Discovery at the Interface of Science and Engineering: Science Matters!

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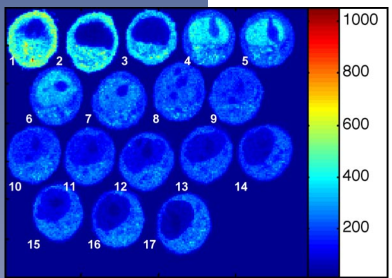
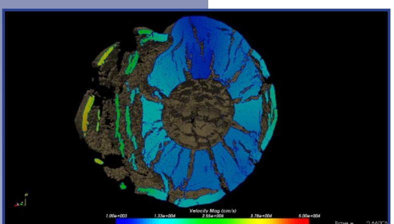
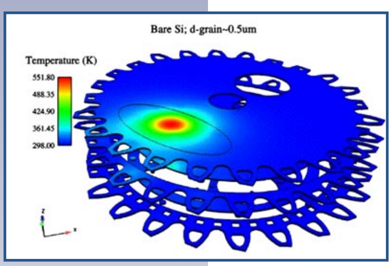
Science, Technology and Engineering

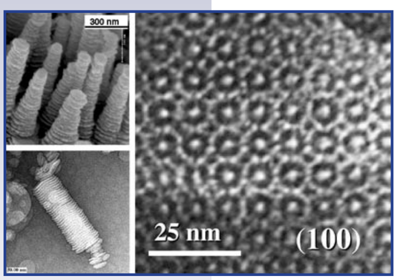


Bioscience

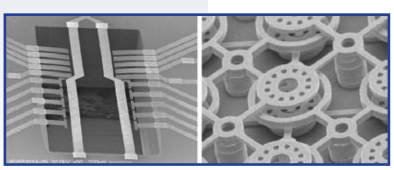

Computers and Information Sciences

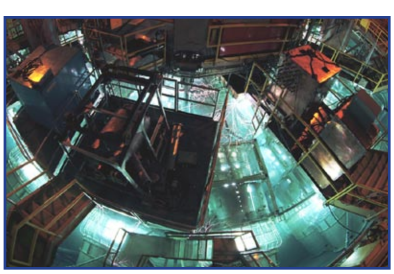


Engineering Sciences



Materials Science and Technology


Microelectronics and Microsystems


Pulsed Power

Vision

Sandia National Laboratories is the provider of innovative, science-based, systems-engineering solutions to our Nation's most challenging national security problems.

Mission

Committed to "science with the mission in mind," Sandia creates innovative, science-based, systems-engineering solutions that

- sustain, modernize, and protect our nuclear arsenal,
- prevent the spread of weapons of mass destruction,
- provide new capabilities for national defense,
- defend against terrorism,
- protect our national infrastructures, and
- ensure stable sources of energy and other critical resources.

Guiding principles for ST&E

- Ensure that the fundamental science and engineering core is vibrant and pushing the forefront of knowledge
- Enable the programs by effective application of that science base
  - responding to current needs
  - anticipating the future

About *Science Matters!*

The purpose of ***Science Matters!*** is to publicize and celebrate recent Sandia accomplishments in science, technology, and engineering. We feature the science that underpins and enables technology for Sandia's missions. We nurture expertise, facilities and equipment to create world-class science that pushes the frontiers of knowledge and anticipates future mission needs. New ***Science Matters!*** are being issued semiannually.

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Sandia National Laboratories

National Nuclear Security Administration

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Biosciences
Ion Channels

How nature discriminates between sodium and potassium ions

ab initio molecular simulations successfully answer long-standing puzzle of critical membrane function

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Natural systems excel at being able to discriminate between molecules on the basis of subtle structural differences. Membrane-spanning protein channels, for example, are exquisitely designed to differentiate between Na^+ (sodium) and K^+ (potassium) ions despite the identical charges and sub-Angstrom differences in size. Consequently, nearly all cells can selectively transport these ions across their membranes, a process that underlies such diverse physiological tasks as cell volume control, nerve cell signaling, heart rhythm control, vision, and kidney function.

Because of their charges, ions are "solvated" or surrounded by ligands to shield the charge. While scientists have long known that ion selectivity often lies in the ability of ion channel proteins to satisfy or frustrate ion solvation requirements, the persistent question revolves around how channel structures give rise to such a subtle effect between Na^+ and K^+. Recent work at Sandia provides a novel explanation. Using quantum chemical methods in a statistical mechanical framework for analysis, we analyzed ion binding to clusters of water and other ligands embedded in various environments. We found that in addition to the specific number and chemistry of ligands coordinating with the ions, the hydrogen-bonding proclivity of the surrounding environment created by the channel protein also plays a crucial role in ion selectivity. Interestingly, octa-coordinated channel binding sites (Figure 1) over-coordinate K^+ to achieve selectivity. Loss in the numbers of coordinating ligands can lead to lost selectivity or transient channel blockage.

These new ideas imply that ion discrimination could be incorporated into synthetic channel design. If we can understand these transport processes at the most fundamental level of ion discrimination by membrane proteins, we can potentially impact the development of drugs designed to counter malfunctions. Furthermore, by understanding how protein structure leads to such a remarkable level of discrimination, we can also aim to harness nature's design principles in nano-scale devices that mimic biological function. For example, Sandia researchers are exploring ways to perform ion discrimination for implantable electric energy sources to power artificial retinas (Figure 2).

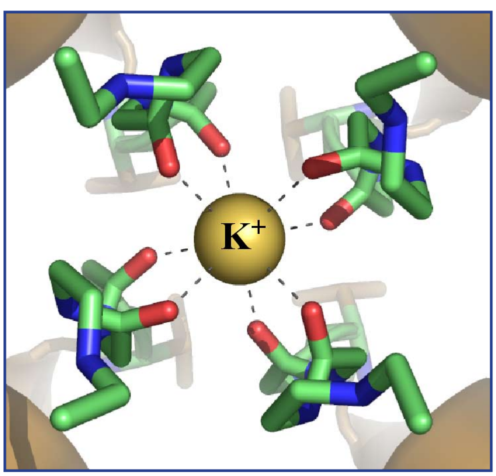

Figure 1: Octa-coordinated channel binding sites achieve K^+ selectivity.

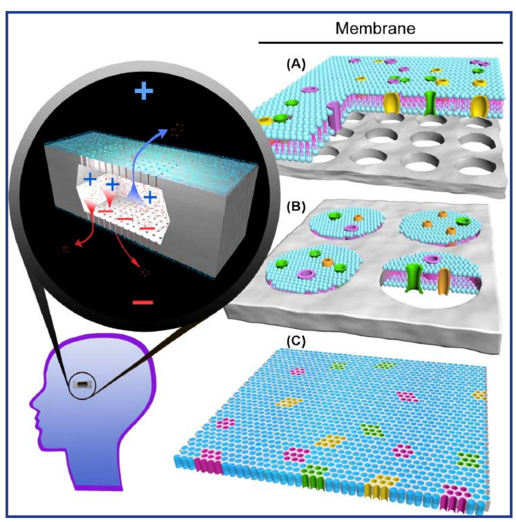

Figure 2. Biomimetic membranes could form components of useful new nanodevices, such as implantable electrical power sources to drive artificial retina.

Publications

S. B. Rempe, D. Asthagiri, and L. R. Pratt, "Inner shell definition and absolute hydration free energy of K^+(aq) on the basis of quasi-chemical theory and *ab initio* molecular dynamics, *Phys. Chem. Chem. Phys.* 6:1966-1969, 2004.

S. Varma and S. B. Rempe, "Coordination numbers of alkali metal ions in aqueous solutions," *Biophys. Chem*. 124:192-199, 2006.

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NNSA National Nuclear Security Administration

Cognitive Science and Technology
Augmented Cognition

Figure 1. Prototype test-bed vehicle Mercedes G500 during the experiments at Marine Corps Base Camp Pendleton

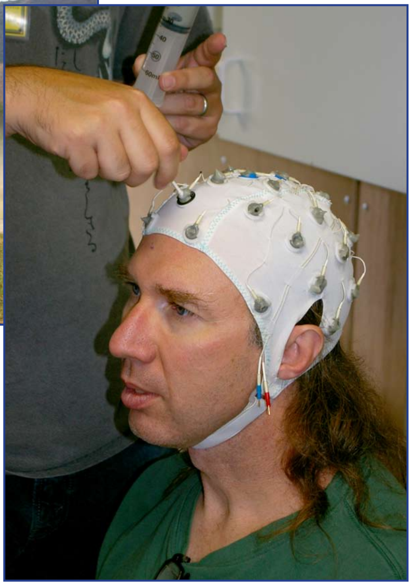

Figure 2. One of the preliminary subjects being fitted with an EEG cap

Augmented Cognition (AugCog) technology improves safety

Improved situational awareness with onboard EEG sensors may protect lives and allow for more rapid responses

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Situational awareness and effectiveness in military vehicles are crucial in today's high technology world. Excessive cognitive stimulation may overload personnel and degrade their operational performance. Sandia's Cognitive Science and Technology (C&ST) program conducts research to understand the neural and cognitive aspects of human decision making in order to build technologies that emulate or augment human performance.

In collaboration with DaimlerChrysler, the CS&T team is working with U.S. Marine Corps vehicle crews, who regularly experience cognitive and physical overload during their missions, to improve their safety, increase their performance, and reduce casualties. This team has developed Augmented Cognition (AugCog) technology that operates in moving vehicles in real time (Figure 1) and includes an electroencephalogram (EEG) gauge (Figure 2) to measure cognitive workloads, as well as a system that determines an individual's physical workload based on data from the vehicle itself (Figure 3, back page). In controlled experiments, subjects were pushed to their limits by engaging targets, categorizing radio traffic, and responding to call signs while their vehicle traversed a course. During the experiments, tasks were varied and assigned to crew members according to three experimental conditions:

- *Experimental* (AugCog): tasks were rerouted when either the EEG or physical-workload classifier indicated a high-load condition on a member of the vehicle crew.
- *Controlled 1*: no routing modifications, irrespective of workload, which tests if there is any value in rerouting.
- *Controlled 2*: modulates tasks to different individuals based on *a priori* knowledge of ongoing tasks, which tests if there is value in measuring EEG signals and physical workload.

The EEG component correctly identified high cognitive workload conditions 84 percent of the time, and the physical workload classifier correctly identified high physical workload 88 percent of the time. In the experimental AugCog condition, the team demonstrated a statistically significant 11 percent improvement in crew performance and situational awareness over both control conditions. This validates the hypothesis that crew performance and situational awareness can be improved by measuring cognitive and physical workloads. These experiments had a relatively light workload. We expect augmented crew performance to be much higher in future experiments where the workload will be much greater.

Figure 3: Two preliminary subjects are providing baseline EEG recordings in a relaxed state prior to experimentation

Figure 4: Interior view of the custom dashboard in the Mercedes prototype during the experiments

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National Nuclear Security Administration

Simulation of early-time head impact leading to traumatic brain injury

Shock physics impact simulations provide medical insights for reducing brain injury

Traumatic brain injuries (TBI) associated with accidental impact may result in a variety of motor and coordination deficits, as well as loss of the brain's capability to perform cognitive and memory tasks and to process information. Consequences of brain trauma begin at the instant of injury as pressure and shear waves propagate through the brain followed by linear and angular accelerations of the brain within the skull. This suggests the existence of threshold levels and/or conditions of mechanical stress experienced by the brain that, if exceeded, lead to neural injury and evolving damage from TBI in the hours and days following an accident.

Sandia, in collaboration with the University of New Mexico Health Sciences Center, is developing numerical simulation models of the human head to study a spectrum of impact and blast wave conditions leading to TBI. Accurate models of the various tissues and geometries of the human head are being created to conduct head injury simulations that will help establish a correlation between incipient levels, rates, and durations of stress experienced by the brain at the onset of TBI. The initial scoping study simulated early-time wave interactions (within 800 micro-seconds after impact) resulting from a 34 mph impact with a plate of glass.

The model is created by importing a digitally processed computer tomography (CT) scan of a healthy female head into the material definition package of a Sandia shock physics hydrocode run on a parallel architecture computer employing 64 processors. The digital process segmented all soft tissue and bone into three distinct materials: skull, brain, and cerebral spinal fluid. Preliminary constitutive models were formulated for the skull, brain, fluid, and glass plate.

Results suggest the occurrence of the classic coup-contrecoup insult to the head, where the frontal lobes experience significant compressive pressure as the shock wave propagates into the brain from the impact. Simulation results display sagittal (side) views of the compressive pressure in the frontal region (Figure 1, back page) and tensile pressure in the occipital region (Figure 2, back page). Regions of significantly elevated deviatoric (shearing) stress are displayed in Figures 3 and 4 (back page), containing plots of the von Mises stress magnitude related to distortional (shearing) strain experienced by the material. The tearing action resulting from this type of stress could lead to cell and tissue damage.

A principal goal of this work is to establish a quantitative correlation between specific levels of stress/strain energy and the neurological conditions that lead to TBI. Once such correlations exist, this approach will be used to investigate mitigating strategies (e.g., protective headgear), which protect against the conditions under which TBI occurs.

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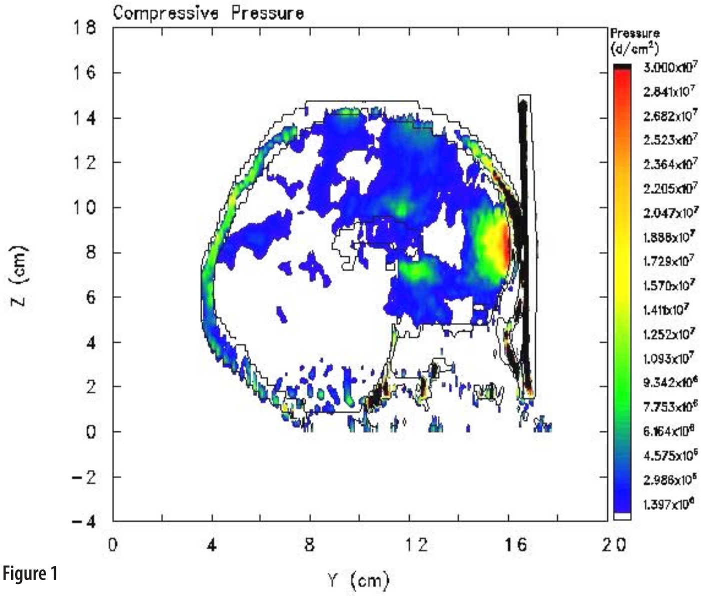

Figure 1

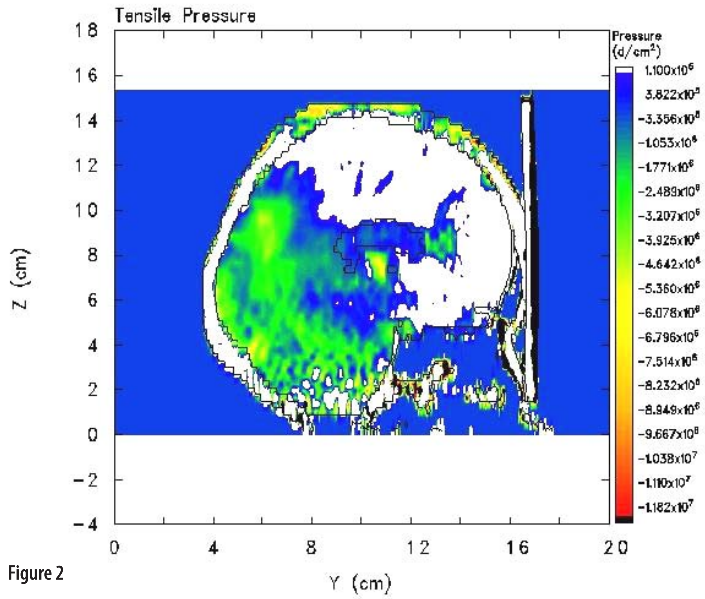

Figure 2

Distribution of compressive and tensile pressures in the sagittal plane (side view) 0.3 msec and 0.4 msec after impact, respectively. Left scale: red: 30 bars, blue: 1 bar; Right scale: red: 12 bars (tensile), blue: 1 bar (compressive).

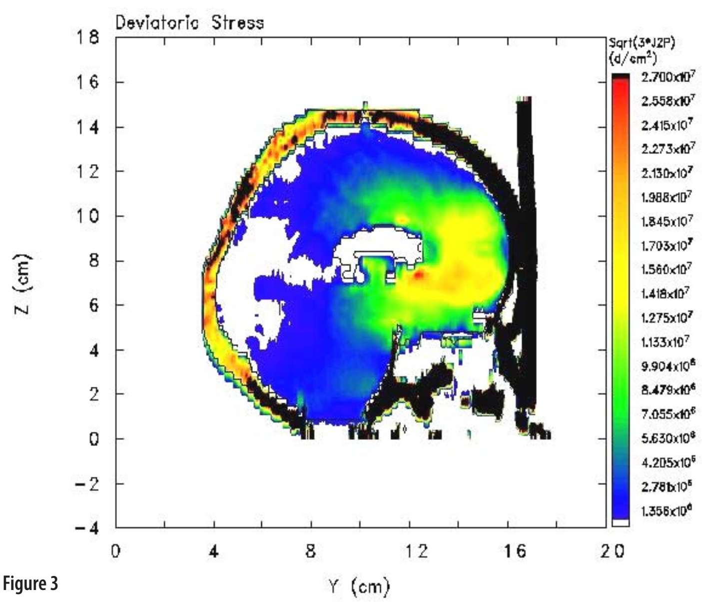

Figure 3

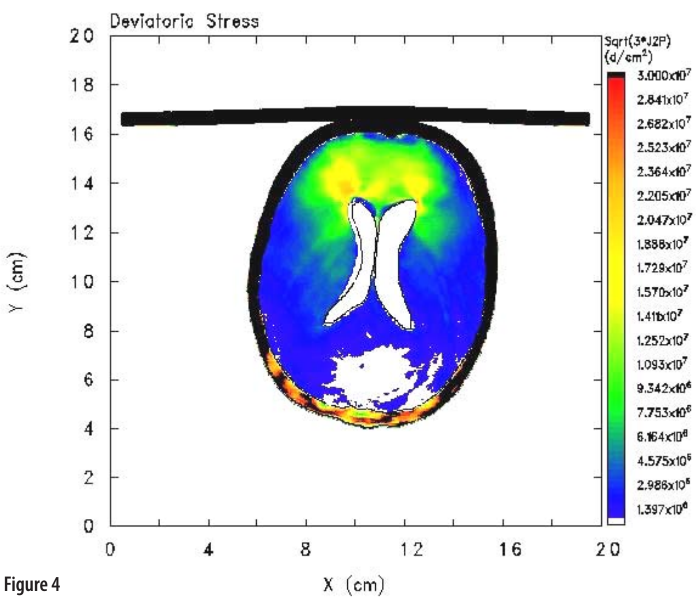

Figure 4

Distribution of deviatoric (shearing) stress in the sagittal and axial planes (side and top views) 0.4 msec after impact. Scale: red: 30 bars, blue: 1 bar.

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National Nuclear Security Administration

Researchers simulate self-focusing beams in high-power fiber lasers

Sandia research significantly impacts power scaling of fiber lasers

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In remote sensing systems, data are often sent via laser light over optical fibers. A unique class of fibers is also used to generate the laser light within the fiber. Increases in the attainable peak power of these rare-earth-doped "fiber lasers" to the megawatt (MW) level have enabled these sources to replace conventional lasers in a variety of applications. However, too much power causes self-focusing (SF), a nonlinear process in which the radial variation in beam intensity causes a corresponding variation in the instantaneous refractive index (RI) in the fiber (see figure). The resultant lens-like RI profile causes the propagating beam to contract. If the power exceeds a certain critical value (P_{crit}), catastrophic SF will occur, causing dielectric breakdown that destroys the fiber.

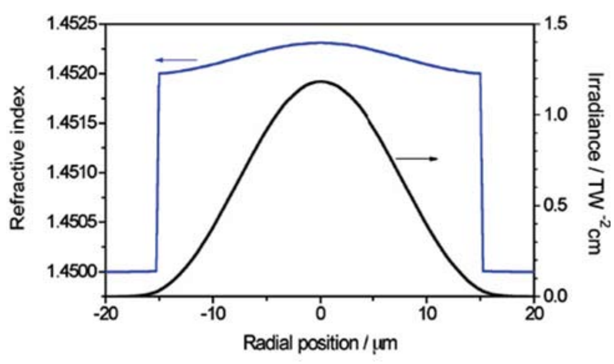
Although SF in bulk media has been well studied, significant confusion exists in the literature concerning SF in optical fibers, and no work has addressed SF in fiber lasers. As such, further power scaling requires an understanding of SF beams in fibers.

Sandia researchers, supported by the Fiber Laser Grand Challenge LDRD program, have addressed the key, fundamental issues associated with SF in fiber lasers via detailed numerical simulations. Their analysis showed the following:

- At all powers below P_{crit}, stationary (non-oscillatory) modes exist that propagate unchanged in the fiber (in contrast to literature reports).
- In a fiber amplifier, the propagating beam will adiabatically evolve through a series of stationary modes.
- The value of P_{crit} is nearly identical in a fiber and in a similar bulk medium.
- These conclusions hold for both straight and coiled fibers.

This work has significant implications for power scaling of fiber lasers. For example, although coiling of the fiber changes the waveguiding properties of the fiber and substantially distorts the fiber modes, this effect will not lower P_{crit}. Similarly, the previously reported oscillatory behavior lowers the effective threshold for parasitic nonlinear processes and optical damage, but real-world fiber lasers will not be subject to this limitation.

In the future, the Sandia codes will be used to analyze the SF behavior of more complex fiber designs, with the goal of exploiting the unique properties of waveguides to increase the attainable power from compact, practical laser systems.



Fundamental-mode irradiance profile (black) and resultant RI profile (blue) for a step-index fiber with a 3 MW beam. The bulge at the center of the RI profile results from the nonlinear response of the RI to the irradiance (Kerr effect), acting as a lens that causes SF.

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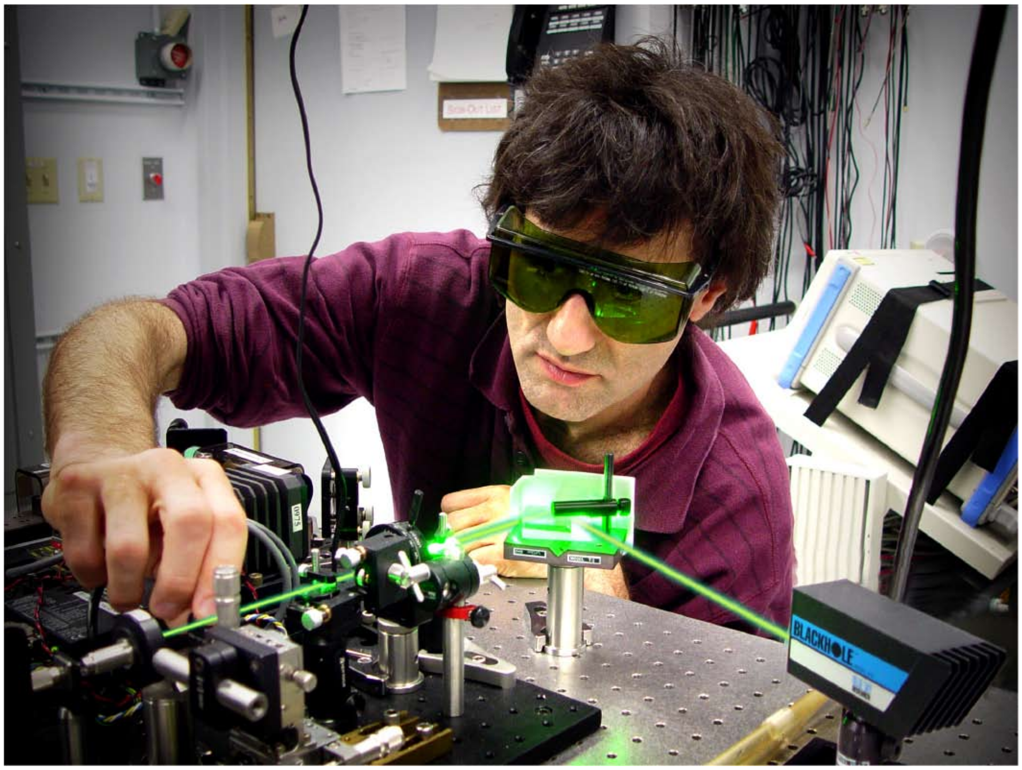
LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT



Sandia researcher, Dahv Kliner, works on a bend-loss-induced mode filtering method that allows the use of large core diameter fibers while maintaining high beam quality.

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National Nuclear Security Administration

Computers and Information Sciences
Compute Process Allocator

Sandia's innovative solutions maximize throughput in parallel supercomputers

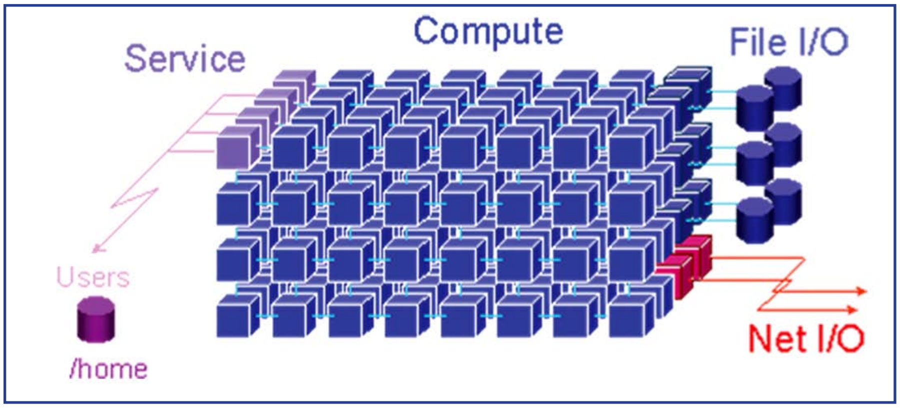

Figure 1: Parallel Supercomputer

CPA's optimized node allocation strategy wins a prestigious 2006 R&D award

In collaboration with researchers from the State University of New York-Stony Brook and the University of Illinois, Urbana-Champaign, Sandia has developed an innovative solution to resource allocation for parallel processing on supercomputers (Figure 1). The Compute Process Allocator (CPA) uses a space-filling curve to reorder a network of processors so that locations remain close in the physical network of processors after reordering (Figure 2). It also uses Best Fit packing (Figure 3, next page), for contiguous allocation and span minimization for non-contiguous allocation. In experiments, the optimized node allocation strategy employed by CPA increased throughput by 23%, thus processing five jobs in the time it takes to process four. The CPA is distributed and scales to over 10,000 nodes while non-distributed allocators scale to 4,096 nodes.

For its superior strategy and scalability over other allocators, the CPA won a prestigious 2006 R&D 100 Award. The CPA's innovative solution was carried to the commercial sector in 2005 when CPA was licensed to Cray Inc. The breadth of impact has been extended through software licensing to numerous laboratory and research centers that bought XT3 systems from Cray. The CPA (at less than one percent of the cost of a parallel computer) is an example of how a relatively small investment in computer algorithms can dramatically leverage the return on a large investment in computer hardware.

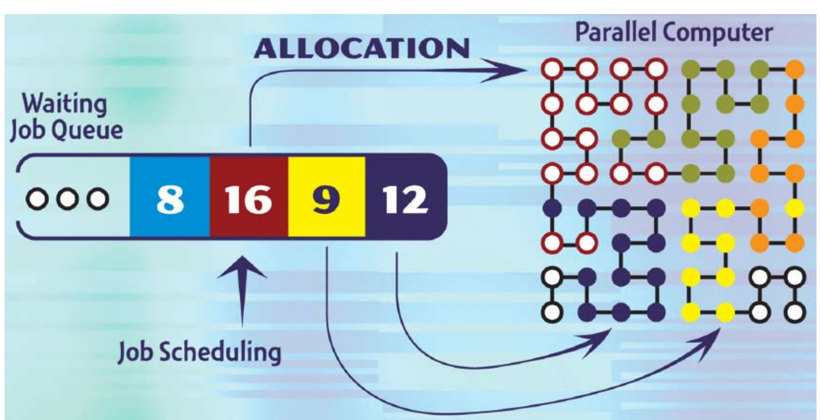

Figure 2. CPA with Hilbert Space-Filling Curve and Span Minimization.

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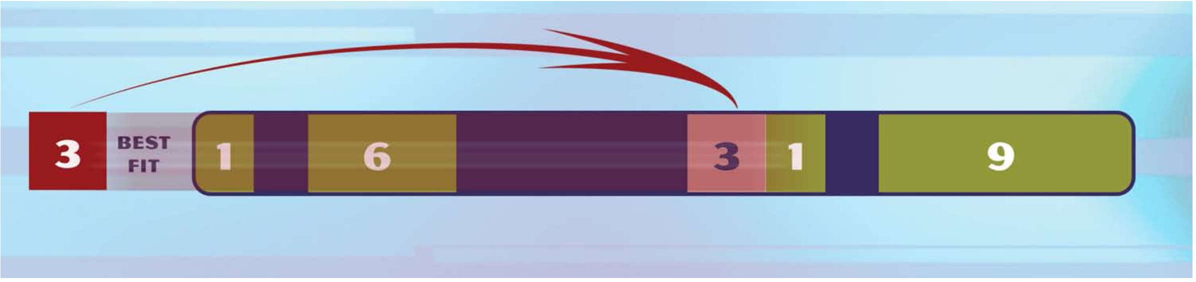

Figure 3. Best Fit Packing

Sites with supercomputers using CPA include:

- Sandia (Red Storm and C-Plant)
- Oak Ridge National Laboratory
- U.S. Army Engineer Research and Development Center
- U.S. Army High Performance Computing Research Center
- UK Atomic Weapons Establishment
- Pittsburgh Supercomputing Center
- Japan Advanced Institute of Science and Technology
- RIKEN Advanced Center for Computing and Communication in Japan.
- Swiss Scientific Computing Center

Publications related to the CPA:

V.J. Leung, E.M. Arkin, M.A. Bender, D.P. Bunde, J. Johnston, A. Lal, J.S.B. Mitchell, C. Phillips, and S.S. Seiden, "Processor Allocation on Cplant: Achieving General Processor Locality Using One-Dimensional Allocation Strategies," 2002 IEEE International Conference on Cluster Computing.

V.J. Leung, C.A. Phillips, M.A. Bender, and D.P. Bunde, "Algorithmic Support for Commodity-Based Parallel Computing Systems," Sandia Report SAND2003-3702, 2003.

D.P. Bunde, V.J. Leung, and J. Mache, "Communication Patterns and Allocation Strategies," 3rd International Workshop on Performance Modeling, Evaluation, and Optimization of Parallel and Distributed Systems, 2004.

M.A. Bender, D.P. Bunde, E.D. Demaine, S.P. Fekete, V.J. Leung, H. Meijer, and C.A. Phillips, "Communication-Aware Processor Allocation for Supercomputers," 9th Workshop on Algorithms and Data Structures, 2005.

Quotes on the R&D 100 Awards and the CPA, in particular:

"I congratulate the researchers who have won these awards, which highlight the power and promise of DOE's investments in science and technology. Through the efforts of dedicated and innovative scientists and engineers at our national laboratories, DOE is helping to enhance our nation's energy, economic and national security." (Samuel W. Bodman, Secretary of Energy).

"At a time when some question whether or not their tax money is delivering results... a time when a few even question the relevance of scientific research in their everyday lives... the R&D 100 Awards serve to recognize excellence, innovation and relevance." (David Garman, Former Acting Under Secretary, U.S. Department of Energy).

"The increased throughput of twenty-three percent that 'CPA' allows and the capability of being scalable to tens of thousands of processors is very impressive. Many prestigious computing centers are already realizing the great benefits of 'CPA'. This well-deserved recognition is an excellent reminder that our laboratories are outstanding science and technology resources for the Nation." (Linton F. Brooks, Former Administrator, National Nuclear Security Administration).

"Congratulations to you and your Sandia colleagues who teamed to win an R&D 100 Award for the project Compute Process Allocator (CPA). I am sure fellow Sandians are very proud of your achievement." (Thomas O. Hunter, President and Laboratories Director).

"These are coveted awards and you should be extremely proud." (Rick Stulen, Chief Technology Officer).

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Picturing Science

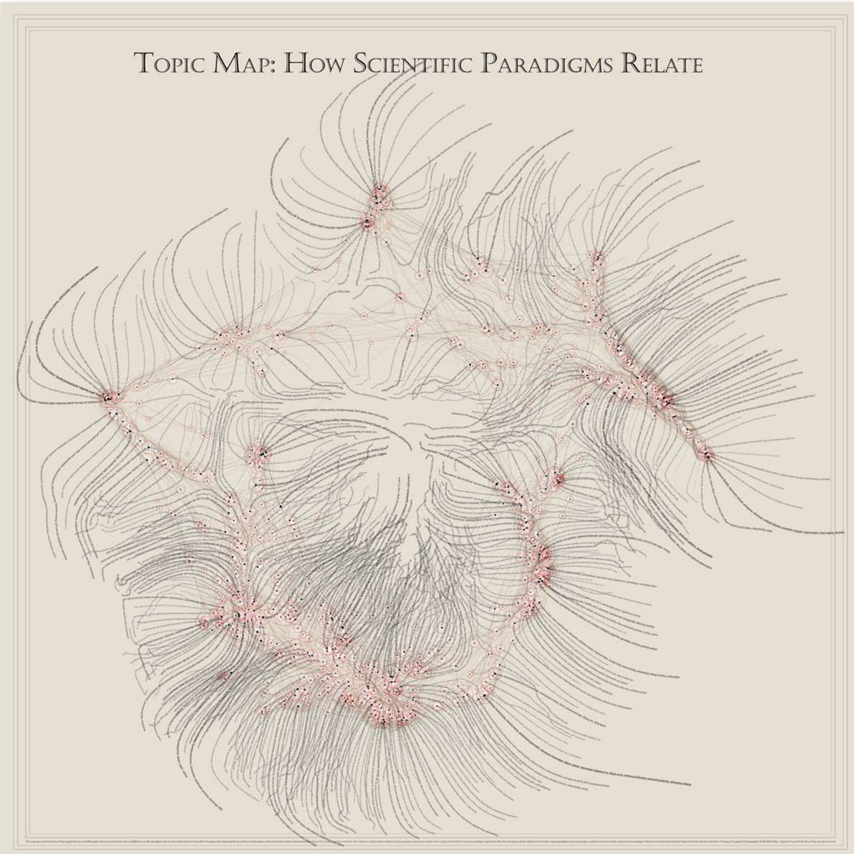

Figure 1. Map of scientific paradigms

Mapping scientific paradigms

Mapping scientific paradigms illustrates the relationships between different scientific disciplines and provides correlated information for planning and evaluation purposes.

With the seemingly limitless amount of information that is now available at one's fingertips, it is increasingly important to evaluate new research ideas with respect to pertinent scientific knowledge databases. Connections between ideas and knowledge are critical and can now be mapped out. Such a map of science resembles a filamentous microorganism you might see under a microscope (Figure 1). The map represents 800,000 scientific papers (portrayed as white dots) and shows relationships between them and different scientific disciplines. The "filaments" are common words unique to each "scientific paradigm," which are depicted as the 776 red circular nodes or clusters of papers (Figure 2, next page). Each node contains papers that are commonly cited together; larger nodes have more papers. The nodes are connected with lines of various lengths and thicknesses, denoting the strength of the citation linkages between them. Layout of the node positions was done with cosine index values generated from co-citation statistics using a recursive process and the VxOrd graph layout routine authored at Sandia. Chemistry papers are found in the right-hand peninsula while astrophysics papers are located at the top. Medicine covers the large region at the lower left.

A four-foot-square version of the map was displayed at the New York Hall of Science as part of the Places & Spaces: Mapping Science exhibition. This image also appeared in the Gallery section of the 2006 year-end issue of *Nature* (vol. 444, p. 985).

Scientists from Sandia and SciTech Strategies, of Berwyn, PA, produced the map using 2003 data from Thomson Scientific. It was enabled by work performed under a Laboratory Directed Research and Development project whose purpose was to generate large-scale maps of science for planning and evaluation purposes.

For more information on interpreting the map, see *http://didi.com/brad/mapOfScience.*

For details on the exhibition, see *www.scimaps.org.*

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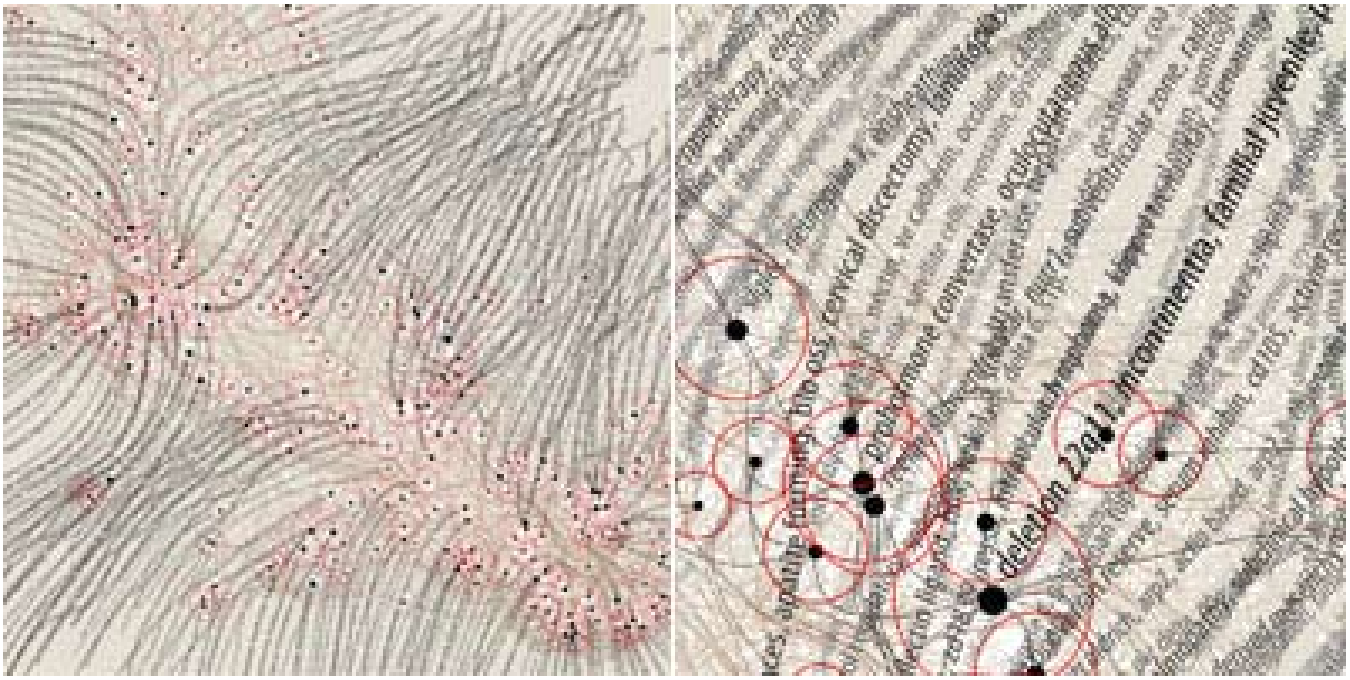

Figure 2. (Left) Enlarged view of a node section. (Right) Magnified view showing common "scientific paradigm" words.

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National Nuclear Security Administration

Engineering Sciences
Aeroscience

Advanced turbulent flow modeling for accurate aerodynamic predictions

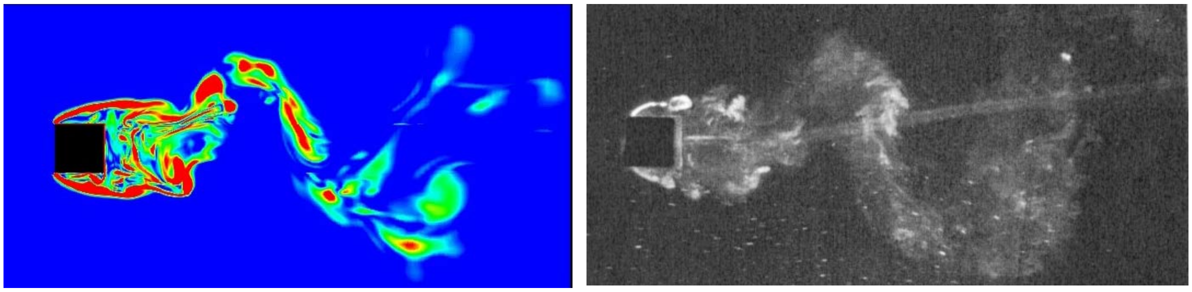

Figure 1: (Left) Instantaneous contours of vorticity magnitude given by a simulation of the turbulent low-speed wake of a square cylinder. (Right) Smoke visualization of the turbulent wake from a water tunnel experiment (Durao et al., Experiments in Fluids, 6(5):298, 1988).

Advances in computer simulations now enable accurate predictions of aerodynamic forces and heating rates

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Although turbulent fluid motion is encountered in countless engineering devices, its complex dynamical behavior has largely defied attempts at a general theoretical description. To tackle this important problem, aeroscience researchers at Sandia are turning to temporally-resolved computer simulations of compressible turbulent flow as a means of improving engineering predictions of aerodynamic forces and heating rates on flight vehicles. Recent advances in computing power have enabled such simulations to tackle the leap from academic research tool to engineering analysis tool.

Sandia's research focuses on development of accurate numerical simulation techniques for compressible gas flows, where gas velocities may approach or exceed the speed of sound. The larger, more energetic, eddy motions of the gas are directly resolved by the simulation, while the smaller, less energetic, turbulent motions are modeled. Results from a validation study involving the low-speed flow of air past a square cylinder (shown in Figures 1 and 2) illustrate the success of this approach for a bluff-body flow. At flight speeds above the speed of sound, a shock wave precedes the bluff body, presenting a severe challenge to the numerical techniques. Figure 3 (see next page) shows the simulation of an Apollo reentry capsule, demonstrating the ability of the simulation to capture the steady bow shock in addition to the unsteady separated wake surrounding the capsule afterbody.

The development of unsteady turbulence simulation technology will allow analysis of weapon delivery system aerodynamics at an unprecedented level of fidelity. It also opens the door to accurate analysis of many other types of complex, unsteady turbulent flows, from wind turbine blades to tractor-trailer vehicles.

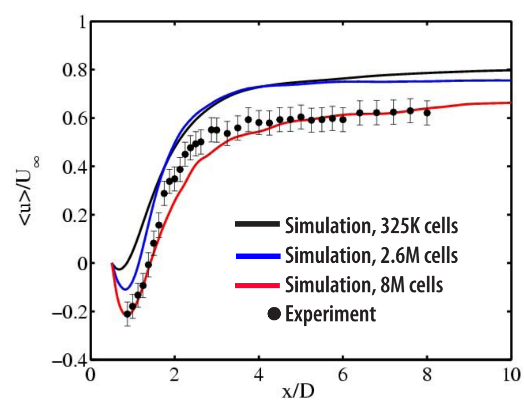

Figure 2. Simulation predictions of the time-averaged streamwise velocity in the square cylinder wake, compared with experimental data.

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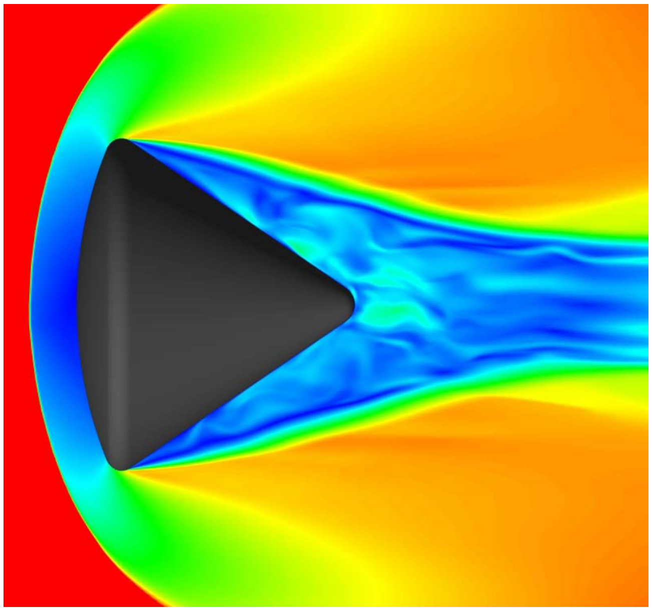
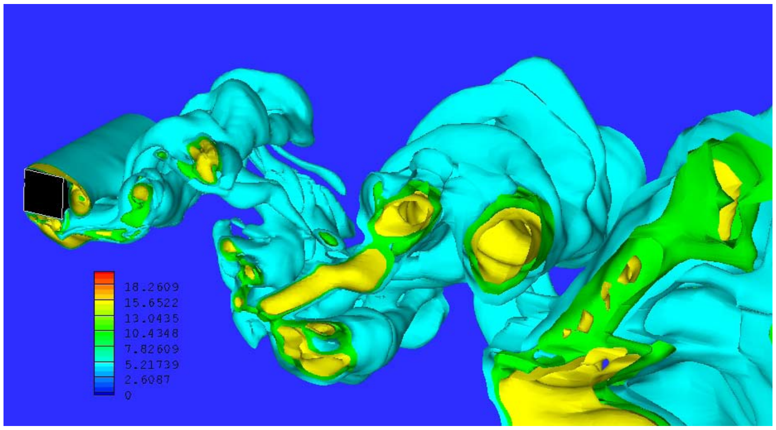


Figure 3. Instantaneous Mach number contours for the flow about an Apollo re-entry capsule, showing the steady bow shock and the turbulent fluctuations in the afterbody wake.



Isosurfaces of the modeled turbulent eddy viscosity in the wake of a square cylinder.

Publications:

M. Barone, "Mesh-independent unsteady turbulent wake simulations using the PANS model," AIAA Paper 2006-3742, 36th AIAA Fluid Dynamics Meeting, San Francisco, CA, June 5-8, 2006.

M. Barone and C. J. Roy, "Evaluation of Detached Eddy Simulation for Turbulent Wake Applications," AIAA J., 44(12):3062-3071, 2006.

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Hydrogen embrittlement mechanisms in metals

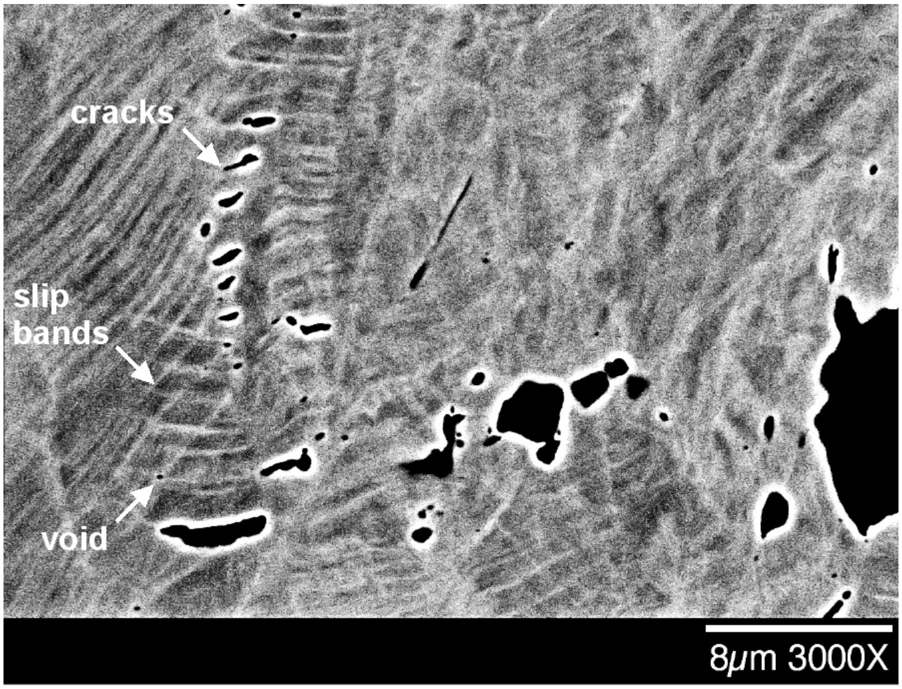

Figure 1. Backscattered electron image from crack growth specimen of stainless steel exposed to hydrogen gas. The image reveals a link between hydrogen-enhanced deformation and cracking.

Hydrogen embrittlement modeling can help ensure structural integrity of hydrogen fuel containers

High-pressure storage is a critical component of the emerging infrastructure for using hydrogen gas as an energy source. One of the key materials issues in storage is hydrogen embrittlement of metals. That happens when metal structures are subjected to concurrent mechanical loading and hydrogen gas exposure, causing the metal to become more susceptible to cracking. Embrittlement is enabled by the ability of hydrogen molecules to dissociate into hydrogen atoms on metal surfaces, which then diffuse into the metal. Hydrogen embrittlement has been explained through several mechanisms involving interactions between the atomic hydrogen and the host metal.

One of the hydrogen-metal interactions associated with embrittlement is hydrogen-enhanced localized plasticity. Compelling evidence from both experiments and modeling demonstrates that hydrogen can facilitate the motion of dislocations and promote slip planarity. However, the link between enhanced deformation and fracture has not been well established.

Sandia researchers conducted crack growth experiments on stainless steels exposed to hydrogen gas to gain insight into how hydrogen-enhanced plasticity can lead to fracture. Post-test examinations using high-magnification backscattered electron imaging (see figure) revealed that voids nucleated at intersecting slip bands and then evolved into cracks, which propagated along the slip bands. Previous results for this stainless steel demonstrated that slip bands were promoted by the presence of hydrogen. Such detailed evidence for the sequence of localized deformation, void formation at intersecting slip bands, and cracking along the slip bands has not been previously reported for full-size crack growth specimens exposed to hydrogen gas.

Ultimately, the motivation for understanding the detailed mechanisms of hydrogen embrittlement is to develop predictive models, and the framework and input parameters must be based on the real physics of deformation and fracture. Hydrogen embrittlement models can aid in designing resistant materials and assessing structural integrity, which will become more important as infrastructure is developed to support the use of hydrogen as a fuel.

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Hydrogen Effects on Materials Laboratory

Sandia National Laboratories has been working on structural design for hydrogen gas containment and hydrogen embrittlement of materials for over 40 years. The Hydrogen Effects on Materials Laboratory is a unique laboratory for measuring mechanical properties of materials exposed to high-pressure hydrogen gas. It has been maintained since the late 1970s and is being expanded. The laboratory has three primary capabilities, which are distinguished by the capabilities for conducting crack growth experiments *in situ* at hydrogen gas pressures exceeding 100 MPa:

- Exposing materials to high-pressure hydrogen gas at pressures up to 140 MPa and temperatures up to 300 ºC. This capability is used to dissolve high concentrations of hydrogen in mechanical test specimens, which are tested *ex situ* and provide data on the effect of high hydrogen concentrations on material properties.
- Testing fracture mechanics specimens that are concurrently exposed to high-pressure hydrogen gas and statically loaded under constant displacement. These *in situ* tests can be conducted in hydrogen gas pressures up to 200 MPa at room temperature and up to 140 MPa at temperatures ranging from -75 ºC to 175 °C. The tests provide data on the crack propagation threshold and crack propagation rates of materials.
- Testing fracture mechanics specimens that are concurrently exposed to high-pressure hydrogen gas and dynamically loaded. These *in situ* tests can be conducted in hydrogen gas pressures up to 140 MPa at room temperature and provide data on the fracture toughness and fatigue crack propagation rates of materials.

Sandia has tested a variety of structural materials in high-pressure hydrogen gas, which have yielded material property data used in structural design for hydrogen gas containment and provided insights into the mechanisms of hydrogen embrittlement. Sandia is actively involved in projects connected to the development of hydrogen energy infrastructure; in particular, providing input on material properties and material testing protocols for codes and standards.

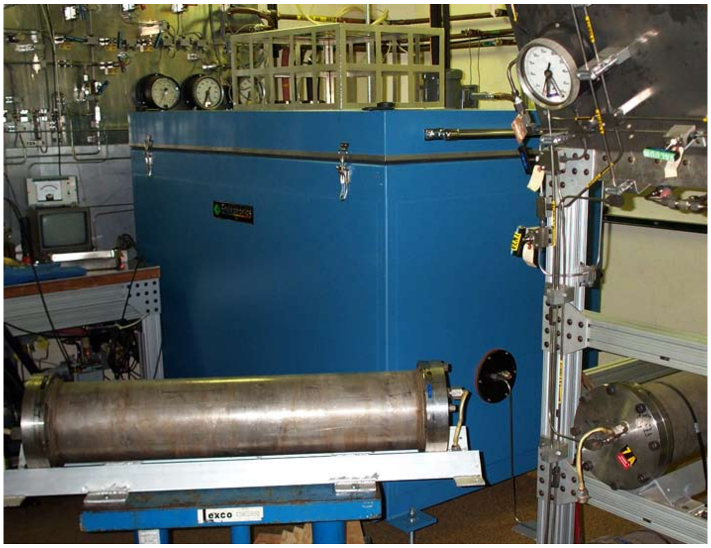

Figure 2. Laboratory for conducting tests on materials in high-pressure hydrogen gas.

Publications

"Technical Reference for Hydrogen Compatibility of Materials", B.P. Somerday and C. San Marchi, Eds., www.ca.sandia.gov/matlsTechRef.

"Effects of High-Pressure Gaseous Hydrogen on Structural Metals", C. San Marchi and B.P. Somerday, SAE 2007 World Congress, Detroit, MI, 2007.

"Mechanical Properties of Super Duplex Stainless Steel 2507 After Gas Phase Thermal Precharging with Hydrogen," C. San Marchi, B.P. Somerday, J. Zelinski, X. Tang, and G.H. Schiroky, submitted to *Metallurgical and Materials Transactions* A, 2007.

"Permeability, Solubility and Diffusivity of Hydrogen Isotopes in Stainless Steels at High Gas Pressures," C. San Marchi, B.P. Somerday, and S.L. Robinson, *International Journal of Hydrogen Energy*, vol. 32, pp. 100-116, 2007.

"Hydrogen Effects on Dislocation Activity in Austenitic Stainless Steel," K.A. Nibur, D.F. Bahr, and B.P. Somerday, *Acta Materialia*, vol. 54, pp. 2677-2684, 2006.

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National Nuclear Security Administration

Shape memory polymers detect changes in temperature or light level

Figure 1. Photo sequence demonstrating the thermally induced shape memory effect for a poly (e-caprolactone dimethacrylate) polymer. Starting from room temperature, the polymer, in its temporary shape (cube, left) is heated up to 70 ºC, which is above its glass-transition temperature. Within 60 seconds, the sample recovers its permanent shape, which is a nearly planar film (right). Reproduced from Lendlein, A. et al. *Encyclopedia of Materials Sci. and Tech*., 1-9.

Sandia scientists are creating composite materials that use shape memory to generate electrical signals

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Active polymer composites are an emerging class of materials offering innovative strategies and readily customized capabilities for intrinsic detection and embedded surveillance. Newly developed active polymer composites for embedded sensors detect and mechanically respond to abnormal thermal and optical environments by combining the capabilities of shape memory polymers (SMP), piezoelectric films, and ceramic fibers. These composites undergo a shape change in response to a specific temperature or light stimuli. The shape change is detected when it simultaneously generates an electrical signal to be transmitted, archived, or implemented. The temperature sensitivity varies with the polymer systems; for example, some current commercial systems are designed to expand at body temperature and have possible medical applications. Sandia is exploring different applications at higher temperatures.

Thermally activated SMPs are characterized by a critical polymer cross-link density and molecular spacing, which enables partial rearrangement of the polymer microstructure in the heated, mobile state, but does not enable full equilibration to a stress-free state. A thermally activated SMP device is processed into a permanent shape and then programmed to fix its temporary shape. The permanent shape is recovered by reheating beyond the transition temperature (Figure 1). Optically induced SMPs are elastomers with cross-links that undergo a photo-reversible chemical change. This process allows the elastomer to reversibly change shape through a microstructural rearrangement of the freed polymer chain segments.

Sandia is combining the sensing and mechanical actuation capabilities of SMPs with the electronic signaling capability of piezoelectrics to create flexible temperature and light-triggered actuators to perform work and generate an electrical signal to verify the actuation event. Thermal SMPs do not possess attractive combinations of processing and performance properties, and novel systems are being formulated and evaluated. The optical SMPs are based on white-light activated spiropyran cross-linkers that are neutral, rigid, ring-closed molecules under ambient light environments. In the dark, the spiropyran converts to the charged, planar, ring-opened, colored merocyanine form (Figure 2, next page). Light sensitive materials are very new, and Sandia plans to optimize and adjust this structural transformation to produce shape changes in a variety of polymers.

Because of the inherent complexity of the material response, we are developing physically based constitutive models of the SMP. We are also using finite element models of the shape memory and electromechanical behavior of active composite structures and devices (Figure 3, next page).

Sandia is seeking new and valuable applications for SMPs, which have many significant features. A unique feature is that SMPs require no power—no battery—as do other sensors. They are self-powered whether used as sensors or in any other way.

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LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

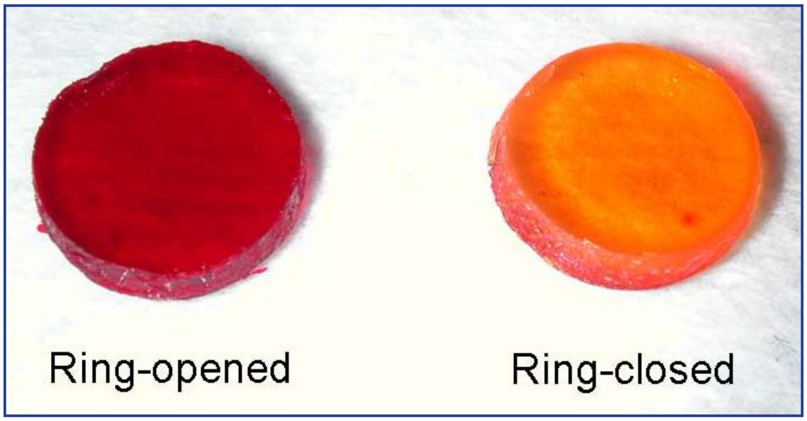

Figure 2. Activated spyropyran gels

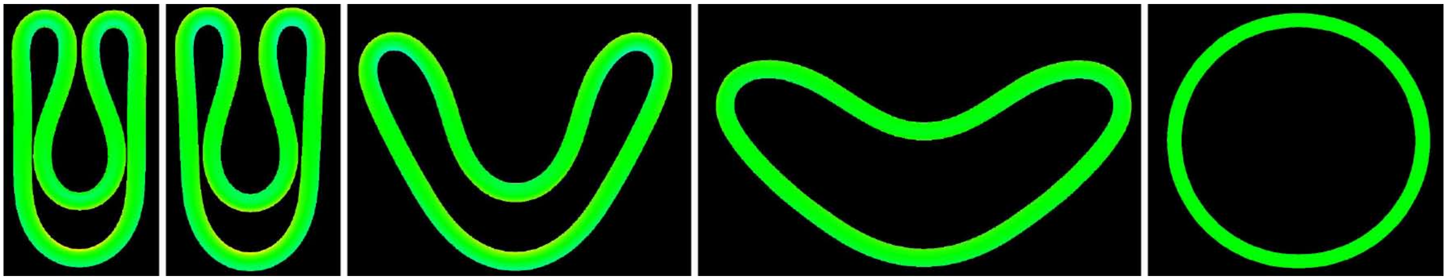

Figure 3. Finite element simulation demonstrating the thermo-viscoelastic relaxation mechanism of the recovery of a thermally induced shape memory polymer. The polymer is initially in its temporary folded shape. It recovers its permanent circular ring shape upon heating to above the glass-transition temperature.

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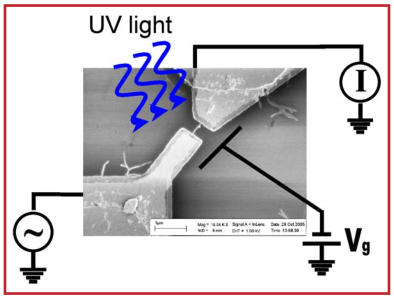

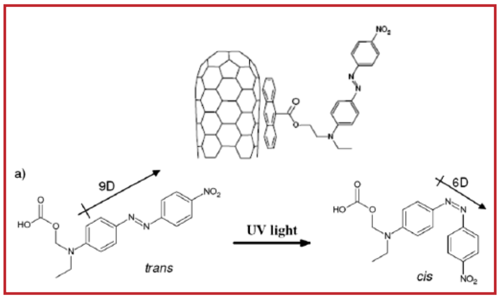

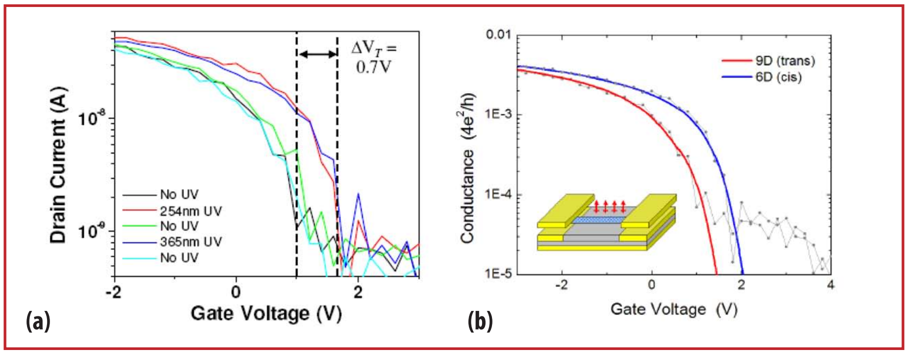

Figure 1: (Top left) Scanning electron micrograph of a chromophore-functionalized nanotube between electrodes. The current through the nanotube can be switched with a back gate (V_g) or by shining UV light.

Figure 2: (Top right) Sketch of carbon nanotube functionalized with azo-benzene. Under UV light, the azo-benzene undergoes a trans to cis transformation accompanied by a large change in dipole moment.

Figure 3: (a) Current-voltage characteristics of functionalized carbon nanotube field-effect transistors. Upon exposure to UV light, the threshold voltage is shifted to more positive values of the gate voltage. (b) Calculated conductance of the nanotube transistor in the presence of surface dipoles (solid lines) showing excellent agreement with the experiments (grey circles).

Red dye makes nanotubes switch in the blue

Photoswitching at the nanoscale can now be performed at low light levels

We are all familiar with the light switch, where an electrical circuit turns the lights ON and OFF. But, what if this concept could be reversed and an electrical circuit could be switched using light? Such a concept is at the heart of modern approaches to enable solar cells, photodetectors, and optical communications. However, conventional materials such as silicon have some fundamental optoelectronic limitations that prevent such applications from being more pervasive. Many of these limitations are overcome with the use of carbon nanotubes. These nanowires of pure carbon have unique optical properties that can be tailored for optoelectronics, and they have the additional ability to rapidly transmit an electrical signal.

Previous approaches to study the optoelectronic properties of carbon nanotubes have focused on bare carbon nanotubes, but large light intensities produced by lasers are required to generate an electrical signal. Sandia scientists, in collaboration with researchers at the University of Wisconsin-Madison, have demonstrated that coating the nanotubes with a common dye makes them sensitive to much lower light intensities—those of simple lamps. Interestingly, while the dye is typically used to impart red color, it makes the nanotubes sensitive to blue light.

The functionalized nanotubes were integrated as channels in field-effect transistors, and these transistors were switched ON and OFF with light. The switching is entirely reversible and repeatable, and the devices are stable in ambient.

A scientific paper with further details, titled "Optically Modulated Conductance in Chromophore-Functionalized Carbon Nanotubes," appeared in the February 23, 2007, issue of *Physical Review Letters*.

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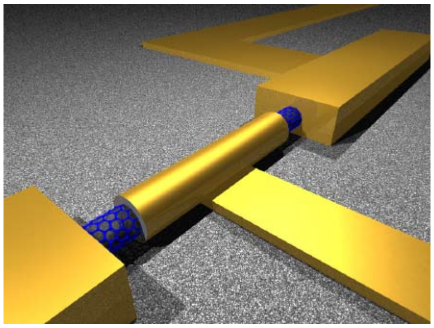
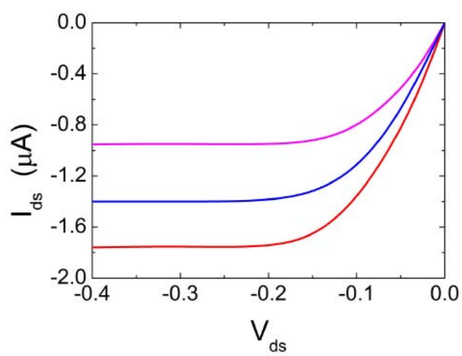
Theory and Modeling of Electronic Transport in Nanostructures

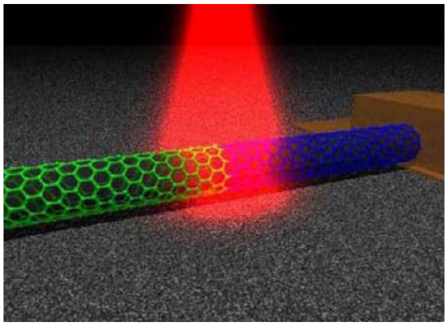
At Sandia, we develop theories and numerical approaches to calculate the electronic transport properties of nanostructures such as carbon nanotubes, nanowires, and single molecules. The goal of our work is to develop a fundamental understanding of the properties of nanostructures and to identify novel behaviors and exploit them in novel nanodevices.

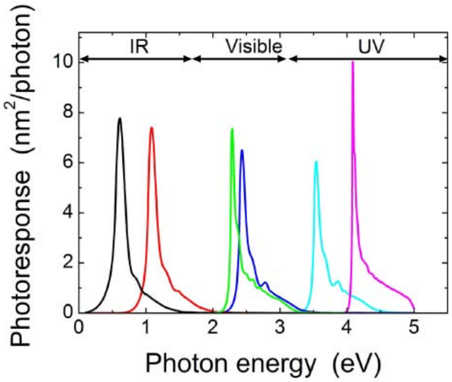
Carbon Nanotube Transistors



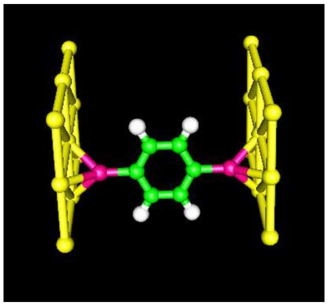


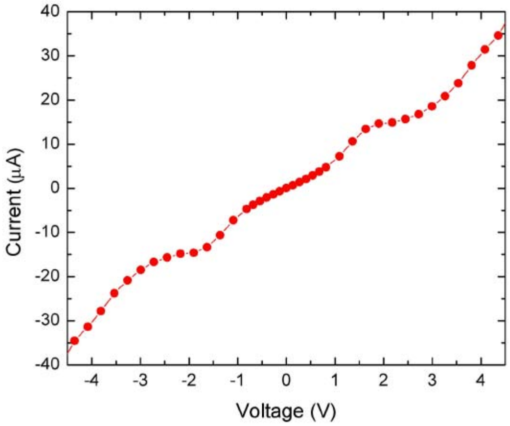
Carbon Nanotube Optoelectronics

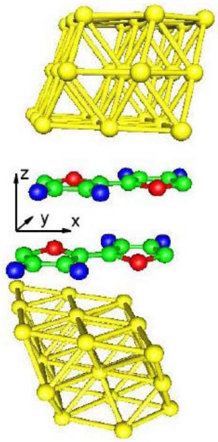




Molecular Electronics







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Physical Science
Ultracold molecules

Sandia opens up new research in the physics of molecules at temperatures near absolute zero

Beam scattering technique produces ultra-cold molecules that will provide insight into the wave-like nature of molecules.

When an atom or molecule is cooled to a temperature below 10 milliKelvin (mK, 1/100 of a degree above absolute zero), its wave-like nature or "wavelength" becomes larger than the particle itself. It thus behaves as a wave as well as a particle. This quantum mechanical effect has many consequences for interaction of particles at these temperatures, such as the formation of new states of matter like Bose Einstein condensates and degenerate Fermi gasses. Although cooling of atoms is now routinely done, no general technique has been available for the production of ultracold molecules.

The added complexity found in molecules—including permanent dipoles and quadrupole moments, and complex rotational and vibrational structure and chemistry—offer the possibility of rich areas of investigation. Moreover, the wave-like nature of ultracold molecules is predicted to lead to a new understanding of weak interactions between molecules, and lead to novel technologies such as quantum computers. All of these possibilities have generally remained unexplored until now.

Sandia researchers have recently produced measurable amounts of ultracold molecules having temperatures ranging from 10-100 mK, using a unique molecular beam scattering technique. The cold molecules are formed at the intersection of an atomic beam and a molecular beam (see figure). The collisions between the beams produce the cold molecules. The researchers have recently demonstrated the ability to produce samples of cold molecules that survive for 100s of microseconds, thereby opening the door to further trapping and detailed studies.

There are four or five techniques in the world that have been able to produce as cold a sample of molecules as has been achieved at Sandia; however, none are as versatile. The technique being developed at Sandia will become general and will lead to the ability to study the wave-like nature of molecules that occurs only at ultracold temperatures.

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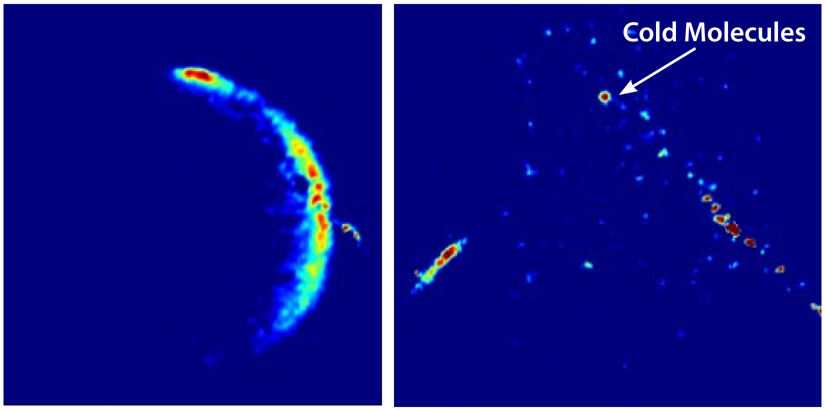

(Left) The production of cold molecules while the atomic and molecular beams are present. (Right) The cold molecules(small spot in the center of the image) remain even 100 microseconds after the atomic and molecular beams have been shut off, indicating a temperature of approximately 30 mK.