first dissolving them in molten halide salts (for example, lithium chloride), under conditions that optimize solubility — and therefore, that enhance the concentration of material that can be dissolved. Subsequently, crystal growth of the relevant nitrides is initiated by electrochemically precipitating the solid material from the molten salt solution. This technique for growing these materials shows promise for generating high-quality materials in a more cost-effective fashion, thus paving the way for the manufacture of LEDs and other high-power solid-state electronics in a fashion that renders the final product sufficiently inexpensive to compete on a market which, in terms of the growing energy crisis, demands such solutions. ■

Exploiting Interfacial Water Properties for Desalination and Purification Applications

Randy Cygan



Comparison of the ordering of water molecules (blue) at an interface with (right) and without (left) the presence of dissolved salt (red "+" circles).

By many measures, potable drinking water may well be the "oil of the 21st Century." While the need for low-carbon, domestic energy generation is obvious and ongoing, the growing shortage of drinking water supplies looms large in the background. At Sandia, numerous projects are underway to address this need, but none, perhaps, so directly as this LDRD project. It begins from the sometimes non-obvious premise that the properties of water, in bulk, are sometimes quite different than its properties at interfaces with other materials (interfacial water). And while the ultimate goal of understanding and modeling such properties is the development of more-energy-efficient desalination membranes, this goal awaits such better understanding and more-representative modeling.

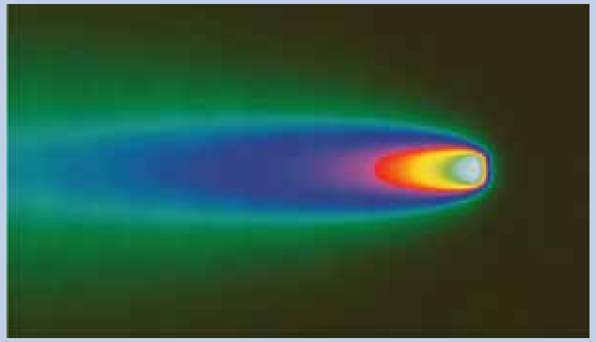
In order to facilitate progress, this project forged programmatic and research ties with the University of Illinois and their National Science Foundation-sponsored Center of Advanced Materials for the Purification of Water with Systems. A Memo of Understanding (MOU) formally acknowledged the exchange of technologies and scientific advances between institutions, and the collaboration of staff.

Project accomplishments included synthesis and characterization of model polymer surfaces such as nylon 6,6, characterization of the structure and properties of interfacial water, and theory and modeling of interfacial water. The results begin to provide a comprehensive picture of how water influences the structure and properties of a polymer membrane, how the polymer influences the structure and properties of water, and how the interactions between the water and the polymer affect the performance of existing membranes. The project also included modeling and development of biologically inspired desalination membranes, in which protein pores known as aquaporins are able to allow the passage of water without allowing passage of associated dissolved salts, such as sodium. Ultimately, one goal of follow-ons to this project would be the formulation and synthesis of enhanced-performance desalination membranes that function in a similar fashion to separate water from its dissolved salts, such that the large quantities of brackish water that exist in aquifers throughout the US can be turned into potable water supplies. This will undoubtedly be a major resource challenge in forthcoming decades. ■

Exothermic Nanolaminates: Structure Property Relationships

David Adams

Nanolaminates are thin films composed of several chemical layers with thicknesses of nanometer dimensions. Exothermic nanolaminate foils are composed of layers of chemically reactive materials that can undergo exothermic (heat releasing) self-propagating reactions when triggered (ignition) by an external energy source. They can therefore serve as local energy sources for applications in joining technologies, sensors/actuators, and other areas.



Predictive modeling of the self-propagating high-temperature synthesis of an Al/Pt multilayer.

However, the fundamental chemistry of such ignition events remains only incompletely understood, and structure-property relationships remain to be fully elucidated, with complex properties, such as oscillatory behavior, possible as laminar structure is altered.

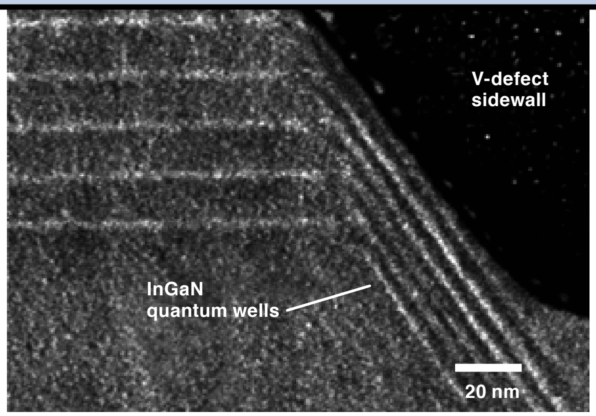
This project is modeling the fundamental chemistry, such that those physical properties can be much more clearly related to nanolaminate structure. Using dynamic transmission electron microscopy and high-speed photography to follow the evolution of reactions, both oscillatory and not, this combination of experiment and modeling should help identify fundamental parameters, as well as clarify such issues as material aging and change in nanolaminate properties with age. In turn, this work should lead to the ability to compose novel nanolaminate films with desired properties.

Nanoscience

Nanoengineering for Solid-state Lighting

Mary Crawford

The ubiquitous presence of light emitting diodes (LEDs) in our lives — in cell phones, mp3 players, TV/stereo remotes, auto taillights, and traffic signals — is actually an understatement of their potential importance as an energy-saving technology. For, if we could cheaply produce efficient LEDs across the visible spectrum, we could enable a new white-light technology for illumination of buildings and homes with significant electricity savings. But developers face the problem that the fundamental physics contributing to light emission from semiconductor materials (such as indium gallium nitride) which form the basis for visible LEDs, are still not well understood. This project, a collaboration with Rensselaer Polytechnic Institute, has pursued several paths to improve the overall efficiency with which electricity is transformed to light in these materials. The project examined critical factors affecting both efficiency of light generation and efficiency of light extraction out of semiconductor chips.



Transmission electron micrograph (courtesy, David Follsteadt) of indium gallium nitride quantum wells grown within a V-defect; this project studied the effect of these defects on optical efficiency.

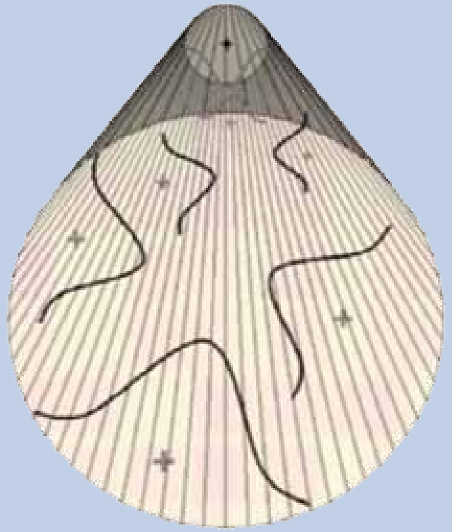
In addition to nanoengineering solutions to increase light extraction efficiency, such as coating LED surfaces with nanorods — graded refractive index coatings that produced a 28% increase in LED efficiency — this project studied the effect of nanoscale material defects on the loss of efficiency observed in InGaN LEDs at higher electrical currents. Ultimately, the goal for LEDs is to reach 50% efficiency, which would represent a doubling of the efficiency attained in current fluorescent light bulbs.

Nanoscience

RF/Microwave Properties of Nanotubes and Nanowires

Clark Highstrete

Increasingly, novel microelectronics applications are being found for nanotubes and nanowires, semiconducting structures whose extremely small size renders them ideal for use in microprocessing chips, allowing for an even greater density of electronic elements on a chip surface than is currently attainable. Problematically, however, there are still great gaps in the understanding of the electrodynamic properties of such nanostructures that preclude their optimal utilization as electronic elements. In this project, the investigative team is seeking to accurately measure the microwave electrodynamic properties of nanotubes, particularly connected to the observation that the electrical conductivity varies with the frequency of the alternating current.



Model derived from this project of disordered nanowire surface charge, which accounts for high DC resistivity and observed frequency response.

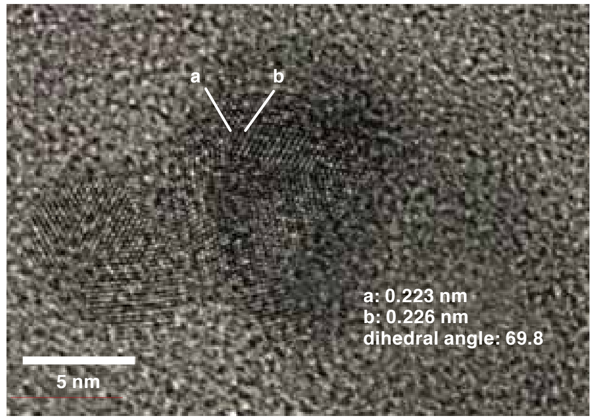
With national security applications in a number of electronic applications, including a variety of sensors, this work is part of an ongoing Sandia effort at thoroughly charactering these nanostructures. In this instance, the team developed a novel microwave conductance spectroscopy method able to measure conductance in arrays of silicon nanowires, as well as of single wall carbon nanotubes. The work has revealed that the conductance properties measured are typical of systems with a disordered distribution of local conductivities, and it suggests directions for researchers interested in developing applications that make use of nanowires.

Nanoscience

Irradiation for the Novel Radiolytic Formation of Superalloy Nanoparticles

Tina Nenoff

Nanoparticle alloys can form at room temperature, when metal ions in solution are irradiated, by either gamma rays or pulsed protons. Subsequent to the reduction of these ions to metal nanoparticles, they combine to form nanoparticle alloys. While theories of the formation chemistry exist, the chemistry is still incompletely understood. This project is investigating that fundamental chemistry, such that, ultimately, better control of formation and composition of these alloys, particularly nickel-based, can be achieved in the absence of traditional mechanisms of alloy formation such as sintering. Underpinned by the defect-free possibilities of the cobalt-60 gamma-irradiation method, the alloys produced by this method are termed “superalloys,” high-performance alloys with high strength and durability, resistance to conditions such as high temperature and oxidation, and a strong resistance to corrosion; they are thus ideal candidates for applications requiring such durability.



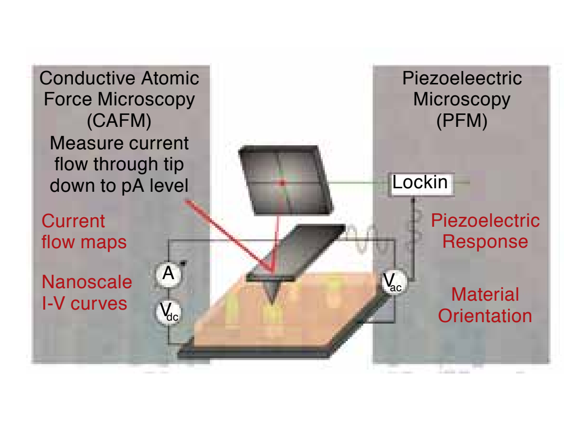
Electron micrograph of silver-nickel nanoparticles.

Silver-nickel and palladium-nickel superalloy nanoparticles have been created and characterized. Applications for such alloys include weapons casings, aircraft parts, satellites, power plants, and gas turbine engines. In addition, membranes to reversibly bind and release hydrogen will be required for hydrogen storage and utilization in hydrogen fuel cells. Nanoparticle superalloys may hold promise in that area as well.

Piezoelectric Properties of Arrayed Nanostructures of Zinc Oxide for Sensor Applications

David Scrymgeour

Funded, in part, by a President Harry S. Truman Fellowship, this project builds on an LDRD Award for Excellence–winning project that succeeded in growing and characterizing zinc oxide (ZnO) nanostructures. These nanostructures have many properties such as the piezoelectric effect that interlink various material states — elastic, optical, and electrical. They are hence ideal for high-sensitivity sensors for hazardous gases, explosive material, and biological agent detection. This project characterizes the the piezoelectric response of ZnO in a wide variety of possible nanoscale geometries 0using scanning force microscopy techniques and nanoscale electrical impedance measurements.



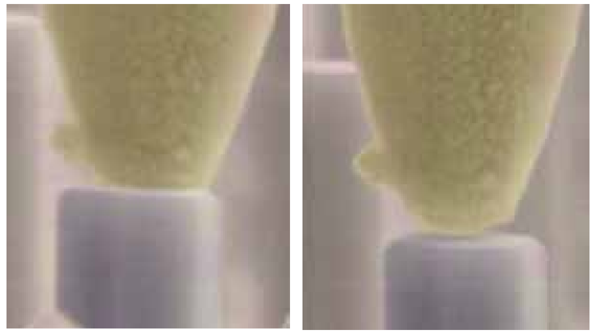
Conceptual drawing of measurement of individual nanorod electrical properties via integrated Conductive Atomic Force Microscopy and Piezoelectric Force Microscopy.

The research has revealed a wide variety of electrical resistivity and piezoelectric properties in individual nanorods that would not be evident in ensemble measurements, and it therefore points a path forward toward achieving better control of nanostructure geometries in order to discover those with the desired high-frequency resonances to function as sensors. The extremely high surface area to volume ratio and the inherently high resonant frequencies of these eventual nanostructures will enable the creation of small, accurate, sensors to target specific chemical and biological agents.

"Bottom-up" Meets "Top-down:" Self-assembly to Direct Manipulation of Nanostructures on Length Scales from Atoms to Microns

Brian Swartzentruber

This project is using low-energy electron microscopy (LEEM) and scanning probe microscopy (SPM) to compare direct imaging of surface features of nanostructures on length scales from atoms to microns. The approach is complemented by the development of a novel nano-manipulator inside of a scanning electron microscope for "top-down" construction and characterization of unique nanostructures such as metallic and semiconducting nanorods and wires. This tool enables not only direct and precise control over the placement of individual nanostructures, but also of their position with respect to each other — unattainable by present techniques.



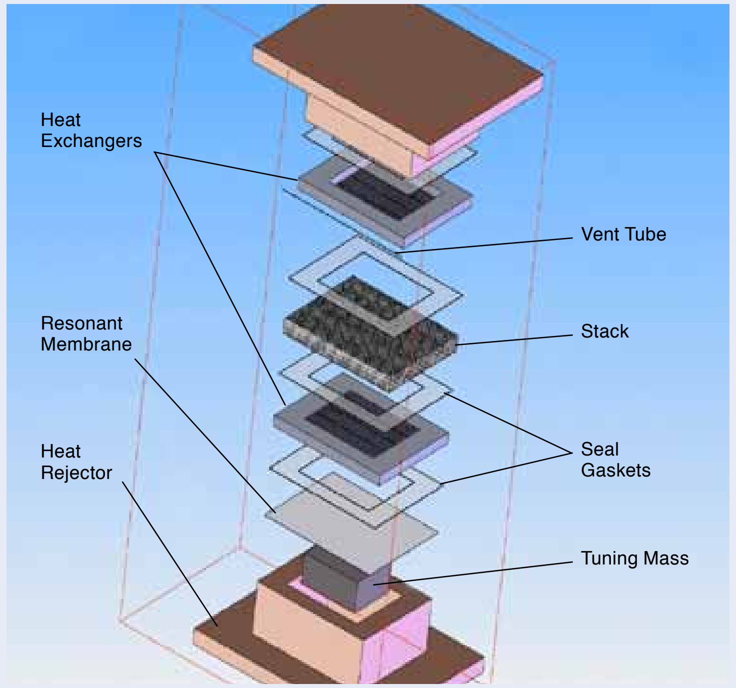
Scanning electron micrograph illustrating precise positioning of the nanomanipulated probe developed in this project.

The project uses these new capabilities to investigate processes underlying the "bottom-up" generation of surface nanostructures on patterned surfaces — the spontaneous formation of one- and two-dimensional features that can serve as templates for three-dimensional nanostructures. This approach, in conjunction with collaborators at the University of Wisconsin, offers a completely novel way of examining, characterizing and controlling nanostructure formation.

A MEMS-based Thermoacoustic Engine

Chris Apblett

Heat engines — systems that derive their energy from heat flowing from hot to cold, analogous to a water wheel deriving mechanical energy from water running downhill — have been built in many different variations and designs. However, until recently, fabricating these heat engines in miniature has posed difficulties, due to issues of heat loss from the relatively high surface-to-volume ratio of small structures, and from friction robbing the engines of power at the small scale. With no moving parts, one particular heat engine, the thermoacoustic engine, does not suffer from many of these limitations and is a prime thermal candidate for miniaturization. A particularly thorny problem is an engine part known as the thermoacoustic stack, similar to the an auto engine's cylinders in that thermal energy is transformed to mechanical work. Utilizing Sandian expertise in microfabrication and extant knowledge of larger thermoacoustic stacks, this project sought to design and prototype a microscale stack, the foundation of a microscale thermoacoustic engine (TAE), in order to verify that the theories of TAEs would be valid at the microscale. Recent advances in very high aspect ratio micromachining technologies allowed the fabrication of a regenerator in thermally insulating materials at microscale dimensions, accomplishments that were unachievable using previous technologies. Prior fabrication methods of high-aspect-ratio stacks were quite expensive, while this new process, using an ultraviolet-light-sensitive polymer, significantly improves the fabrication at much lower cost.



Exploded view of the components of the MEMS-based TAE.

Given the applicability of these theories, it should be possible to harvest relatively small thermal gradients (temperature differences of only 10 °C) from the environment to produce electrical power, a potentially significant contribution to US energy security. The project involved a collaborative effort with Los Alamos, whose larger Stirling heat engine had been successfully fabricated in the late 1990s.

As a heat scavenger, the MEMS-based TAE would also enable a variety of long-term remote sensing applications that are not currently possible with current battery technology. Mating the TAE to a radioisotopic heat source could possibly even present a power source option with a higher power density than current radioisotopic thermoelectric generators (RTGs). ■

Remotely Interrogated Passive Polarizing Dosimeter

Rob Boye

Ionizing radiation, such as x-rays, and the alpha and gamma radiation deriving from certain radioisotopes can be extremely harmful to human cells, and detecting such sources of radiation in a benign fashion is an ongoing challenge. This project is developing an ultrathin (a fraction of a millimeter) imaging chip for detecting and measuring the dose of ionizing radiation, which can be remotely interrogated to reduce danger to personnel.

The team has developed a conductive polymer film, a polarizer of infrared (IR) light, whose conductivity changes as a function of absorbed radiation dose. Relating this change in conductivity to the extinction ratio of the polarizer for IR allows for remote interrogation. For example, innocuous optical tags placed on a shipping container could be interrogated from a distance, by a special "camera," a polarimetric imager. While no visible change would occur on such labels, the absorption of ionizing radiation would change the labels' appearance to the polarimetric imager, which then can be related to the dose of ionizing radiation necessary to evoke that change. Since imaging is done at a distance, this greatly reduces danger to personnel.

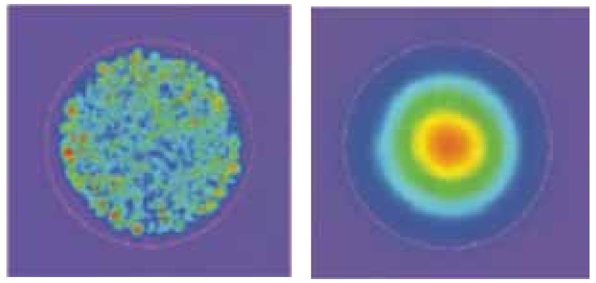
At-a-distance polarimetric imaging of radiation-sensitive tags on shipping containers.

Fiber Laser Grand Challenge

Jeff Koplow

Three years of prior Grand Challenge work featured the validation of the technique of mode-filtering for accomplishing high power (exceeding 1 MW) in a fiber laser. In this follow-up year of research, the project is experimentally determining the ultimate limits of mode-filtering for power scaling, and in doing so, more-deeply understanding the underlying physics. The team is, additionally, developing an optimized double-cladding fiber architecture, and has developed fiber laser modeling software, which suggests that there are nonlinear effects in mode filtering that impose a limit on the maximum fiber core diameter to which the technique can be applied. The software will eventually be made available to the large and ever-growing global fiber laser community.

In addition to extending and refining the results of the first three years, the team has also approached the issue of air-cooling is an innovative fashion. This is a key issue because of the attractiveness of portability of fiber lasers, which because of their far better efficiency, do not necessarily require the elaborate water-cooling systems of traditional laser systems. This line of research resulted in a patent submission for this fundamentally novel approach to air cooling.



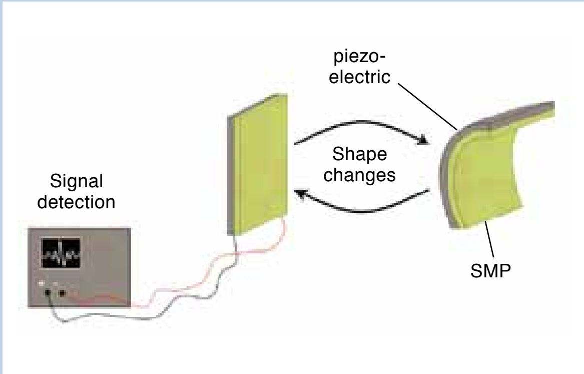
Comparison of beam quality in uncoiled versus coiled fiber lasers.

Active Polymer Composites for Detection of Abnormal Thermal and Optical Environments

Greg O'Bryan

Piezoelectric materials, which generate an electrical current with changes in shape, have potential as sensors, if, as in this project, they can be combined with materials known as shape-memory polymers (SMP), which are flexible and can be deformed from a quasi-permanent shape, then promoted to return to that shape by exposure to light or heat. This project is investigating such a combination of piezoelectric and Sandia-created SMPs to serve as future sensors of abnormal thermal and optical environments.

The concept is to deform an SMP-piezoelectric combination, where the SMP is sensitive to a particular wavelength of light. That light, when present, will trigger a return of the SMP to its quasi-permanent shape, during that shape-change process also changing the shape of the attached piezoelectric, thus generating an electric current and signal. In addition to light-sensitive SMPs, the team has also performed experiments with temperature-sensitive SMPs, and it is developing an SMP material model, which will allow refinement of the work, as it proceeds to develop the desired SMP-piezoelectric interactions for sensors that show sensitivity for monitoring desired environmental changes.



Layered composite of shape memory polymer (SMP) and piezolectric material illustrating how changes in shape produce an electrical signal.

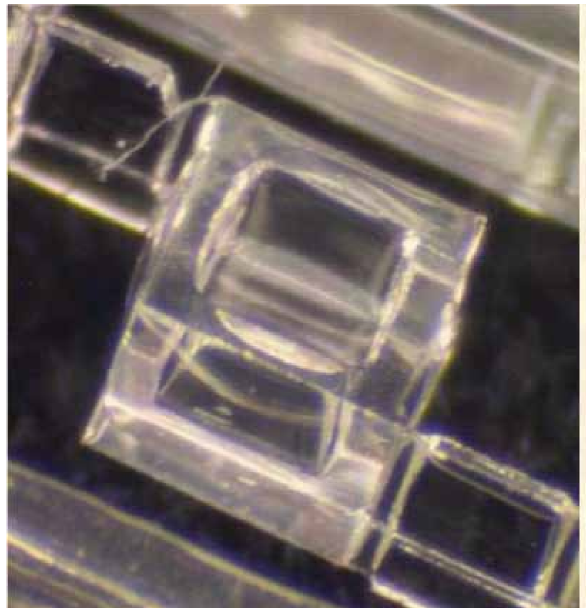
Tuned Micro-cavity Magnetometer

Murat Okandan

Magnetometers, which measure magnetic fields, are important tools in various applications requiring ultrahigh-sensitivity measurement, such as the location of unexploded ordnance, the mapping of underground facilities, and the monitoring of brain activity (Magnetoencephalography or MEG) by way of the small magnetic fields set up as ionic charges move into and out of nerve cell during their activity. Some magnetometers, such as those for MEG, require extremely low temperatures for operation, and this increases cost and limits functionality. This project team is developing a miniaturized atomic magnetometer with the potential to function at high sensitivity and without cryogenic cooling.

By using a closed cell containing cesium vapor and lasers to align the atomic spins, the spin-aligned cesium atoms can then sense a small magnetic field, as their spins change (precess) in response. A probe laser can then detect that precession, which will be a reflection of the strength of the magnetic field.

In addition to the applications in underground detection and brain measurements, other applications for miniaturized, highly sensitive magnetometers arise in satellite systems, and navigation, as well as in fundamental scientific research.



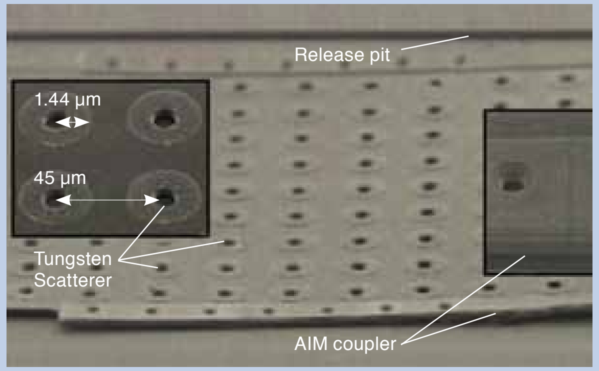
A prototype vapor cell for cesium vapor within the magnetometer.

Micro-sized Acoustic Bandgap Structures

Roy Olsson

Phononic crystals are the acoustic equivalent of photonic crystals (light). In this project, the team is microfabricating acoustic crystals that will hopefully realize the first bulk acoustic wave (BAW) bandgap technology at frequencies commonly used in acoustic imaging and radiofrequency (RF) communications (the 1 MHz to 1GHz range). In the process, the goal is to develop a fundamental understanding of micro-acoustic bandgap physics (analogous to photonic bandgaps, an acoustic bandgap [ABG] is range of acoustic frequencies or phonons forbidden to exist in a structured material [phononic crystal]).

In addition to providing a unique opportunity to study phonon interactions, this research is relevant to acoustic devices, such as RF resonators and filters, medical ultrasound and thermal management. To this point in time, ABG research has been limited to large structures operating at acoustic frequencies below 1 MHz. By using a combination of microfabrication and modeling, this team is scaling ABG structures to submicron



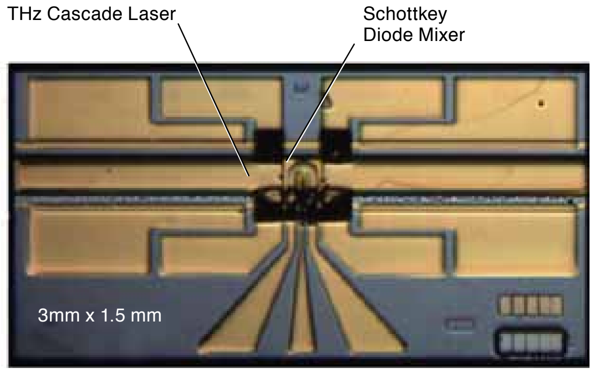
Scanning electron micrograph of a 67 MHz acoustic crystal fabricated as part of this research.

length scales. The project has demonstrated the first micromachined ABGs at frequencies as high as 1 GHz. Such devices enable filters with unprecedented small size and frequency selectivity, swell as higher-sensitivity, jam-resistant RF communications.

Terahertz Microelectronic Transceiver (TµT) System

Michael Wanke

See-through imaging through opaque materials for concealed weapons, high-specificity chemical detection of explosives and other chemical signatures, lightweight, high-spatial-resolution airborne radar and remote detection platforms, and secure high-speed communication links — these are just a few of the promises of a terahertz transceiver. This frequency range between infrared and microwave has been difficult to utilize productively to this point in time, and has relied on fragile and expensive vacuum or gas tube components. But this project has demonstrated an integrated THz microelectronic transceiver (TµT) using all solid-state components and fabrication methods compatible with modern semiconductor processing. Requiring participation of a multidisciplinary team, fabrication has produced these components, reliably and at relatively low cost. In addition, the project team developed unique device-modeling codes. And research into THz quantum cascade lasers produced



Integrated solid-state THz Mixer developed in this project.

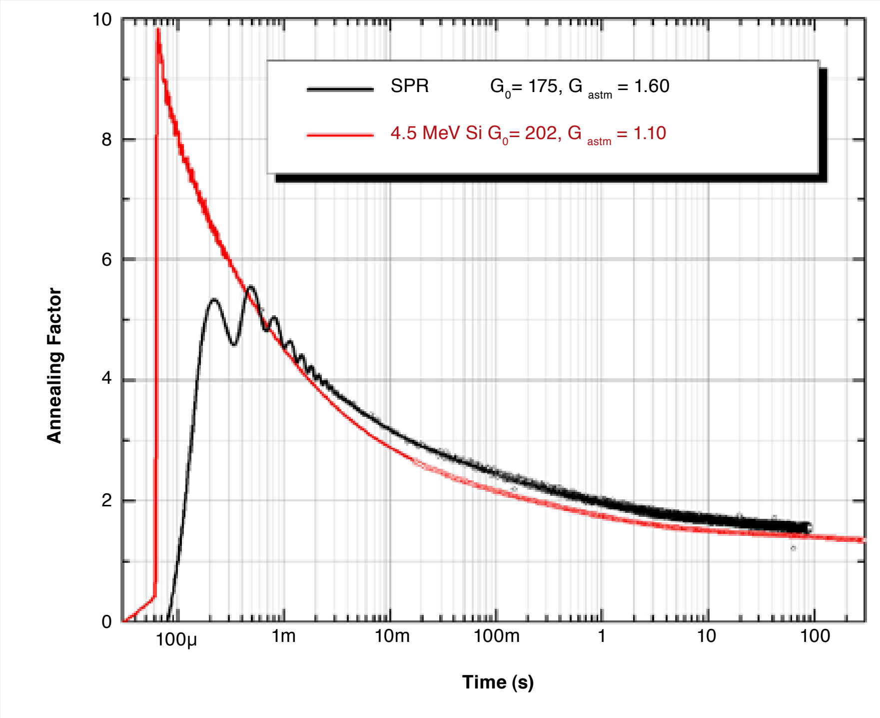
an 8% gain-bandwidth and demonstrated high-resolution spectroscopy of molecular vapor.

The possibilities for military and civilian uses of a stable, compact, all-solid-state terahertz transceiver are numerous, and the technological results of this Grand Challenge project will undoubtedly be significant in forthcoming years, placing Sandia in the forefront of this microelectronics arena.

Ion Neutron SIMulation – INSIM

George Vizkelethy

One of Sandia's oldest and most-important core missions is the certification of electronic components for strategic nuclear weapons. One aspect of such certification involves the fact that such weapons will almost certainly encounter hostile countermeasures — including short intense neutron bursts — designed to disable the functioning of weapons electronics. In the past, pulsed nuclear reactors, such as the Sandia Pulsed Reactor (SPR III) have been used, for certification, to produce such neutron bursts to test weapon-electronics resistance. Since this reactor, and others are to be closed because of concerns around terrorist access to special nuclear materials (SNM), and since new types of neutron threats have been identified, which the reactors cannot simulate, methods are needed to emulate such neutron damage to weapons electronics, without the use of SNM. This project has developed precisely such a method, the Ion Neutron SIMulation or INSIM technique.



Data illustrating that the annealing factor transients of SPR-III neutron irradiations can be simulated by heavy ion irradiation.

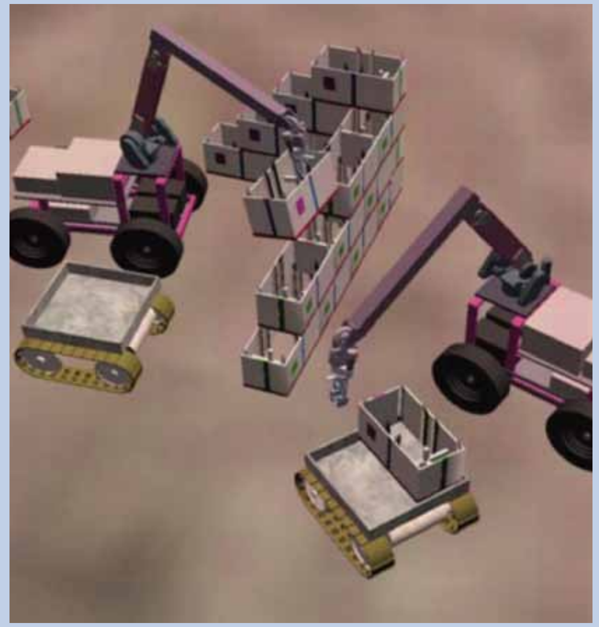
This technique of using high-energy heavy ions to emulate neutron damage allows the testing of discreet electronic components and is fast, inexpensive, and very flexible. The duration and intensity of the pulse can be widely varied with ease, to study and validate models of the time-dependent response of transistors to short intense neutron pulses. As important, there are no radiation concerns to personnel or surroundings using ion beams, by contrast to using reactors and SNM.

Including modeling in this project makes it more flexible, in terms of anticipating new threats. By comparing the results of the ion beam irradiation with actual neutron data and to results of simulation from continuum codes, the latter can serve as guides for verifying the validity of the technique for weapons electronic certification. This combination of techniques enable the adaptation of the specifics of the technique — in terms of specific ions utilized and their energetic parameters — to achieve valid emulations of novel enemy countermeasures as they arise. ■

Autonomous Intelligent Assembly Systems

Robert Anderson

Robotic assembly of structures in locations where human life might be at risk or not yet present — in space, on ocean bottoms, in combat zones: such is the ultimate goal of this project, which seeks to develop new algorithms to increase the autonomous functioning of robotic agents in unstructured environments. Even sophisticated robotic systems currently require an at-risk human operator to function; even high-bandwidth and GPS navigation is insufficient to accomplish truly effective robot operation, once the robot has stopped moving at its destination. In this project, visual, command-and-control, and communication algorithms are being developed to improve the functioning of both individual and teams of collaborating robots. Commands have been developed for visual servo-ing, waypoint following, and arm and gripper control.



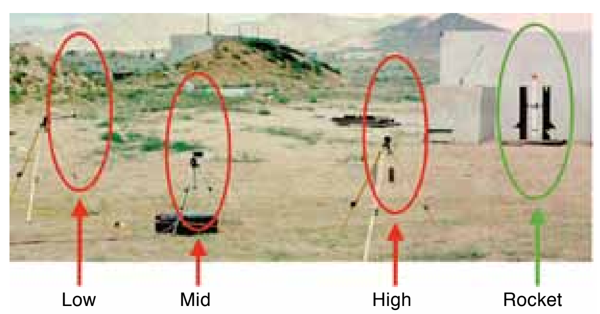
Conceptual drawing of teaming robots building a brick wall.

In a preliminary demonstration, a robot autonomously took a series of overlapping photographs to generate a visual map of its test site. The control precision is adequate to the tasks of sensor array deployment and brick-wall building, demonstrating the core project competencies. During these demonstrations, robots must cope with real-world illumination variations, communication issues, and vehicle platform uncertainties.

Electromagnetic Properties of Plumes and Plasma Jets for High-power Microwave Applications

Larry Bacon

Detonation or burning of energetic materials such as shaped charges result in the formation of plasmas with electromagnetic signatures (such as radiofrequency [RF] emissions) that are potentially exploitable. Through both experiment and simulation, this project is investigating the plasma physics of plumes and plasma jets to enable more-effective exploitation. This team had designed and fielded an RF sensor system with three separate channels to cover desired bandwidth. By measuring RF emissions during live-fire tests of rocket systems and small-caliber firearms, the project has acquired a dataset containing unique and identifiable RF signatures for such events. The goals ultimately include characterization of these phenomena, the conditions that may enhance or diminish the signals received by the sensors, and the accuracy with which these signals can be discriminated.



RF sensor system with low-, midrange-, and high-frequency antennas.

In addition to the diagnostic uses of such information in tracking weapons testing and use, an additional application is the enablement of tactical weapons within artillery shells or small rockets. By utilizing the knowledge of such signatures to produce plasmas generating high-power microwave (HPM) pulses, these devices could be delivered by shell or rocket to the site of any device that required an "electronic kill."

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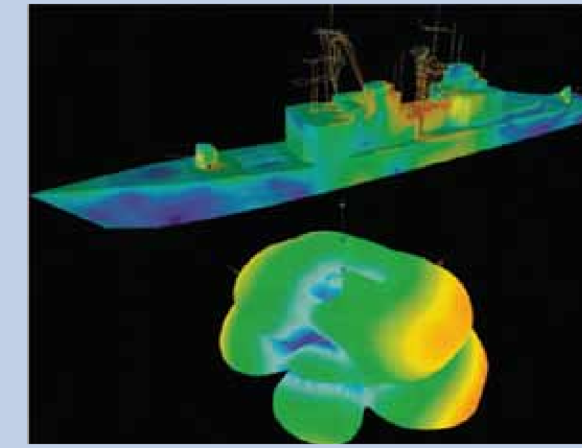
Creation of a First-principles Simulation of Weapons Generated Electromagnetic Pulse

Robert Campbell

This computational modeling initiative has potential impact in a number of Sandia's national security missions, including the design of microsystem-based components for nuclear weapons, the radiation hardening program, and various aspects of the Electromagnetic Program. It specifically addresses threat assessment and asset protection from electromagnetic pulses. Utilizing state-of-the-art computational capabilities, the project is developing a code that can model spatial scales from a few microns to hundreds of kilometers, and that is being validated through comparison with published experimental data. In addition, advanced models of electromagnetic pulses developed in this project can be compared with those formerly treated by legacy codes.



EIGER modeling software has been used to predict the installed performance of antennas in complicated environments, such as on-board a destroyer.

Focusing on high-altitude electromagnetic pulses (EMPs), the project's models contributed to validation efforts by the Defense Threat Reduction Agency (DTRA). Such models assist in the prediction of EMP environments relative to the necessary measures required to ensure that military systems are adequate to withstand threats from EMPs. The models are, therefore, crucial to adjudicating appropriate levels of investment in countermeasures. There is, also, an ongoing need for the capability to predict the properties of novel transient field environments that might arise in the future.

Enhanced Simulation for Homeland Security Training

Donna Djordjevich

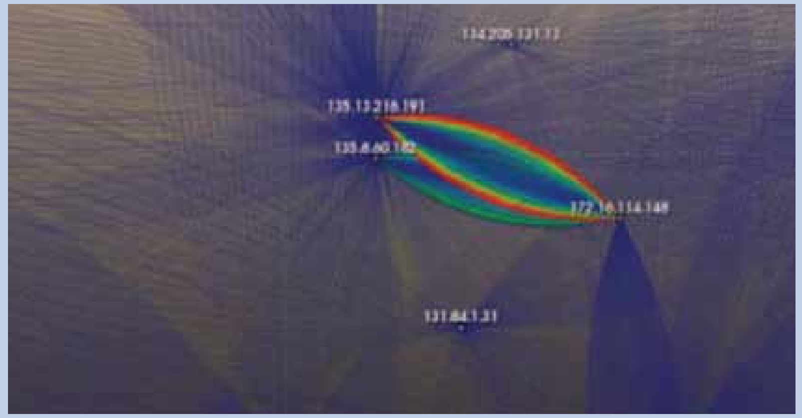
Initiating and sustaining the training of DHS and other US and local government personnel who are responsible for responding to emergency situations, particularly those involving weapons of mass destruction (WMD), is a key challenge facing training personnel. Among the available options — from full-scale exercises to simulation and others — trainers are faced with the less-obvious constraints of time and manpower, in addition to the more-obvious ones of the effectiveness of situational training in preparing for the real thing. In this project, the advantages of game-based training have been explored in the context of several types of police force and public health HazMat responders.

Simulation of chlorine gas release from a tanker in an urban environment.

The advantages of this type of game-based simulation include the ability to train in short bursts, thus taking advantage of time limitations by allowing personnel to train during windows of available time. Utilizing short scenario run-time allows trainees to run more scenarios in available time, all of which train decision-making skills that are only acquired through experience. Furthermore, by leveraging adaptive artificial intelligence elements, scenarios can be slightly altered to provide innovative variants that enhance the training experience.

Network Discovery, Characterization, and Prediction Grand Challenge

Bruce Hendrickson



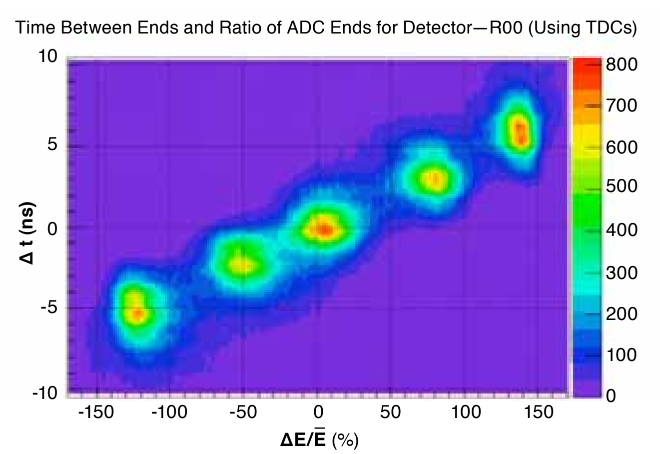
Cyber-analysis prototyping of an intelligence dataset.

On the surface, the threats to national security appear to manifest in a diversity of forms, and may also appear to be individualized and not intimately connected — the suicide bomber, the cyber-intruder, the illegal weapons salesman. Despite the apparently minimally connected perpetrators, underpinning this loose, dynamic aggregation are networks that support and finance these activities — supply, recruitment, and shipment networks, as well as financial and communications (including computer) networks. This Grand Challenge project seeks to begin the process of defeating these adversarial networks through discovery, organization, and characterization of the huge amount of extant intelligence data, using resources thoroughly developed at Sandia.

Beginning from the recognition that the human intelligence analyst is pivotal to such discovery and analysis, this team seeks to apply a broad repertoire of capabilities to this challenge: from advanced information visualization, to high-performance graph queries and algorithms, to uncertainty characterization and predictive modeling. All these analytical tools are combined with a human factors perspective to integrate the tools with the expertise of the intelligence analyst. Several prototype scenarios have already illustrated the value of this approach and pointed a path forward.

Active Coded-aperture Neutron Imaging

Nathan Hilton



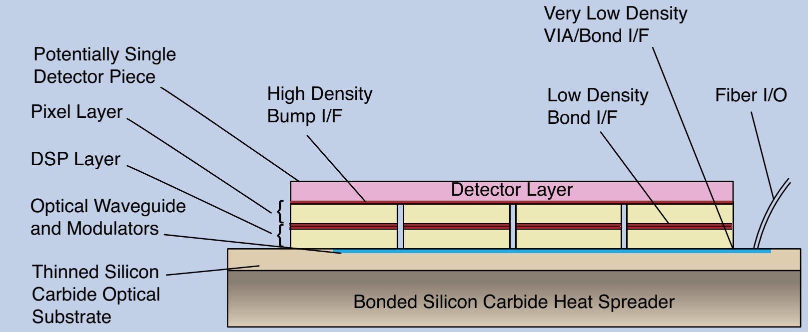
Experimental results, assessing sensitivities of a prototype detector.

Discovering and accurately locating, from a distance, sources of special nuclear materials (SNM, such as enriched uranium and plutonium) are pressing national security needs, from the standpoint of both state-sponsored and rogue attempts to create weapons of mass destruction. However, to this point, measurement of gamma rays released by such SNM is the primary diagnostic methodology. Meanwhile, energetic neutrons, which are more penetrating, and thus, should be easier to detect remotely are not used in detection because no efficient imagers of such neutrons exist. This project team is working toward the creation and refinement of just such a neutron imager.

Simultaneously performing one-dimensional coded-aperture and two-dimensional double-scatter imaging will impart greater sensitivity to the device. Experimental measurements of neutron sources are being combined with simulations to enhance the evolution from smaller to larger prototype detectors. Experiments with combined neutron and gamma ray sources have shown the ability of prototype detectors to distinguish between neutrons and gamma rays. DTRA, DHS, and DOE are actively seeking such a capability, and this project will hopefully offer a uniquely effective solution to this important national security need.

Highly Pixelated Hypertemporal Sensors for Global Awareness Grand Challenge

Rex Kay



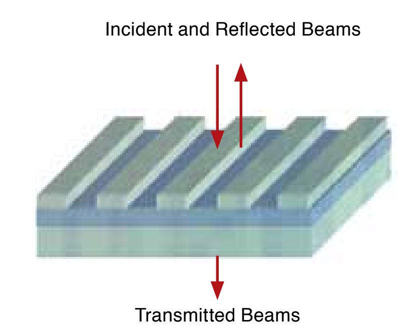
Conceptual drawing of hypertemporal sensor technology developed in this project.

Remote sensing and surveillance of the environment and of outer space for full-earth persistent monitoring of transient events (e.g., explosions) that might be important to intelligence and to national security is best accomplished through focal-plane arrays (FPAs), that sample the environment repeatedly and rapidly, such that even the smallest and most-transient event of interest will not be missed. In this Grand Challenge project, the team focused on development of the critical enabling technologies necessary to accelerate the realization of future FPAs that will be key to persistent whole-earth monitoring.

These technologies include two- and three-layer daisy-chained structures, (each layer a 4 x 4 array), silicon circuitry, and high-speed data interconnects, including a transmitter/receiver prototype and optical interconnects. The system has a very small footprint, is rugged, and its scalable packaging paves the way for fabrication of larger FPAs, which will be crucial to challenging national security remote sensing missions. Its advanced circuit architectures consume small amounts of power and its optical fiber interfaces can move terapixels of data per second.

High-speed Spectral Sensor

Shanalyn Kemme/Aaron Gin



An Active Resonant Subwavelength Grating Device.

This project seeks to engineer and fabricate a sensor that can quickly and accurately detect wavelengths of radiation — the spectral content of light — coming from an object or scene on a moment-to-moment basis The technology has no moving parts, and is therefore rugged and agile; it has several applications in national defense and security, for example, in kill assessment — the determination of the efficacy of an interception of an incoming enemy missile.

The critical component is a tunable optical filter that uses resonant subwavelength gratings (RSG), which act to transmit certain wavelengths and reflect others. These RSGs can also become active systems, by using an electric field to shift the wavelength response. This feature allows detection of a range of wavelengths from infrared through ultraviolet. For example, in a missile kill, the emitted wavelengths would rapidly change from visible and ultraviolet (UV) in the initial fireball flash, and to infrared (IR) in the subsequent debris cloud. A sensor utilizing active RSG technologies will be able to quickly access all of these wavelength regimes to make fast characterizations of an intercept event. Using Sandia's microfabrication capability, the team is assessing different materials to ascertain the most favorable for use in RSGs, as well as any design modifications necessary to yield optimal functionality.

Direct Approaches for Recycling Carbon Dioxide into Synthetic Fuel

James E. Miller

Two interrelated and extremely urgent issues threatening national and global security are rapid depletion of petroleum, mostly exported from the Middle East, and the growing climate change effects of CO_2 accumulation resulting from fossil fuel combustion. A Sandia team is approaching both these threats by developing a solar-thermal energy–driven process for re-energizing CO_2 .

Project staff member adjusts solar tracking heliostat on a solar thermal collecting dish.

The resulting CO (carbon monoxide) can be used with hydrogen derived from water to synthesize liquid transportation fuels by well-known syngas processes. The re-energizing process utilizes a metal oxide thermochemical cycle driven by concentrating solar power and operating at temperatures as high as 1500 °C in a device such as the Counter-Rotating-Ring Receiver/Reactor/Recuperator to split water and carbon dioxide. This mimics photosynthesis, and in effect, reverses combustion, which introduces CO_2 into the atmosphere. Strategic university collaborations are an important part of this effort. The actualization of this process at an adequate efficiency would represent a giant step for US energy independence and freedom from the grasp of foreign oil.

DSA Intelligent Transformational Systems: Real-time Individualized Training Vectors for Experiential Learning

Elaine Raybourn

One of the US Army's top-five outcomes in future warfighter training is adaptive self-paced anytime-anywhere training. This project applies social learning theory to conduct human-subject experiments for identifying training vectors in game-based training, for both competent and novice levels, in an experiential learning environment. "Can in-game performance be correlated with training level" is a key question for this type of research study. A number of Sandia, US Army, and DARPA training implements were utilized, in order to observe study participants.

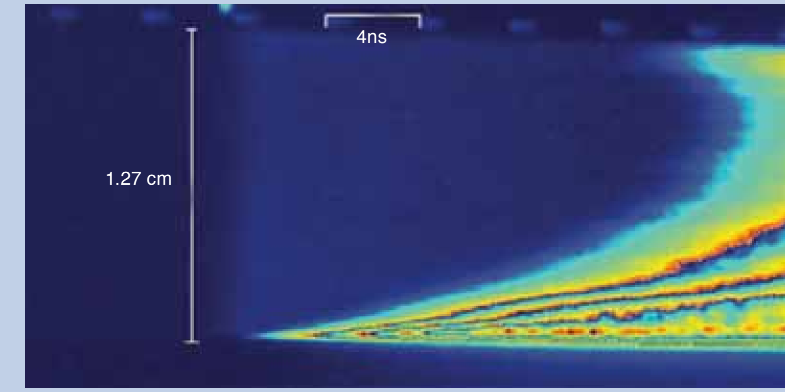
Instructor interface for the DARWARS ambush training module.

An initial sample of 90 study participants indicates important outcomes for trainees who observe interaction strategies in these training vehicles — whether or not they model the behaviors, such trainees tend toward better performance. The project team has assembled an external advisory board with military, industrial, and DOE participants, and has also identified a transition partner in the US Army Armor Center Directorate of Training, Doctrine, Combat Development and Experimentation at Fort Knox, such that the further results of this study can be applied in improving the impact of these experiential learning vehicles.

Understanding Surface Breakdown in Electronegative Gases

Larry Warne

Pulsed power machines rely on gas breakdown phenomena. High-power gas breakdown switches are critical components in the ZR upgrade of the Z machine, for example, and will likely play roles in future larger power drivers. Gas switches rely on high-density electronegative gases and insulator barriers, which are often weak links in the lifetime of the components and are the most-common sources of failure in these machines. This project is attempting to secure a more-fundamental understanding of how discharges interact with surfaces in dense electronegative gases from both modeling and experimental perspectives.



Streak camera image of an electrical discharge progressing across a gap in air.

Working with Sulfur hexafluoride (SF_6), surface ionization waves (streamers) are analyzed for both the gas itself and different surfaces with which it interacts (e.g., Teflon); this source of breakdown is being analyzed from a fundamental physics perspective. Defects and external stimuli (such as UV) are included in this set of analytical studies. Future pulsed power machines should benefit from the acquired understanding.

Supercritical CO_2 Brayton Cycle Test-loop Development, Controls, Testing, and Model Validation

Steven Wright

The overall aim of this project is to move in the direction of maximizing the energy efficiency and cost effectiveness of next-generation nuclear power plants. The supercritical carbon-dioxide (S-CO_2) Brayton Cycle is considered one of the most promising power conversion cycles because it can achieve very high efficiency (40-50%) at relatively low reactor coolant exit temperatures (< 600 °C). The cycle involves compression near the critical point of CO_2 . Carbon dioxide is a dense fluid in this regime, so a high power density is achievable in a compact configuration.

CO_2 Brayton Cycle Test Loop.

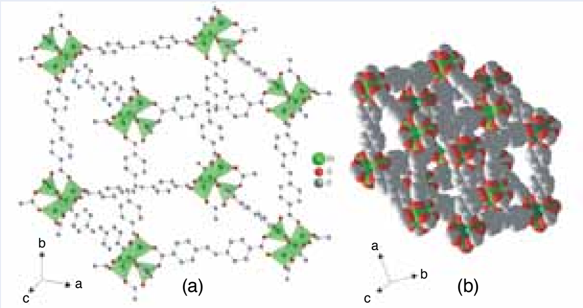
A small-scale test loop has been configured and tested. In addition to control components, the project team must engineer bearings, compressors, turbines, alternators, shafts, and seals that must operate at high speed and in the dense supercritical fluid. Successful accomplishment of these goals will lead to the construction of a full-scale loop, and testing over a large range of loop operating conditions and loop configurations. The outcomes of this project will lay the groundwork for a next generation of efficient reactors that can be used both to generate electricity and to power the formation of transportation fuels such as hydrogen.

Creating a Discovery Platform for Defined-space Chemistry and Materials: Metal Organic Frameworks

Mark Allendorf

Removal of environmental pollutants, sequestration of chemical weapons, breath analysis, radiation detection/surveillance, water decontamination/desalination: these possibilities exemplify the mission-relevant applications of the class of chemical compounds known as Metal-organic Frameworks (MOF). Composed of inorganic metal clusters (such as Zn_4O) on a backbone of rigid organic "linkers" (such as benzene dicarboxylate groups), MOFs display a crystalline structure with monolithic pores that do not collapse when solvent is removed. Depending on the specific chemistry, this structure can be tuned to create a diversity of porous nanostructures and films, whose complete range of applications remains to be explored. However, from nanosieves for separation chemistry, to binders of gases such as methane and carbon monoxide, to creation of MOF films on semiconductors and optical devices, the number of potential applications is quite large.

The key to realizing such applications is a fundamental understanding of the chemical interactions governing MOF properties, and to use this knowledge to create models of that nanochemistry to guide current and future exploration. Collaborating with Washington State University, New Mexico Highlands University, Georgia Tech, and the University of California Berkeley, this project team significantly advanced the synthetic chemistry, physical characterization, and modeling of MOFs. Among the discoveries is a series of new fluorescent MOFs, created using a range of metals and linkers, promising for uses such as chemical weapon detection and personal exposure monitors. Another important development is the first "flexible force-field" model, which the team is now using to rationally design new MOFs for specific uses.



Molecular structure of a zinc oxide MOF: extended (a) and space-filling (b).

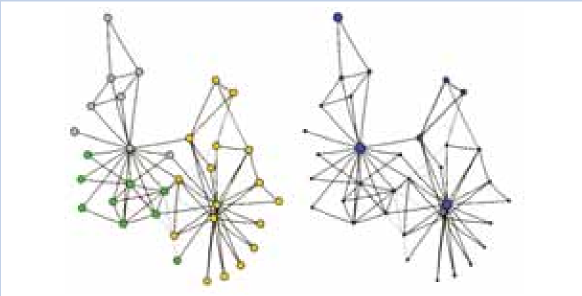
The project also benefited from the serendipitous discovery that some of the initially synthesized fluorescent MOFs exhibit intense proton-beam-induced luminescence. This creates the potential for a completely new application, namely, the detection of radionuclides for homeland security and nuclear nonproliferation. In the best scientific tradition of pursuing serendipity to advantage, the team submitted a patent application, representing the first truly new category of radiation detection materials since the early 1950s. Additionally, this team successfully integrated a MOF film with the surface of a microcantilever, paving the way for applications in microchip sensors and electronic devices.

This work opens the way for a diverse array of solutions in important Sandia mission areas, exactly the type of discovery initiative that reflects the finest in LDRD-funded research at Sandia. ■

Massive Multithreading Applied to National Infrastructure and Informatics

Jonathan Berry

Sandia's massively parallel computing resources have numerous applications, ranging from the modeling and simulation of physical processes to informatics, the analysis of large datasets such as electricity grids or the World-Wide Web. While massively parallel computers with distributed memory architectures such as Red Storm (in which data are partitioned by programmers onto each of the thousands of processors in the machine) are excellent at modeling and simulating physical processes, they are not as generally useful in informatics applications. Massively multithreaded machines with shared-memory architectures are well-suited for these problems. This team is developing algorithms and open-source software to run on the Cray XMT, a massively multithreaded machine soon to be in operation at Sandia.



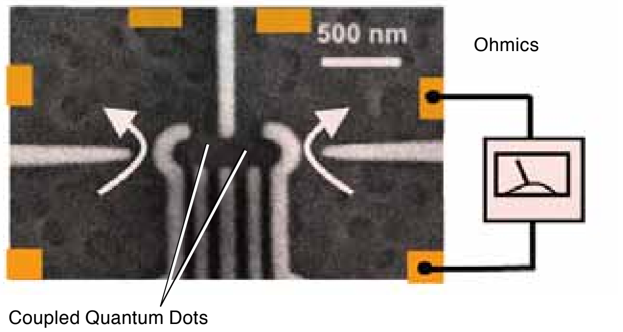
Graphical representation of network structures.

Multithreading systems are especially valuable when the datasets do not have physical structure. Homeland security applications such as the analysis of important networks for cybersecurity and the analysis of economic transaction networks from the National Infrastructure Simulation and Analysis Center (NISAC) feature such datasets.

Quantum Information Science and Technology Grand Challenge

Malcolm Carroll

This project is developing a physical quantum bit (qubit) in silicon using a dual quantum dot (studied at Sandia for several years) to isolate a single electron and encode quantum information in its spin state, a well-described quantum property of all electrons. A quantum bit is the fundamental unit of quantum information, able, because of quantum properties such as superposition, to encode more information states than a classical (0,1) computer bit. A silicon-based qubit is the key step toward developing quantum computers that can interface with silicon-based semiconductor electronic circuitry. Hence, this grand challenge is taking key steps necessary to actualize quantum computing.



Micrograph of silicon-based nanoscale arrangement of quantum dots coupled with interfacing circuitry.

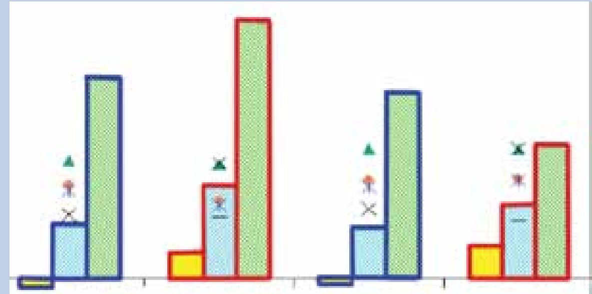
There are several types of national security problems that can be rapidly solved by quantum computers, which either run untenably slowly or are insoluble on classical computers. Efficient simulation of quantum systems is an application expected to benefit Sandia's core missions; in addition, a quantum computer could significantly improve simulation of complex physical systems, impacting several civilian and military applications.

Because quantum computers will require operation at extremely low temperatures to preserve information states for a longer duration, they will complement, rather than replacing classical computers, called upon in the solution of the aforementioned classically intractable problems.

Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

Whitney Colella

Optimal energy efficiency in heating buildings — this is one important goal of an improved energy policy. One key methodology of heating buildings is via stationary cogenerative fuel-cell systems (FCS), fueled either by natural gas or hydrogen. The CO_2 produced by natural gas combustion can be cut to one-third of that created by conventional natural gas-combustion systems if the fuel-cell systems burning natural gas can both heat a building and generate electricity for that building's use, thereby conserving energy and reducing emissions. The question is how to do so most efficiently. This project, funded, in part by a President Harry S. Truman Fellowship, has created a model that evaluates 12 novel operating strategies for designing, installing, and controlling stationary fuel cell systems to provide electricity and heat to buildings.



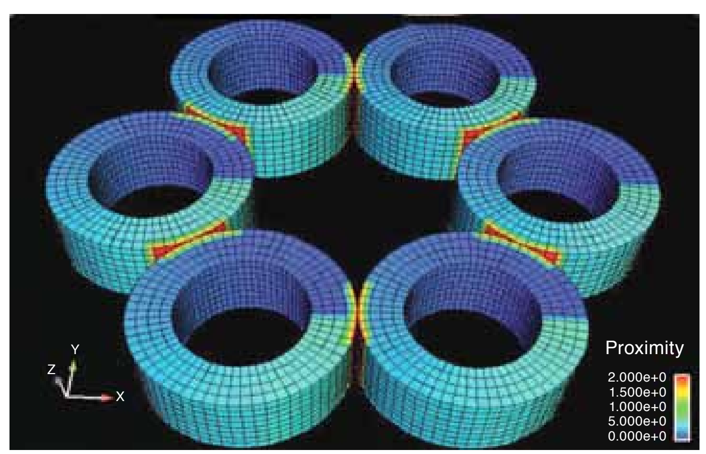
Examples of the comparative assessments of CO_2 emissions, coast savings, and efficiency of some of the fuel cell configurations examined in this project.

The model finds that networked FCS are superior to standalone FCS in terms of both CO_2 reduction and cost savings; likewise for the superiority of variable heat-to-power ratio over fixed heat-to-power ratio FCS. Unfortunately most currently installed FCS are standalone and of fixed heat-to-power ratio. Hence, this model suggests a different path forward to both save heating and electricity costs and minimize CO_2 emissions. In fact, the study concludes, changing to novel strategies can augment a carbon tax's impact on cost savings.

HPC Application Performance Analysis and Prediction

Michael Heroux

With the arrival of multicore processors to already massively parallel computers, like Sandia's Red Storm, the world of high-performance computing now faces both great possibilities and great challenges. In high-performance machines with thousands of individual processors, the arrival of multicore processors must be assessed from several angles to ensure that the most productive hardware choices and the best operating-system software are combined to provide optimal computing resources to users. This project, named "Mantevo," from the Greek, connoting prediction, is an attempt to develop benchmarks and simulators to assess the performance of applications within this multicore, parallel processing environment.



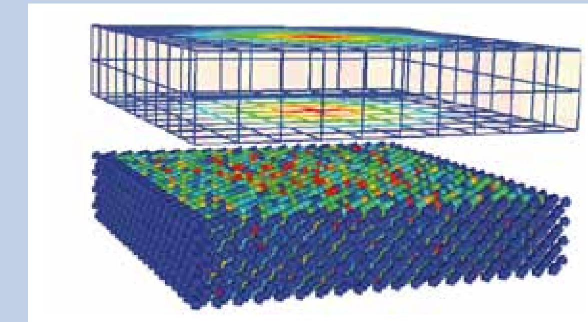
Mesh simulation of a six-counter-rotating-gear problem.

In addition to assessing node hardware architectures, the project is simulating the operation of several different application types , providing a test-bed for programming models, and quantifying the performance advantages of different models. Using Prolego, a compact performance-prediction application, the team is collecting and comparing predicted performance data, thereby continually refining its ability to assist developers as this architecture becomes a reality at Sandia. Making these efforts available to the external community as open source, enhances visibility and draws in valuable insight from external experts.

Enhanced Molecular Dynamics for Simulating Thermal and Charge Transport Phenomena in Metals and Semiconductors

Reese Jones

There are several approaches to simulating materials, each of which emphasizes particular fundamental properties. Such modeling is especially important for materials such as metals and semiconductors, whose properties, particularly at the nanoscale, are key to electronics. This project is developing a method to couple the simulations created by molecular dynamics (MD), which focus on phonons and defects, with those created by finite-element theory (FE), which focus on electrons, charge transport, and thermoelectric phenomena. The outcome will be a new class of predictive models that should greatly assist in the design of nanoscale devices.



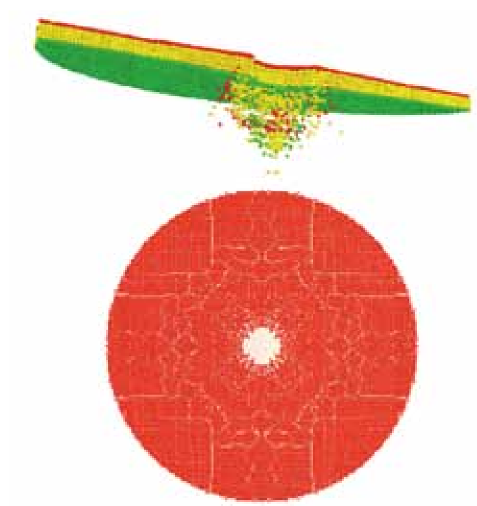
FE Mesh and MD Lattice.

The tight coupling between MD and FE paradigms utilizes the inherent strengths of each, and in doing so, this project seeks to enable predictive simulation for applications such as nanowire lasers, components of integrated semiconductor circuits and super lattice thermoelectrics, where the effects of nanoscale structures and electronic transport are equally important. The coupling paradigm is called the "Two-temperature Model" (TTM); the team used three approaches to calculated parameters required in the TTM, including a critical electron-phonon exchange coefficient. The first application will be to simulate electron-phonon–mediated energy transport in a conducting carbon nanotube. Eventually, the code will be released with user documentation.

Peridynamics as a Rigorous Coarse-graining of Atomistics for Multiscale Materials Design

Rich Lehouq

Critical to the understanding of materials and their macroscopic properties is the mathematical formulation of continuum mechanics, which approximates materials as continua of matter, filling all empty space, to some extent ignoring the atomic and molecular nature of matter as being, in fact, largely empty space. Peridynamics is a reformulation of the mathematics of continuum mechanics to permit a rigorous mathematical approach to discontinuities such as cracks and fractures.



A peridynamics representation of a layered material, implemented within LAMMPS.

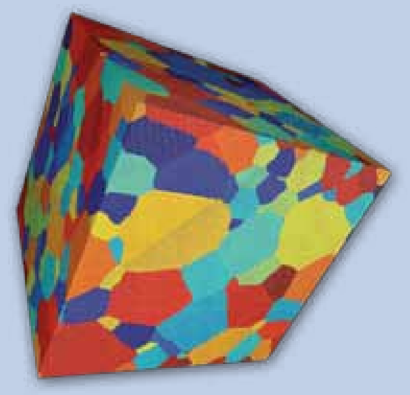
Given the importance of materials design at Sandia, and the fact that unanticipated discontinuities such as cracks often spontaneously arise in materials, the availability of a reliable and useful mathematical descriptor is of extreme importance. Proposed about 10 years ago by Sandian, Stewart Silling, this work finds continuity in the current LDRD, which is deriving and validating peridynamics in the context of the First Law of Thermodynamics (the conservation of energy). This entails the implementation of peridynamics within the LAMMPS computer code, thereby enabling applications to test-bed this ingenious new mathematical approach to materials such as those important to both weapons and nonweapons R&D at Sandia and elsewhere in the DOE and NNSA complex.

Crossing the Mesoscale No-man's Land: Parallel Kinetic Monte Carlo Simulation

Steve Plimpton

This project focuses on the development of a general purpose parallel code for new modeling initiatives at the materials mesoscale. There are numerous parallel codes that model at the atomic/molecular or nanoscale, both those based on Molecular Dynamics and those based on Density Functional Theory. And at the macroscale, there are, likewise, a variety of parallel codes from different perspectives. However, at intermediate length scales, there exist solely special-purpose codes, which do not address the need for a general-purpose code to support new modeling initiatives at that scale.

This team initially developed an approximate parallel Kinetic Monte Carlo (KMC) algorithm, which spatially decomposes a physical domain to a group of parallel processors. This enabled a Grain Growth application, capable of addressing very large sample sizes. The SPPARKS Kinetic Monte Carlo Code makes it easy to add new applications to its basic framework, to define events and their probabilities; it will soon be released as open-source code.



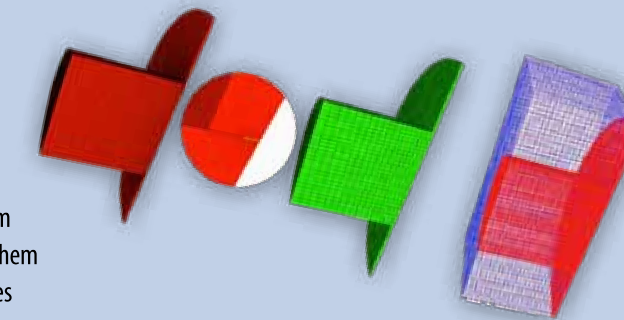
Mesoscale Grain Growth Simulation.

Multi-Length Scale Algorithms for Failure Modeling in Solid Mechanics

Benjamin Spencer

Engineered mechanical systems often fail at locations such as bolts and welds, yet these features are often omitted from computational models of these systems because including them makes computation much more costly. This project addresses this problem by developing new algorithms to enable efficient modeling of such systems that contain multiple length scales. This allows system models to include the most likely structural failure points.

In explicit solid dynamics, the time step (a slice of computer-processing time in generating the model) is controlled by the smallest elements in the model. As a result, models with fine details can require extremely small time steps, which results in more processing, and thus, high computational expense. This team has developed a method employing a coarse mesh that overlays a fine mesh that contains details of interest. Because the time step is governed by the size of the coarse mesh rather than that of the fine mesh, this results in dramatic improvements in computational efficiency. The team has implemented this method in the Presto finite element code — part of the Sierra Mechanics suite of codes — and has demonstrated the efficiency and accuracy of the method on many applications.



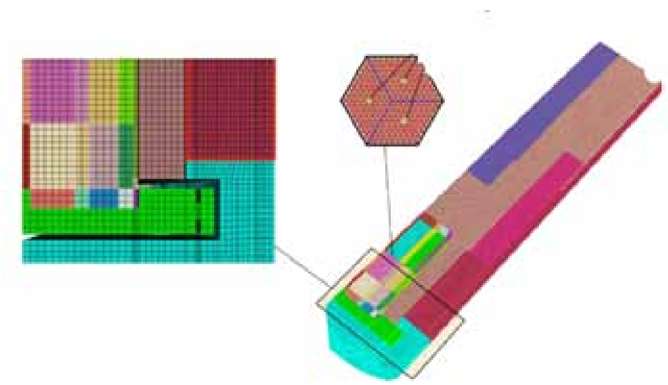
Fine mesh of component with laser weld (left, with detail shown in circle), together with two different coarse meshes used in multiscale method (center and right).

Foundational Development of an Advanced Burner Reactor Integrated Safety Code

Rodney Schmidt

The burgeoning concern about fossil fuel depletion and its burning's effect on climate change has made it imperative that nuclear reactor–driven electricity generation be revisited; and in conjunction with that return to nuclear, the closing of the fuel cycle to burn long half-lived actinides is essential. In the nuclear fuel cycle envisioned for the future, an Advanced Burner Reactor (ABR) based on fast reactor technology is expected to play a key role. However, the improved system designs being proposed have not been subjected to the thorough safety analysis or risk assessment that will be required. Legacy reactor safety codes have received only minimal investment since the early 1990s, and modeling approaches have not kept pace with computational technology.

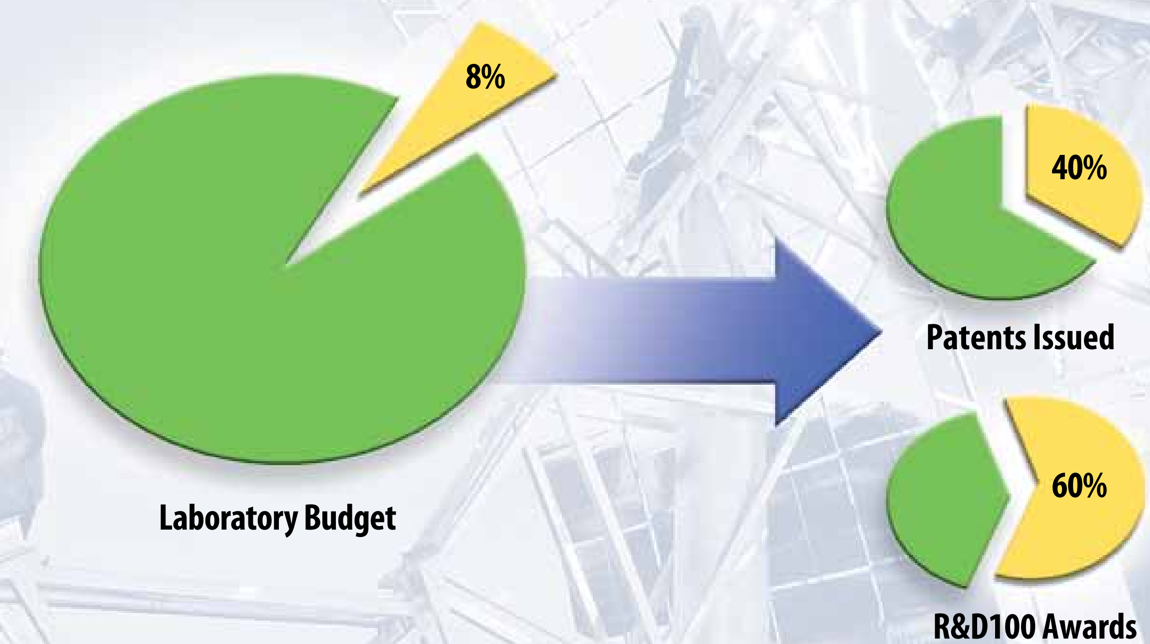
In this project, an integrated safety code is being developed — advanced multifidelity Burner Reactor Integrated Safety Code (BRISC) — crucial to performing the rigorous nuclear reactor safety analysis that will be required. Using an Argonne National Laboratory preconceptual design for a burner reactor, the BRISC code approaches the issue in a three-tiered multiscale fashion, with consideration given to the issue of uncertainty quantification, necessary to give results a greater measure of assurance.



Mesoscale mesh used to represent in-vessel regions of reactor model.

LDRD Program

Impacts Far Outstrip Its Cost



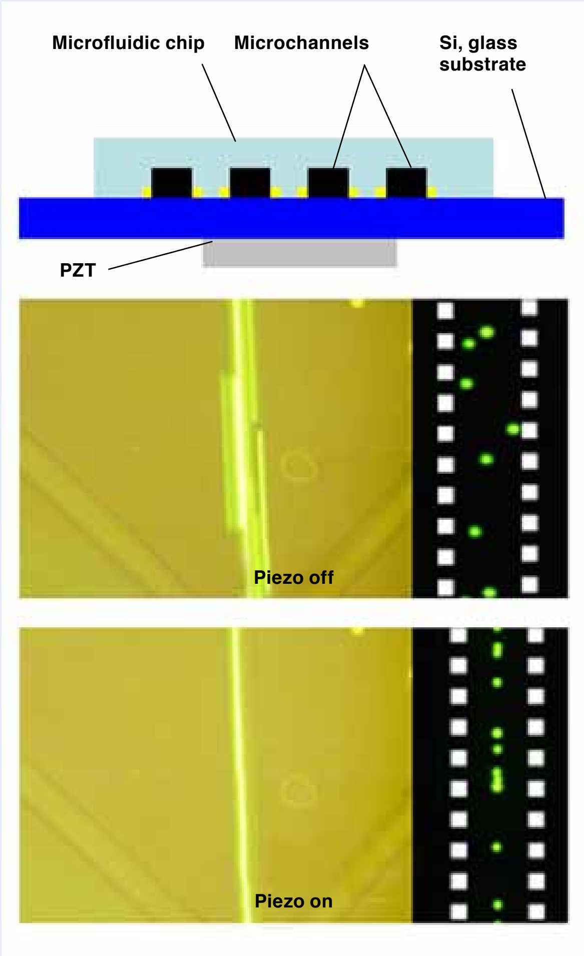
Miniature Flow Cytometer for Medical Diagnostics and Pathogen Detection

Igal Brener

Since the 1970s, flow cytometry, the hydrodynamic focusing of streams of microscopic particles, very often live human or bacterial cells for analysis, and their fluorescence interrogation by laser beams, has been a cornerstone technology in both research and in clinical diagnostics, particularly of infectious diseases.

This project has developed a microsystem flow cytometer based upon a combination of microfluidics and microacoustics. The microfluidics components allow for coarse routing of particles to necessary optical interrogation points and the sophisticated microacoustics allow precise positioning of particles in the center of a microchannel, as required for accurate fluorescent readout. By setting up acoustic standing waves, polystyrene beads, and ultimately, living cells can be delicately and precisely controlled within a microfluidics system, such that single-file queues can be reproducibly achieved; this will allow accurate optical interrogation of individual cells. Designing and engineering piezoelectric transducers and a sealed portable self-contained platform using Silicon-based microfluidics, this project team created a portable, low-cost, and simple system ideal for several applications that require precise particle positioning and integrated fluorescence readout.

When integrated with optical detection, the miniature flow cytometer can serve as a low-cost, portable platform for performing sophisticated cellular assays and rapid disease diagnostics. The reduced cost and simplification of operation will enable the system to be fielded in clinical settings around the world, especially in remote locations and combat environments where trained technicians are unavailable. This would greatly increase the potential for early detection and diagnostics of pathogens, both endemic to a population and deriving from bioterrorism. It thus has great potential benefits to both poor, indigenous populations and to US military personnel serving in remote locations. ■



Schematic of the miniature flow cytometer chip (top) in which acoustic standing waves are used to control particle position within micromachined microchannels; when the acoustic transducer is turned on, flowing beads or cells move to the channel's center (bottom) where there is an acoustic pressure node.

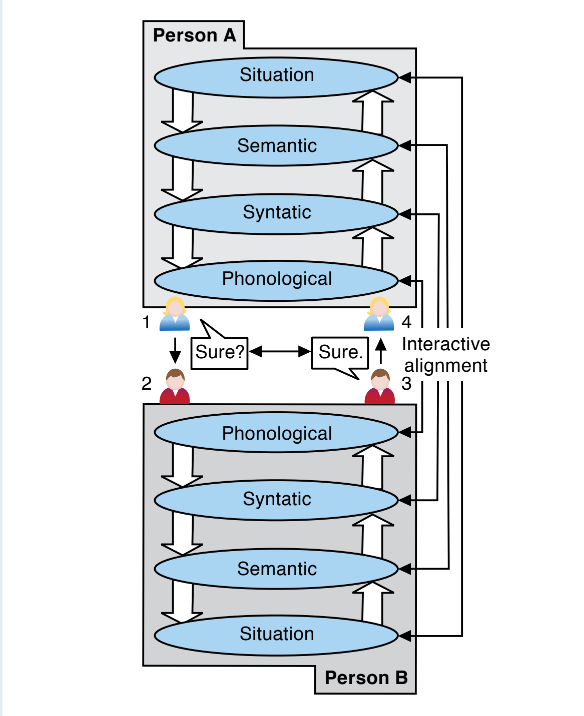
Collaborative Situational Awareness in Network-Centric Operations and Pathogen Detection

John Ganter

With the enormous intelligence available to the US military from diverse sensors and surveillance devices, responding to an overt threat or focusing a strike on a military target is a relatively straightforward exercise in military logistics. The new challenge is disguised precursor activities and targets camouflaged in normal civilian activities, particularly in peacekeeping and conflict monitoring. To detect and categorize these blended, ever-evolving threats requires cooperative analysis not unlike multidisciplinary scientific research. Network centric operations (NCO) link dispersed teams who pool their data and verbalize their thinking to develop multiple working hypotheses that steer data collection and analysis. As one might expect, intellectual diversity is not easy: each community of sensor operators and data analysts has developed it own set of linguistics, almost a tribal set of customs, responses, and descriptors.

This project's focus was collaborative situational awareness (SA) in NCO intelligence, surveillance, and reconnaissance (ISR) operations involving multiple types of sensors (Multi-Int) operated by historically insular teams having their own cultural and linguistic standards. Under conditions of acute time constraints faced during escalating conflict, such cultural communication barriers can increase ambiguity rather than clarity. Since command decisions rely on making sense of all sensor data from multiple perspectives, it is problematic that the very tribal characteristics that facilitate communication among the members of a single tribe in a mutually familiar context — for example, analysts who deal only with radio spectrum sensors — can often inhibit cross-tribe communication.

To some extent, this problem is one of understanding the situational, semantic, syntactic, and phonological components that comprise human dialogue, particularly in the enormously time-compressed regime of NCO situational awareness. In order to understand these issues more thoroughly, team members in this project conducted hundreds of hours of observation of intra- and inter-tribal dialogue as a basis for developing a detailed systems analysis technique to inform policy, training, and potentially improved or new sensor and analysis technologies. This work is positioned to ultimately help lower the barriers that cause standoffs and frustrate military decision-makers in time-compressed response situations. ■



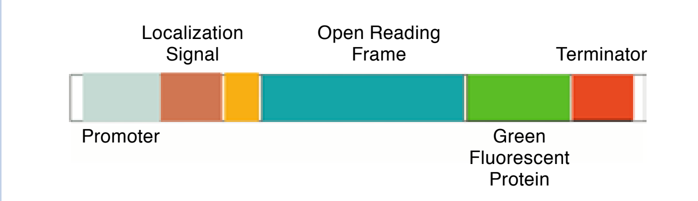
One of the new cognitive science models of human dialogue used in this research. In each person, the same sequence of processing levels that refines concrete speech to abstract situational meanings also operates in reverse to generate speech. Although rapid, this system can also lead to cross-cultural misunderstanding. (Redrawn after Trends in Cognitive Sciences, 8(1), S. Garrod & M.J. Pickering, "Why is conversation so easy?", p. 10, ©2004, with permission from Elsevier.)

"Trojan Horse" Strategy for Deconstruction of Biomass for Biofuels Production

Masood Hadi

Biofuels such as ethanol represent a key component of an evolutionary energy policy, moving the US away from dependence on foreign fossil fuel. A major hurdle is the efficiency with which "waste" plant biomass can be degraded to simple sugars and subsequently fermented to ethanol. This project is developing a completely novel approach to providing the enzymatic tools to carry out these biochemical reactions.

Genes for these enzymes are derived from extremophilic bacteria, which live in either very acidic or very hot conditions. These genes are incorporated into plants, but are not expressed as the plants grow and mature. Instead, the genes are activated after the plant is harvested, as the temperature is raised to the optimal one for activity of the extremophilic enzymes thus producing the enzymes that begin to degrade cellulose from the inside.



Example of the arrangement of genetic elements within one of the recombinant DNA molecules used to transform plants with the enzymes of extremophilic archaean bacteria.

A signal sequence of amino acids targets the enzymes to a location ("the apoplast") in the plant cell where they can be optimally efficacious at carrying-out cellulose degradation to glucose, which is subsequently fermented to ethanol. The project has achieved targeted expression of the genes, and with further refinement, the system is well-positioned for eventual use in the ethanol industry.

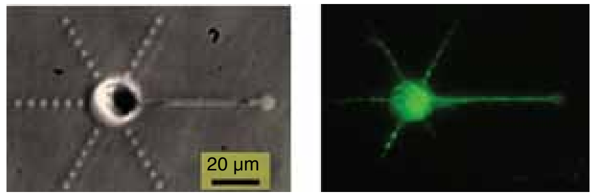
Life and Cognative Sciences

Enhanced Performance of Engineered Neural Networks using Microfabricated Guidance Cues and Predictive Computational Modeling

Conrad James

Advances in the ability to manipulate central nervous system neurons have moved researchers closer to the possibility that, ultimately, functional enhancement and/or repair of nervous system damage in human patients could become reality. One key area must be an improvement of the understanding of how networks of neurons develop their interconnected architecture and how that synaptic network determines their electrophysiological properties. This project is developing methodologies to engineer networks of neurons in vitro, control the architecture of the networks, and measure their electrophysiological properties, thus enabling a study of the relationship between network architecture and function.

Rat brain neurons are explanted into culture and provided guidance cues, as they extend output (axons) and input (dendrites) nerves fibers. By varying these cues, the nerve fiber patterns of individual neurons and groups of neurons can be controlled to produce communicating networks of different



An explanted neuron growing and extending its nerve fibers upon a patterned glass substrate; left, optical microscopy; right, fluorescence microscopy.

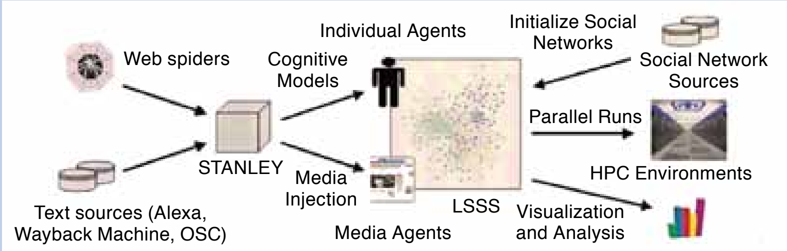
architectures. The flow of information is then measured electrophysiologically in these networks as the phenomena of long-term potentiation (LTP) and long-term depression (LTD) are recreated and modeled using Sandia's Xyce software. The understanding gained from such a study is fundamental to a deeper understanding of structure-function relationships that will ultimately be necessary to intervene in human nervous system damage.

Life and Cognative Sciences

Large-scale Simulation for Human Behavior Modeling

Eric Parker

Analysts, daily, face real-world situations, in which populations exhibit behaviors, often in a reactive mode, toward social and economic situations that may threaten US national security. To provide more-realistic models, based on human cognitive models and the behavior observed in human social networks, this project is using and developing new analytical tools and simulations. Utilizing web spiders and STANLEY software to collect and process information from online media sources, Cognitive Foundry software is used to create psychologically plausible cognitive models.



The architecture supporting "Cognitive Seldon."

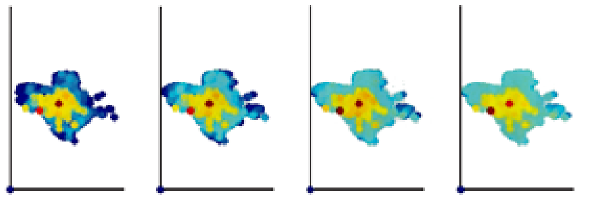
The Cognitive Foundry is integrated with a social simulation toolkit called "Seldon," which allows for dynamic social network evolution and has been used to study terrorist recruitment. This combination, "Cognitive Seldon," is used to study how media reports affect societies, and it automatically generates models from media text. Through the employment of Sandia's high-performance computing resources, large-scale simulations of entire populations are possible. This represents the first time that cognitive models have been incorporated into a social simulation. Beyond its application to analysts, important consequences of this project occur in the training of military officers in a new combat area, and improved techniques for communications personnel regarding the most propitious ways to release news or other event information.

Life and Cognative Sciences

Distributed Micro-releases of Bioterror Pathogens: Threat Characterization and Epidemiology from Uncertain Patient Observables

Jaideep Ray

From the standpoints of both bioterrorism and of climate change with its evolving array of infectious organisms at different latitudes, it is more important than ever to be able to make predictions about the genesis and progress of epidemics. This project is creating an epidemiological model that can yield significant information about an epidemic's genesis and pathogenic characteristics from only incomplete information, partial observations. The overall approach is to create a stochastic, individual-based epidemiological model separating social and pathogenic contributions.



A portion of a 21-day simulation of smallpox spread in an urban setting.

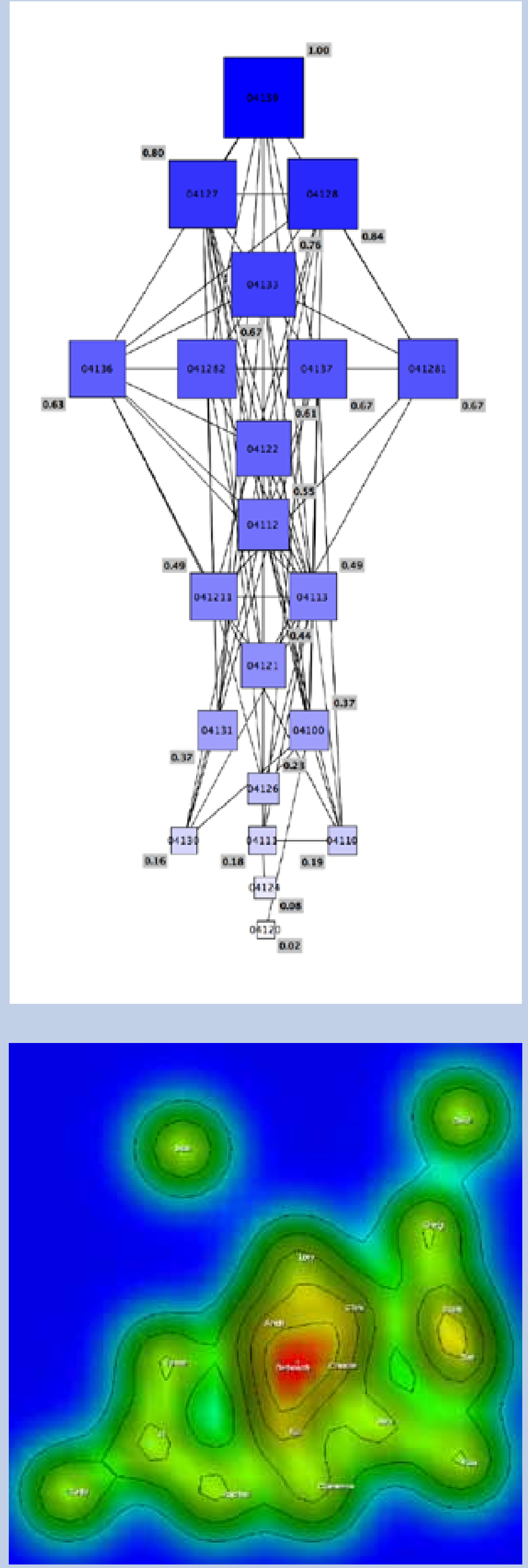
Important to models such as this one is a good knowledge of the social structure of the population through which an epidemic is spreading, since the social network parameters constitute a separate, albeit inextricably interwoven set of variables with the pathogenic characteristics of the organism in question. The model has been tested with several different epidemics, including an anthrax outbreak in 1979, and a smallpox outbreak in 1967. With refinement, the goal is to be able to model an unknown situation from sparse data.

Quantifiable and Objective Approach to Organizational Performance Enhancement

Andy Scholand

Pressure to do better work at lower cost is likely to be a ubiquitous feature of the federally funded environment for the foreseeable future, creating a need to find new ways to increase efficiency and effectiveness. Furthermore, much of an organization's technical expertise in successfully executing work is not written down precisely because this information is developed, shared, and acted upon in an operational context through informal conversations among groups of individuals. Hence, appropriately addressing organizational and interpersonal issues is likely to provide the highest probability of return within technically skilled organizations. In collaboration with the University of Texas, this research investigates socially informed quantitative measurements of work, through analysis of the digital records arising from interactions in the "as-is" organization.

Results identify work-centered social dynamics, such as distributed cognition, execution of group work, and various aspects of organizational power and control. By providing a means to inform efforts to better execute collaborative technical work, the research will contribute to the DOE Science Strategic Goal and NNSA's vision for complex transformation, as well as showing potential application to DoD's mission effectiveness efforts by enabling improvements to compel cohesion and efficiency.



Work-related communication patterns between departments (top) and individuals (bottom).

Sandia National Laboratories

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