
UR
UNIVERSITY RESEARCH
ANNUAL REPORT
2007
SANDIA NATIONAL LABORATORIES
$S = 2RI_s(\lambda)\left[1+\gamma\cos\left(\frac{4\pi L}{\lambda}+\varphi_0\right)\right]$
Sandia National Laboratories
A Department of Energy National Laboratory

# Abstract

Sandia National Laboratories has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons. Sandia and its strategic university partners are seizing the opportunity to establish enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and develop national constituency and name recognition. Sandia's university research investments are made, for the most part, by individual technical programs. The University Research Programs Office serves as the point of contact for all university research issues and creates and implements those processes and tools that enable university partnerships. The office also manages several university-related programs (Campus Executive Program, Sandia University Research Program, and the Presidential Early Career Award for Scientists and Engineers), through which investments are made in students and faculty via contract research and graduate research projects. In addition, the University Research Programs Office, in partnership with Human Resources, oversees the President Harry S. Truman Fellowship in National Security Science and Engineering Program (Truman Fellowship) and programs that forge new strategic relationships in critical skills areas. The FY2007 University Research Annual Report details the projects supported by Sandia in these university-related partnerships programs.

Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94-AL85000.





SAND 2008-2770P
April 2008
Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

## 2007 University Research Annual Report Team

Marie L. Garcia, Sandia National Laboratories
Yolanda Moreno, Sandia National Laboratories

Editor: Vin LoPresti, Sandia National Laboratories

Design: Douglas Prout, Technically Write, Inc.

# CONTENTS

## An Overview of Sandia National Laboratories' University Research Investments

Marie L. Garcia

The nation's investment in science has been in crisis for some time, especially in the physical and engineering sciences. Federal support for academic R&D began falling in 2005 for the first time in a quarter century, while Federal and industry support for their own basic research has stagnated over the last several years.[1] R&D investment from industry has not filled the gap, perhaps because industry views such investments as strongly slanted toward development, when application is a closer match to their shareholder-driven requirements. In addition to leading to a weakened technology base for both U.S. industry and the national defense enterprise, these declines in support set the stage for future challenges in attracting the scientific research talent we need in this critical area.

Our nation's business and academic leaders came together in 2005 to issue a series of reports that convincingly document the threats to continued U.S. economic primacy and, more important, offer an action agenda to address the many global challenges facing our country today. In particular, the National Academies released a report, Rising Above the Gathering Storm, which reinforces an urgent message: if trends in U.S. research and education continue, our nation will squander its economic leadership, and the result will be a lower standard of living for the American people.

Many other countries are pouring money into building their science and technology enterprises. In fact, many of these countries are emulating our innovation model-leveraging investment in science and technology to create market leadership—with remarkable success. America's leaders and its citizens have traditionally pursued policies that encouraged innovation by funding Federal investment in basic research, improving education at all levels, allowing the U.S. to attract the best and the brightest from around the world. Today, we must follow those footsteps and take the actions necessary to keep the U.S. at the forefront of an increasingly competitive global economy. Partnerships with universities, industry, and other national laboratories are essential to address this issue.

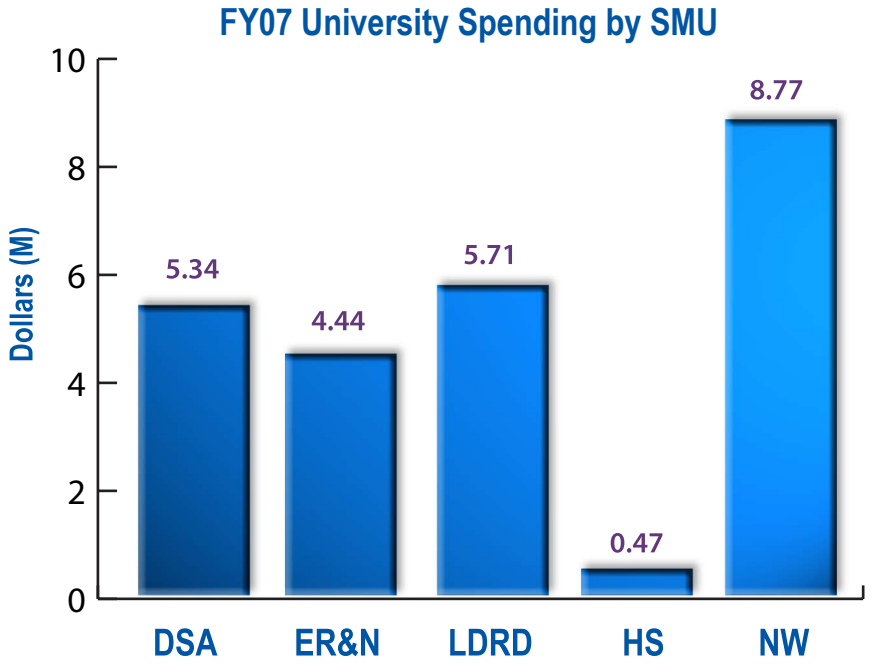



Figure 1. Sandia investments in university research in FY07, by Strategic Management Units[2]

For over fifty years, Sandia National Laboratories (Sandia) has focused on being the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. University partnerships have been and will continue to be a critical element in achieving this goal. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons.

Sandia and its strategic university partners are seizing the opportunity to establish deeper, enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and build national visibility and name recognition. In FY2007, Sandia invested approximately $24.7 million in 514 joint research projects with 103 universities (Figure 1) in five mission-related areas. The research projects reported in the following pages represent the corporate investment portion of Sandia's total investment in research collaborations. Sandia invests additional monies for graduate student support, tuition assistance for employees, and university and K-12 science outreach. The strategic partnerships of the future will be additionally be directed towards those

[1]National Science Foundation, National Science Board, Science & Engineering Indicators 2008, p.1
[2]Defense Systems & Assessments (DSA), Energy, Resources & Nonproliferation (ER&N), Laboratory Directed Research and Development (LDRD), Homeland Security (HS), Nuclear Weapons (NW)

joint activities that will help ensure national competitiveness in the twenty-first century.

The University Research Programs Office provides the leadership and framework for execution of the Laboratories' university partnerships strategy, as well as leadership within the Nuclear Weapons Complex regarding the role of university partnerships in supporting Complex Transformation. The Programs Office executes this strategy primarily through management of the Campus Executive Program, the umbrella under which corporate investments in research, recruiting and education are aligned with the Campus Executive universities. The Programs Office also manages several other university-related programs including the Graduate Research Program, Sandia University Research Program, Presidential Early Career Award for Scientists and Engineers, and the Truman Fellowship. Through these programs, investments are made in students and faculty via contract research and graduate research projects. These investments are intended to help accelerate the creation of world-class research, produce future generations of scientists and engineers, and grow competencies and new businesses for Sandia.

The Programs Office serves as the point of contact for university research issues and develops and implements those tools and processes that enable university partnerships. One major area of emphasis includes further development of the partnership between Sandia and the University of Texas System (UTS). The overarching goal is to achieve a greater mutual impact on national security issues. Its strategic purpose is to participate with Sandia scientists on collaborative research projects, to provide peer review for Sandia's research programs, and to provide specialized courses taught by UTS professors to increase educational opportunities for Sandians.

In FY2007, the President Harry S. Truman Fellowship in National Security Science and Engineering Program (Truman Fellowship) entered its fourth year. This new program provides an opportunity each year for exceptional scholars to join Sandia in the continuation of Sandia's tradition of excellence. Two new Truman Fellows joined Sandia in late 2007. They came from the University of Colorado at Boulder and Oxford University.

Investments in university research continue to pay off handsomely for Sandia and for U.S. taxpayers. This University Research Annual Report showcases the excellent results of these investments. Our joint accomplishments can be measured by the number of journal articles published, patents and copyrights issued, and new employees hired. New collaborations include the University of Texas Medical Branch, DOE Basic Energy Sciences, National Science Foundation, the Defense Advanced Research Projects Agency (DARPA), the National Institutes of Health, the Science and Technology Center for Sustainability of semi-Arid Hydrology and Riparian Areas (SAHRA), the Colorado School of Mines, the University of Buffalo, Pacific Northwest National Laboratory, and the High End Computing University Research Activity (a partnership between Sandia, Oak Ridge National Laboratory, University of New Mexico and Georgia Institute of Technology). Three provisional patents have been filed as a result of research collaborations through the Graduate Research Projects partnerships.

As a national laboratory, Sandia is proud to continue on the path established by Vannevar Bush, science advisor to Presidents Franklin D. Roosevelt and Harry S. Truman, who asserted that the Federal government should facilitate science and technology by funding researchers in the nation's universities and national laboratories, and by supporting the training of the next generation of scientists. Bush's advice to President Roosevelt became the seminal study, Science: The Endless Frontier, issued by the Executive Office of Scientific Research and Development in 1945, and led to the establishment of the National Science Foundation in 1950.

## CAMPUS EXECUTIVE PROGRAM

Sandia National Laboratories (Sandia) has as its highest goal to become the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. University partnerships are a critical element in achieving this goal. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons. Opportunities exist beyond this status quo. Both Sandia and universities share a need to accelerate the creation of world-class research, produce scientists and engineers, and grow competencies and new businesses. Today, Sandia partners with key universities to achieve three major objectives: conduct world-class science, hire world-class scientists and engineers, and develop strategic collaborations in focused research areas.

The Sandia Campus Executive Program was established in 1997 as a means to help accomplish these objectives. It provides a framework for Sandia to focus its research goals and helps create the 21st century workforce needed to perform the technical jobs crucial to fulfilling its national security mission. Sandia executives, acting in the role of ambassadors, are paired with top university officials (usually vice presidents of research and/or deans of engineering) at schools that have synergistic research interests and capabilities with Sandia. These Sandia executives are tasked with the responsibility of working with the universities to implement programs established for the express purpose of furthering the goals of both Sandia and the universities.

This program encourages the Campus Executives to work with their university counterparts to develop and implement action plans that satisfy the needs of each institution. They employ an integrated investment approach where research, talent, and advocacy needs are worked simultaneously, not independently. The Campus Executives schedule visits to their assigned universities once or twice each year, serve on university advisory boards, and attend special events. They interface with campus recruiting teams to actively support placing students in the numerous Sandia programs. The Campus Executives also interface with university faculty to promote sabbaticals, placements, and exchanges. This program enables the Campus Executives to deliver a coordinated message to educate key university personnel regarding the infrastructure and programs being put in place to mutually benefit both Sandia and its strategic university partners. In 2007, 20 universities were considered the corporate key/regional universities with which campus executives interacted.

Each Campus Executive has $50K of Laboratory Directed Research and Development (LDRD) funding earmarked for investments in either graduate research projects or contract research at their university. Based on the plan developed for each university, the Campus Executive determines the appropriate investment of that money. At some schools, the Campus Executive, working with the deans of engineering or arts and sciences, may employ the strategy of establishing graduate research projects for doctoral students doing research in areas in which the Labs has an interest. In these instances, the student and a Sandia Principal Investigator are matched to identify a research project and conduct the research. In many cases, the Sandia Principal Investigator or the Campus Executive becomes a member of the student's doctoral committee. With the Sandian on the doctoral committee, the Labs not only builds relationships with other professors but also is able to offer direct input in the research direction. The desired result of these research projects is to develop a long-term relationship with students that show promise of becoming future Sandia employees, educated and trained in areas of importance to Sandia. At other universities, the Campus Executive elects to invest his/her money in a research project as a means to "seed" an area that looks promising, with the strategy of Sandia and the university eventually collaborating for third-party funding.

For 2007, the following were the Campus Executive/University assignments.

| University | Campus Executive | Deputy Campus Executive | Research Focus Area |
|---|---|---|---|
| **Caltech** | Gerry Yonas | John Cummings | Cognitive Neuroscience |
| **Carnegie Mellon** | Steve Roehrig | Larry Shipers | Computer Science/Robotics |
| **Cornell** | Gerry Yonas | John Cummings | Cognitive Neuroscience |
| **Georgia Tech** | Jill Hruby | Dave Womble | Microsystems Research |
| **MIT** | Jim Woodard | Gerry Sleefe | Infrastructure Surety |
| **New Mexico State University** | Steve Rottler | Anthony Medina | Water Research |
| **New Mexico Tech** | Jim Chavez | Paul Shoemaker | Explosives/Energetic Materials |
| **Purdue** | Joe Polito | Marcey Abate | Nanotechnologies & Microsystems Res |
| **Stanford** | Joan Woodard | Glenn Kubiak | Materials Mechanics Modeling |
| **Texas A&M University** | Les Shephard | James Peery | Global Nuclear Security |
| **University of Arizona** | Duane Dimos | Ray Finley | Water Systems Modeling |
| **University of California at Berkeley** | Terry Michalske | Blake Simmons | Microsystems Research/Energy |
| **University of California at Davis** | Corey Knapp | Mike Hardwick | Info Security/Embedded Reasoning |
| **University of Colorado at Boulder** | David Plummer | | Microsystems Research |
| **University of Illinois at Urbana-Champaign** | Dave Carlson | Russ Skocypec | Nano Science/Cognitive Neuroscience |
| **University of Michigan** | Bob Carling | Brandon Levey | Microsystems Research |
| **University of New Mexico** | Rick Stulen | Rob Leland | Nano Science & Engineering/ModSim |
| **University of Texas at Austin** | Jerry McDowell | Art Ratzel | Nano Science & Engineering |
| **University of Texas at El Paso** | Gil Herrera | Ernest Garcia | Advanced Manufacturing |
| **University of Wisconsin** | John Stichman | Mark S. Allen | Nuclear Eng/Computational Sciences |

## Kinetics and Mechanisms of Nanowire Synthesis

Teresa Clement
Arizona State University

Julia Hsu (Org. 1114)
Sandia Principal Investigator

### Project Purpose

This project with Arizona State University (ASU) seeks to develop a mechanistic understanding of the heteroepitaxial growth of semiconducting nanowires and nanowire arrays for potential applications in nanoscale electronic, photonic, and sensor devices. Our studies focus on systematically investigating and understanding nanowire growth kinetics of epitaxial silicon and germanium nanowires by ultrahigh vacuum (UHV) chemical vapor deposition (CVD) using the vapor-liquid-solid (VLS) growth technique, such that we can controllably grow specific nanowire heterostructures. These investigations have shown that in situ real-time monitoring of nanowire nucleation and growth is essential to understanding nanowire growth kinetics, and as such, we developed an observation method using optical reflectometry to measure nanowire growth in real time. In this technique, we treat the growing nanowire layer as an effective dielectric layer and correlate scanning electron microscopy measurements with optical reflection modeling. The technique has surprisingly good sensitivity to observing quantitatively the onset of nanowire growth, the nanowire growth rate, and the average length of the nanowires. This technique is expected to allow us to accurately control, in situ, the fabrication of nanowire heterostructures. By manipulating the inherent strains within specific Si/Ge heterostructures, we can controllably tune the band structure properties of the nanowires. At ASU, we have focused on the key issues such as the nucleation and growth of the nanowires, the spatially specific location of nanowires into lithographically defined arrays, the factors affecting the synthesis of sharp epitaxial nanowire heterointerfaces, and the resulting strain in these novel structures.

### Accomplishments

We have investigated the nucleation and growth kinetics of Si and Ge nanowires and Si/Ge heterostructures on Si(111). These studies are focused on understanding the fundamental mechanisms of vapor-liquid-solid (VLS) synthesis of Group IV semiconducting nanowires and exploiting this understanding for the synthesis of novel Si/Ge nanowire heterostructures with new materials properties. The research is being conducted in the specially designed UHV CVD system at ASU. We developed an optical reflectometry technique for in situ monitoring during VLS nanowire growth, and demonstrated Si/Ge nanowire growth for both linear and core-shell heterostructures. The CVD system has the unique capabilities of in situ metal deposition for the formation of Au catalytic seeds on atomically clean surfaces, and has been extended to provide for millitorr regime growth with up to 4 precursors (silane, germane, disilane, and digermane) simultaneously. Over the last year, our project accomplishments include the following:

1. Highly vertical silicon <111> nanowire growth has been achieved using silane precursors following high-temperature pre-annealing treatment of the Au catalytic seeds on Si(111) substrates. With increasing pre-anneal time and temperature, larger-diameter nanowires are formed which exhibit greatly reduced kinking, resulting in an increase in the percentage of vertical nanowires from 60% without pre-anneal to 100% vertical nanowires.
2. The in situ nanowire monitoring tools developed in previous years of this project were used to monitor the synthesis of axial Si/Ge nanowire heterojunctions, while specifically investigating silane and germane in addition to our original disilane and digermane gas sources. Energetic differences between such gases enable greater flexibility in the nanowire heterostructure growth conditions.
3. In collaboration with ASU's Electrical Engineering Department, we successfully demonstrated the growth of vertical silicon nanowires in regular arrays using electron beam lithographically patterned oxides on silicon (111) substrates.

### Significance

A key research and development accomplishment of this project is the determination that the electronic band-structure of semiconducting nanowires can be tuned over a significant range of properties. Large modifications in the electronic band-structure can be achieved through the growth of nanowire core-shell and axial heterostructures using conventional electronic materials such as silicon and germanium. The changes in band-structure are predicted to make possible electronic and optoelectronic properties not previously attainable. These modifications in electronic properties are due to the large strains that can be incorporated without the introduction of strain-relieving defects, something that cannot be achieved in normal semiconductor processing such as conventional CVD or MBE layered growth. While

additional work is required to clearly demonstrate the various aspects of this important result, it is apparent that new electronic properties will be achievable in nanowire electronics. Potential implications and future applications of this result include room temperature resonant tunneling diodes made from Si/Ge, nanowire logic circuits at ultrasmall dimensions, ultrasensitive chemical sensor arrays, and high-performance thermoelectric devices. Such advances would have beneficial impact on national security and energy utilization areas.

Additional new results obtained in the last year, advancing the area of ultrasensitive chemical sensors, are methods to achieve highly vertical nanowire growth and preliminary results demonstrating vertical epitaxial nanowire growth from oxide windows. These elements of nanowire processing are considered critical for creating manufactureable high density, nanowire sensor systems. For this reason, such vertical nanowire arrays are anticipated to be a key enabling element for low-power, electronic-based chemical and biochemical sensors. They have the potential for ultrasensitive detection limits (down to the few molecule level) and through functionalized arrays to greatly limit false positives. This work is highly relevant to the national security and threat reduction areas.

*Refereed Communications*

T. Clement, S. Ingole, S. Ketharanathan, J. Drucker, and S.T. Picraux, "In Situ Study of Semiconductor Nanowire Growth Using Optical Reflectometry," Applied Physics Letters, vol. 89, p. 163125, 2006.

*Other Communications*

S.G. Choi, T. Clement, and S.T. Picraux, "Ex-Situ Doping and Characterization of Silicon Nanowires," presented at Materials Research Society Spring Meeting, San Francisco, CA, April 2007.

T. Clement, D.J. Smith, J. Drucker, and S.T. Picraux, "Synthesis of Si/Ge Nanowire Heterostructures for Strain-Controlled Bandstructure Modification," presented at Materials Research Society Spring Meeting, San Francisco, CA, April 2007.

R.P. Prasankumar, G.T. Wang, T. Clement, S.G. Choi, S.T. Picraux, and A.J. Taylor, "Ultrafast Carrier Dynamics in Semiconductor Nanowires," presented at Conference on Lasers and Electro-Optics, Baltimore, MD, May 2007.

## Neural Correlates of Attention and Intention in Decision-Making of Macaques and Humans: Selective Lesioning of Posterior Parietal Areas during Electrophysiology and fMRI

Tamara Knutsen
California Institute of Technology

John Cummings (Org. 7000)
Sandia Principal Investigator

### Project Purpose

This project is a collaboration between researchers at the California Institute of Technology (Caltech) and Sandia. It seeks to exploit recent advances in the ability to chemically induce reversible cortical lesions to study spatial attention and motor intention in monkeys, and studies the same brain regions and behavior in humans using electromagnetically induced temporary lesions. During decision-making, there are three serial processing steps: an initial perceptual representation of the stimuli, a subsequent association of this perceptual representation with motivation and reward expectancy, and a final central representation of an organism's dispositions and preparations to behave towards the stimuli. An important aspect of decision-making is the prior allocation of attention and intention before an action is performed. Decision-making is a spatiotemporal process, requiring spatial elements of sensory information and motor planning as well as temporal elements of reward expectancy and learning (error-correction).

The work not only offers potential advances in understanding decision-making in the brain, but also demonstrates and validates advancing methodologies in neuroscience. The study of both macaque monkeys and humans is extremely ambitious and relatively high risk.

### Accomplishments

A mature male macaque monkey was chosen and trained for the "decision" and "reach" functions required for these experiments. Touchscreen, arm-tracking, eye-tracking, and reward systems for the macaque were installed and optimized. Surgery was performed on the macaque and a set of removable electrodes was installed in the appropriate regions of his brain. The recently developed technique of selective, reversible lesioning in primate cortex was used to elucidate the influence of various functional areas within the intraparietal sulcus during electrophysiological recording. An extensively used stimulus of cued target locations with asynchronous onsets, variable delay periods and reward schedules was employed in initial experiments to probe attention

and intention during sensorimotor integration.

Preparation (experimental procedure and human testing approvals) for the technique of transcranial magnetic stimulation (TMS) was begun. TMS will be employed in FY 2008 for equivalent experiments in humans, with brain activity recorded using functional magnetic resonance imaging (fMRI).

### Significance

A significant part of what DOE and DHS do for the nation involves risk-informed decision-making. This project addresses the human cognition element of those critical national and homeland security decisions. It will examine cognition under uncertainty in decision-making (especially in areas such as intelligence and policy making). Issues include attentional demands, ambiguity, physiological state, individual ontogeny, role of intuition, and memory.

## Improving Robot Navigation Through Self-Supervised Online Learning

Boris Sofman
Carnegie Mellon University

Ray Byrne (Org. 6634)
Sandia Principal Investigator

### Project Purpose

In mobile robotics, there are often sources of information that, while potentially powerful for improving navigation, prove difficult to profit from as they generalize poorly to novel situations. Overhead imagery data, for example, has the potential to greatly enhance autonomous robot navigation in complex outdoor environments. In practice, reliable and effective automated interpretation of imagery from diverse terrain, environmental conditions, and sensor varieties proves challenging. Similarly, fixed techniques that successfully interpret on-board sensor data across many environments begin to fail beyond short ranges, as the density and accuracy necessary for such computation quickly degrade and features that can be computed from distant data are very domain-specific. This research, conducted in collaboration with Carnegie Mellon University, is focused on utilizing online, probabilistic models to effectively learn to use such scope-limited sources of information by leveraging other sources of information that, while perhaps more limited, generalize reliably. The goal is to apply such approaches to provide efficient, self-supervised learning algorithms that allow robots in various domains to utilize the information at their disposal in order to better interact with their environment. Results are generated from field testing on board a rugged robot operating over large distances in various off-road environments. Such approaches have the potential to significantly improve the versatility of many unmanned ground vehicles by allowing them to traverse highly varied terrains with increased performance.

### Accomplishments

We were able to successfully develop and implement a self-supervised online learning algorithm to allow a mobile robot to improve its on-board perception system through experience. Fixed techniques that successfully interpret on-board sensor data across many environments begin to fail past short ranges as the density and accuracy necessary for such computation quickly degrade and features that can be computed from distant data are very domain-specific. We developed an online, probabilistic model to effectively learn to use these scope-limited features by taking advantage of other features that, while perhaps otherwise more limited, generalize reliably. We were able to apply our approach to provide an efficient, self-supervised learning method that leverages the capabilities of the robot's on-board perception system to accurately predict traversal costs over much larger areas from either overhead data or far-range sensor data. The system was fielded on a large autonomous outdoor robot as part of the UGCV PerceptOR Integrated (UPI) Program at Carnegie Mellon University and showed significant improvements to the navigational capabilities and versatility of our system over hundreds of autonomous kilometers of traversal in complex, natural environments.

### Significance

Autonomous robot navigation is an important technology for several Sandia mission areas. These include military systems, nonproliferation and assessments, and homeland security. For nonproliferation and assessments, autonomous robot technology can be used to aid robots performing site assessments. Similarly, there are many military applications for autonomous robots. For homeland security, robots are used in a wide range of activities that include emergency response and physical security. We have engaged in discussions with NASA regarding possible use of this technology, at some point in the future, to aid in the construction of global path plans for the Mars rovers. The autonomous navigation technologies developed under this project will enhance robot performance for this wide range of applications.

*Refereed Communications*

B. Sofman, E. Lin, A. Bagnell, J. Cole, N. Vandapel, and A. Stentz, "Improving Robot Navigation Through Self-Supervised Online Learning," *Journal of Field Robotics*, vol. 23, pp. 1059–1075, December 2006.

## File System Performance Optimization for Supercomputing Applications

Jay Lofstead
Georgia Institute of Technology

Ron Oldfield (Org. 1423)
Sandia Principal Investigator

### Project Purpose

The purpose of this work with the Georgia Institute of Technology is to explore and experiment with ways in which applications interface to and make use of future scalable file systems, in particular addressing quality of service guarantees. Specifically, we are investigating techniques for achieving input/output (I/O) performance at rates as close to the hardware specifications as possible using real codes as our test cases. We will replace the existing I/O calls within the codes to use our new application programming interface (API) that affords flexibility in transport, data organization, storage destination, and in-transit processing, all without having to alter the calls within the codes. In addition to managing the immediate data movement out of the compute nodes, managing concurrent access to shared storage subsystems is critical for optimal performance. Competing use for storage resources in high performance computing (HPC) codes can cause dramatic negative impacts on performance. By monitoring and adapting I/O usage, overall end-to-end performance for all users of the HPC storage resource can be improved. We investigated approaches for determining effective interleaving of I/O usage, and the advantages of instrumenting and integrating with the storage system as an aid in this investigation. Ideally, this will also provide feedback into the HPC codes to adjust the rate and transmission of data.

### Accomplishments

We analyzed all of the different types of I/O performed by the parallel codes GTC, GTC_S, Chimera, and XGC1 in an effort to design a I/O API that is both simple and provides a rich feature set. It was acknowledged that an AMR (adaptive mesh refinement) code would be needed to provide a fully general solution. Based on the analysis results, we designed and developed the adaptable I/O system (ADIOS) API. In ADIOS, the programmer accesses data through a fixed API and the user decides on appropriate access methods and libraries with a configuration file. We demonstrated the efficacy of the system by replacing all of the I/O in the above parallel codes with our new API calls. We tested them using POSIX I/O, MPI Collective I/O, and our own asynchronous methods. We showed that we could get equal or better performance using the same executable code compared with hard-coded versions of the same I/O routines. Our current investigations look at how to incorporate necessary descriptive data hooks for visualization engines using the same source code API.

### Significance

This asynchronous I/O API provides a clean way to integrate with scientific codes while affording us the opportunity to perform various experiments. While preliminary efforts have focused on particular needs of fusion simulations, the technologies and techniques developed apply to a much broader class of scientific applications.

This work also relates to the goals of the High End Computing University Research Activity (HECURA) project with Sandia, Oak Ridge, University of New Mexico, and Georgia Institute of Technology by investigating data transfer performance issues key to driving adoption by and cooperation with scientists.

## Reliable and Secure Communication in Wireless Sensor Networks

Vishal Doshi
Massachusetts Institute of Technology

Nina Berry (Org. 8961)
Sandia Principal Investigator

### Project Purpose

We are studying distributed data compression algorithms for use in sensor networks. Oftentimes, in such networks, there exists a central node that receives information from the other nodes. Further, this central node computes some function of that data measured by the other nodes, which it then relays somewhere else. When only the function value is important at the receiver, why send everything? By reducing the amount of information sent, one can reduce the bandwidth and power constraints of the system.

The goal of this research, with the Massachusetts Institute of Technology,

is to exploit the computational requirements of the system to achieve compression gains, not merely the inherent probabilistic correlation in the data, as is the case with contemporary systems.

The optimal compression gains available from the correlation in the data were precisely elaborated in the prior work of others. While current systems employ these compression gains, they do not account for the computation. This project has sought to build an understanding of this aspect of compression. The major difficulty is that the function need not be separable; in fact, our research considers functions with no restrictions (except that they are nonrandom) and has discovered novel algorithms that solve the problem in special cases over the past year.

We hope to delve more deeply into the general problem. We wish to consider the distributed compression of several sources, such that a central receiver node can compute a nonrandom function of those sources. We would like to describe the optimal rates for the problem as well as simple algorithms that can achieve almost optimal rates. We suspect the simple algorithms from the special cases will not immediately extend to the general case. Nevertheless, our insight of using graph-coloring techniques will provide us with novel results for the more general problem.

### Accomplishments

There are two main avenues of compression. First, one can exploit the correlation between the data collected at the various nodes. Second, one can exploit the relative simplicity of the function to be computed at the receiver side. Earlier research in this area made precise the exploitation of the correlation in the data. However, contemporary distributed data compression schemes fail to account for receiver-side goal, often the computation of a simple function of the data received. The research addressed this problem to make precise the exploitation of the function and implement such a compression scheme.

This compression scheme introduced a small probability of error. This research explored a better understand of this probability of error in order to ensure it will always be "small." This involved more extensive simulations of the scheme with more varied functions and more than two sources.

The design and development of the methodology for how the data compression will be accomplished is based on the following series of steps:

1. Based on the knowledge of the given function use graphs to distinguish amongst the function values.

2. Given a function and the statistics of a set of sources, a graph for each source could be constructed which carried all the information relevant to distributed encoding. Each vertex for the graphs would identify with a particular source word. The compression then comes from the idea of coloring the vertices of the graph. The graph is constructed in such a way that the colors are sufficient statistics of the sources.

The two-part scheme, using two binary functions, was simulated using vehicle-tracking data. The results showed coding gains of 20% or more over contemporary methods when using a simple greedy coloring algorithm (with probability of error less than 0.1%).

### Significance

In our work, we have made significant progress toward solving a problem that has eluded the communications theory community for 30 years. This work is of theoretical interest to the science and technology community, but also of interest to those trying to improve communications schemes. More important than the actual theorems we prove is the framework through which they are derived. This general framework for solving problems of functional compression for any general function would work in a variety of situations, not limited to sensor network communication, and would provide database privacy. Given a problem within these contexts, one simply needs to apply our work and the framework will detail the optimal system to solve the problem as well as provide heuristics that can be quickly implemented.

## Effect of Pressure and Particle Size on Microstructure and Properties of Vacuum-Plasma-Sprayed Yttria-Stabilized-Zirconia Solid Oxide Fuel Cell Electrolytes

Nick Spinhirne
New Mexico Institute of Mining and Technology

Aaron Hall (Org. 1813)
Sandia Principal Investigator

### Project Purpose

Solid oxide fuel cell (SOFC) electrolyte research has focused on reducing the thickness and increasing the density of electrolytes in order to reduce ionic resistance losses [1]. Low-pressure plasma

spraying (LPPS) and very low pressure plasma spraying (VLPPS) have been shown to be capable of applying thin, dense coatings over large surface areas in a short amount of time for both SOFC and thermal barrier coating applications (TBC). Recently, VLPPS has been used to create homogeneous coatings with unique columnar microstructures that have not been created using other plasma spray methods [2]. The coatings were designed for TBC applications, and therefore, the electrochemical properties of the coatings were not investigated. It is known that a columnar microstructure is advantageous for TBCs due to its increased thermal strain capacity compared to lamellar microstructures typical of plasma sprayed coatings. However, the effect of microstructure on the electrochemical characteristics of LPPS yttria-stabilized zirconia (YSZ) coatings for SOFC electrolytes has not been thoroughly studied.

The purpose of this study with the New Mexico Institute of Mining and Technology (NMT) is to investigate the effect of pressure and particle size on the microstructure and the mechanical, thermal, and electrochemical characteristics of VLPPS YSZ. Specifically, the properties of traditional lamellar microstructure coatings are compared to columnar microstructure coatings. Investigating this research topic will advance understanding of ion transport in plasma sprayed YSZ electrolytes.

## Accomplishments

Experiments were conducted using the controlled atmosphere plasma spray (CAPS) system at Thermal Spray Research Laboratory in an effort to duplicate the columnar microstructure observed by other researchers [2]. Two 8 mol % YSZ powders were sprayed onto stainless steel substrates at chamber pressures of approximately 2 torr. The powders were characterized using particle size analysis, x-ray diffraction (XRD), and scanning electron microscopy (SEM). Several spray parameters have been investigated, including upstream versus downstream injection, standoff distance, and helium plasma gas flow rate. XRD and SEM have also been used to analyze the coatings. SEM results showed that coating microstructure can be greatly altered by changing helium flow rate. Lamellar microstructures have been observed in addition to a mixed columnar structure. The mixed columnar microstructure consists of a mixture of splats and loosely defined columnar growth. Progress has been made in determining which spray factors contribute the most to columnar microstructures.

## Significance

This project will further knowledge and understanding of the VLPPS process and how the coatings are formed. Present research has only suggested some parameters that might influence columnar grain growth. These parameters include substrate temperature and roughness, plasma gas flow rates, and powder feedstock size. Still, much of the mechanism behind columnar growth of plasma sprayed YSZ is not understood. Quantifying the parameters responsible for columnar growth is the first step in understanding the mechanism creating the columnar structure.

The project also involves the advancement of SOFC technology. SOFCs are still not an economically viable source of energy for several reasons, including low power densities. Power densities can be increased and operating temperatures can be decreased by improving the ionic conductivity of the electrolyte. Decreasing operating temperatures also improves the economy of SOFCs by allowing less-expensive materials to be used. The columnar microstructure being investigated could greatly increase the ionic conductivity of the coating. Additionally, once the process can be controlled, the same VLPPS system could be used to develop coatings in other areas such as electronics and optics.

### *References*

[1] Lang, et al., "Development and Characterization of Vacuum Plasma Sprayed Thin Film Solid Oxide Fuel Cells," *Journal of Thermal Spray Technology*, vol. 10, no. 4, pp. 618-625, December 2001.

[2] A. Refke and R.K. Schmid, "Low-Pressure Plasma Spraying for High-Temperature Fuel Cells," *Technical Review Sulzer* (English Edition), vol. 87, no. 2, pp. 8-10, 2005

### *Other Communications*

N. Spinhirne, D.A. Hirschfeld, R. Williamson, and A. Hall, "Comparison of Vacuum Plasma Spray (VPS) and Low Pressure Plasma Spray (LPPS) for Deposition of Yttria-Stabilized Zirconia (YSZ)," presented at Materials Science and Technology, Detroit, MI, 2007.

A.C. Hall, R. Williamson, E. Muheleberger, D.A. Hirschfeld, T.J. Roemer, D. Beatty, A. Mayer, N. Spinhirne, "Solving an Anode Burning Problem in a Low-Pressure Plasma Spray System," presented at Materials Science and Technology, Detroit, MI, 2007.

## Micro-Rheology of Polymeric Materials at High Strain Rates

Taylor Dotson
New Mexico Institute of Mining and Technology

Doug Adolf (Org. 1821)
Sandia Principal Investigator

### Project Purpose

A number of technologically important processes, from the design of bulletproof vests, to the fabrication of plastic films and bottles, to the implosion dynamics of nuclear weapons and plastic-bonded high explosives (PBX), depend in a critical way on the dynamic response of polymeric materials when subjected to a strong impulse. Polymers constitute an especially difficult class of materials to describe due to their complex rheological behavior (ranging from semi-crystalline, to glassy, to rubbery, to liquid) and the highly entangled nature of their constituent molecules. Indeed, depending on the temperature and the timescale of observation, the same polymer can exhibit glassy, rubbery, or liquid-like dynamic response. Moreover, chain entanglements make the response not only dependent on the current state of the material (e.g., temperature, density, strain rate) but also on its past history.

Our goals are to understand the interplay between molecular architecture, nano- and micro-rheology, and macroscopic response of bulk materials leading, over time, to a predictive capability for the dynamic response of polymers undergoing deformation.

This project coordinates the work of a graduate student at New Mexico Institute of Mining and Technology (NMT) with mentors at Sandia to study polymer dynamics at the atomistic level with molecular dynamics.

### Accomplishments

Computer modeling techniques were used to study polymer dynamics. The principle one of these was molecular dynamics, implemented through the LAMMPS (large-scale atomic/molecular massively parallel simulator) software. The particle trajectories thus generated were analyzed with a suite of "in-house" programs for both static and dynamic quantities. The static quantities included the pair correlation function, the packing fraction, and the scattering function. The dynamics quantities included the mean-squared-displacement of particles, rotational relaxation functions, and the relaxation of the dihedral angle correlation function. Each of these relaxation functions has an associated response function given by the negative of the derivative of the relaxation function.

A survey of methodologies and models for fitting the relaxation functions was performed. The functions, themselves, were found to be relatively featureless nonexponential decays and thus very difficult to fit. That is, the inversion of the relaxation data to obtain unique and physically significant parameters is a seriously ill-posed problem. We decided that the assumption of a stretched-exponential form in addition to a novel method for determining the stretched exponential model's region of applicability provided a sufficient constraint on the fit to produce not only very good but also unique choices of parameters. However, the method has not yet been applied to wide range of polymer models or types of relaxation functions.

In order for time-temperature superposition to hold, the function form of the stretch-exponential expression must remain fixed across state-points. In particular, the stretching-exponent, ß, assumes a constant value in the case of time-temperature superposition. In our simulations of simple chain models, we find clear evidence of changes in ß; indicating a violation of time-temperature superposition.

### Significance

Plastic bound explosive (PBX) 9501 is an important component in existing weapon systems. PBX 9501 is roughly 95% high melting point explosive (HMX), 2.5% Estane, and 2.5% nitroplasticizer. Estane 5703, made by B. F. Goodrich, is a polyesterurethane elastomer and is used as a binder to decrease the mechanical sensitivity. It is a copolymer, and its chain consists of alternating "soft segments" and "hard segments." The soft segments are short polymers (oligomers) of the ester of adipic acid with 1,4 butanediol (BDO). The hard segments consist of very short polyurethanes. The soft segments are rubbery to quite low temperatures (Tg= –31 °C), while the hard segments serve as thermoplastic crosslinkers below 85 °C. Above this temperature the PBX can, with care, be molded. Although a small percentage of the whole, the Estane has a marked effect on the Young's modulus, lowering it from 15 GPa for neat HMX near room temperature to 1 MPa for PBX 9501 (a reduction by a factor of 15000). Of course, this dominant influence of the Estane on the mechanical properties of PBX introduces a strong overall viscoelastic behavior. Moreover, the chemical and physical aging of Estane changes the mechanical behavior of PBX. The atomic level modeling of PBX aging is multifaceted. The current project addresses the relationship between molecular structure of an elastomer and its complex modulus, that is, with its viscoelastic behavior. This will permit studies of, for instance, the chemical aging of PBX to be linked to the mechanical properties of the material.

*Refereed Communications*
J.V. Heffernan, J. Budzien, F. Avila, T.C. Dotson, V.J. Aston, J.D. McCoy, and D.B. Adolf, "Rotational Relaxation in Simple Chain Models," to be published in Journal of Chemical Physics.

## Modeling River-Aquifer Interaction with Application to the Rio Grande

Suzanne Tillery
New Mexico State University

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

### Project Purpose

Interactions between surface water and groundwater systems are complex, and these flow systems are not isolated components of the hydrologic cycle, but interact in a variety of ways. Development or contamination of one system commonly affects the other, such that understanding the interactions between the flow systems is necessary for effective water resource management. However, surface and groundwater models have traditionally been developed and calibrated independently of each other. Another discrepancy in the models is in the time-steps used—typical stream-flow models use days or hours, while groundwater models use months or years. Linking the separate models works well when the interactions are weak, but when the interactions are significant they need to be simulated in an integrated model.

This project, a partnership with New Mexico State University, has been established to develop an integrated surface-groundwater model providing improved computational efficiency and mathematical fidelity. Specifically, the new approach solves the surface and subsurface flow equations simultaneously within the same global matrix structure, thus eliminating the need for iterative solution of the governing equations. However, simultaneous solution requires that the stream and groundwater equations be solved at the same time-step. In the vicinity of the strong stream-aquifer interaction, a small time-step is required to simulate the interactions properly, while at distance, a much larger time-step could accurately simulate groundwater flow. Therefore, a local time-stepping procedure has been adopted. Finally, if the grid spacing throughout the domain is defined to be relatively small to meet the accuracy needs in the regions of strong stream-aquifer interaction, there are inefficient and redundant calculations being performed in the regions away from the area of strong interaction. Thus, we have proposed embedded mesh refinements to cluster grid points in regions where they are most needed, while allowing coarser grid resolution in regions with minimal interaction.

### Accomplishments

The Riverware model for the Rio Grande between Caballo Dam and El Paso was completed using monthly flow data and autoregressive integrated moving average (ARIMA) transfer function models. The interaction between surface water and ground water was implemented via the transfer functions that define the relationships between the diversions and the major drain return flows in the Rio Grande.

The results of the literature review and governing equation classification research was documented in full detail, with the goal of submitting the manuscript as a review article. This document provides the framework for numerical analysis of high-resolution surface water/groundwater modeling.

An extensive literature review was performed on topics related to modeling systems with variable grid spacing (grid adaptation) and variable time-steps (local time-stepping). It was found that these methods are currently being used separately in stream analysis and in groundwater analysis, but are not typically applied to coupled systems. Research into methods for coupling surface and groundwater systems was also performed, with a special emphasis on studying simultaneous solution methods that allow for the surface and groundwater equations to be solved at the same time.

A plan was developed to implement these three methods (simultaneous solution, grid adaptation and local time-stepping) into the existing United States Geological Survey (USGS) software for modeling groundwater (MODFLOW-2000), streamflow (BRANCH), and linking the groundwater and streamflow models together (MODBRANCH).

We began modifying the USGS software, by first updating the MODBRANCH and BRANCH software from interfacing with MODFLOW-96 to interface with MODFLOW-2000. Baseline runs were started to compare results from model simulations using MODFLOW-2000 and MODBRANCH prior to any modifications. To ensure consistency of the comparisons between model runs, modifications were made to the MODBRANCH software to provide input for the stream setup package instead of having to create separate files in MODBRANCH.

### Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries as well as regarding the distribution of water

among irrigators, urban developers and environmentalists. This work focuses on developing tools to better manage our limited resources; specifically, to quantify the magnitude as well as the spatial and temporal variability in exchanges between streams and their adjoining aquifers. For most water courses, these exchanges represent a significant contribution to the overall water budget. Additionally, these exchanges play an important role in defining water quality (including temperature) as well as controlling biologic processes in the hyphoreic zone. Unfortunately, it is very difficult to accurately measure these exchanges. Significant difficulties often arise in water planning exercises over uncertainties in surface-groundwater exchanges. To further complicate the water planning process, these uncertainties extend to issues concerning how these exchanges respond to changes in agricultural practices and/or land use within the flood plain.

This project is focused on developing computational tools that better quantify surface water/groundwater exchanges. Work over the last year has yielded an improved computational framework for simulating river-aquifer interaction. The new approach solves the surface and subsurface flow equations simultaneously within the same global matrix structure, while improving computational efficiencies by way of local time-stepping and embedded mesh refinement. These computational improvements will allow analysis of currently intractable river-aquifer dynamics. Additionally, such methods should hold promise for other coupled engineering problems.

*Other Communications*

S. Tillery, Z. Sheng, J.P. King, B. Creel, C. Brown, A. Michelsen, R. Srinivasan, and A. Granados, "The Development of a Coordinated Database for Water Resources and Flow Model in the Paso Del Norte Watershed," No. 337, New Mexico Water Resources Research Institute, Las Cruces, NM, December 2006.

S. Tillery, Z. Sheng, J.P. King, B. Creel, C. Brown, A. Michelsen, R. Srinivasan, and A. Granados, "Lower Rio Grande Flood Control Model [LRGFMC] River Ware Model Development," NM Water Resources Research Institute, Las Cruces, NM, March 2007.

S. Tillery, Z. Sheng, J.P. King, B. Creel, C. Brown, A. Michelsen, R. Srinivasan, and A. Granados, "Availability of Flow and Water Quality Data for the Rio Grande Project Area," NM Water Resources Research Institute, Las Cruces, NM, March 2007.

## Tunnel Gap Modulation Spectroscopy: An Ultrasensitive Technique for Measuring Small Mass Change

Laura Biedermann
Purdue University

Steve Howell (Org. 1744)
Sandia Principal Investigator

### Project Purpose

The feasibility of using carbon nanotubes (CNTs) as ultrasensitive mass sensors will be explored in this project using both electrical and optical means. Electrically, we are investigating tunnel gap modulation spectroscopy (TGMS) for measuring high-frequency oscillations of conducting nanowires. To verify TGMS, a laser interferometer technique is being investigated to independently measure the oscillation frequencies of suspended nanowires.

TGMS measures the oscillation spectra of a single CNT at room temperature by monitoring the electron tunnel current between the CNT and a conducting substrate using scanning tunneling microscopy (STM) derived techniques.

The laser interferometer can detect oscillation amplitudes as small as tens of picometers and oscillation frequencies from 0–20 MHz. In collaboration with Purdue University, we have successfully measured the oscillation spectrum of a multiwalled carbon nanotube (MWNT) with a 4-µm glass bead affixed to one end.

This research is being driven by the desire to measure an ultralow amount (< 1 fg) of a target analyte that selectively binds to a functionalized CNT. The CNT's natural frequency of vibration will shift due to the CNT's small mass (< 1 pg). To demonstrate useful sensors, individual CNTs will be functionalized with Sandia's unique enabling diazonium/iodonium chemistries that will selectively bind various analytes. We estimate that using a functionalized CNT, a frequency shift of 0.57 MHz will result when a single virus ($10^{-15}$ g) is attached to the end of the CNT.

Although initial experiments are using MWNTs, the methods under development are generally applicable to most nanowires. This research has the capability to determine the elastic properties of an oscillating nanowire in an unobtrusive way. Successful completion of this project will enhance Sandia's ongoing nanosensing programs by enabling fundamental research in carbon nanotube-based sensing and device development.

### Accomplishments

We built and tested the experimental apparatus required for tunnel gap modulation spectroscopy (TGMS).

- In addition to the current-to-voltage converter required by all STMs to monitor and amplify the tunnel current, this radiofrequency (RF)-STM head included an inductor/capacitor pair to shunt the high-frequency signals into a pair of wideband fixed-gain amplifiers.
- Testing revealed that the high-frequency portion of the RF-STM board is self-oscillating at 50 MHz. This portion of the circuit board has been bypassed; RF signals are now amplified by a cascade of three external amplifiers.
- We wrote LabView and Matlab programs to partially automate TGMS peak detection.

We investigated alternate methods to measure the oscillation frequency of a MWNT.

- MWNTs were driven through mechanical resonance using electrostatic excitation. We determined the approximate resonance frequency by monitoring the oscillations in a dark-field microscope and noting the frequency corresponding to maximum oscillation amplitude.
- Using a laser interferometer, we measured the oscillation frequency, 83 kHz, of a MWNT decorated with a glass bead. The bead was added because the bare MWNT is too small to reflect enough laser signal for detection.

We evaluated an alternate oscillator for calibration of TGMS sensitivity.

- A 5-MHz quartz crystal is known to undergo a transverse oscillation amplitude of ~0.1 nm and serves as a calibration for feedback stability tests. As expected, the RF-STM maintained a stable tunnel current. Unfortunately, leakage EMI from the crystal and associated electronics overwhelmed any TGMS signal from the vibrating quartz substrate.

We evaluated MWNT-Ni STM tips.

- We recorded topographic STM scans and current-voltage curves using MWNT-Ni STM tips.
- Tip fabrication time was greatly reduced by adding a small amount of adhesive to the Ni STM tip, which improved MWNT adhesion.

### Significance

In order to increase the sensitivity of cantilevered microsensors and nanosensors, the mass of the cantilever must be decreased. Multiwalled carbon nanotubes (MWNTs) are ideal cantilevered nanosensors due to their small mass (~ 1 pg) and high quality factor (Q ~ 500). Even the smallest amount of analyte bonded to a MWNT will cause a detectable shift in the MWNT's oscillation frequency. With the unique enabling diazonium/iodonium sensor chemistry developed by Sandia, MWNTs can be functionalized to detect the presence of chemical warfare (CW) stimulants and toxic industrial compounds (TICs). Once the reliability of measurements of the oscillation frequency of MWNTs has been demonstrated, the MWNTs can be functionalized for use as nanoscale chemical and biological sensors. In addition to their improved sensitivity, cantilever nanoscale sensors offer a low-power (microwatts) sensing platform. Sandia's mission areas of Nonproliferation and Assessments and Homeland Security and Defense, specifically monitoring and detection of chemicals, will benefit from the sensitivity and low-power consumption of these MWNT-based sensors.

## Optical Properties of Plasmonic Metal-Dielectric Composites

Mark Thoreson
Purdue University

Arlee Smith (Org. 1128)
Sandia Principal Investigator

### Project Purpose

One purpose of this collaborative project with Purdue University is to apply plasmonic resonances of small metal particles to enhance stimulated Raman scattering and thus improve the sensitivity of Raman spectroscopy. The fabrication of thin films containing the particles will be optimized for this application. Another purpose is to explore the application of plasmonic resonance to developing negative refractive index material. Such material might be useful in subwavelength resolution, near-field imaging.

### Accomplishments

Our work with semicontinuous films for infrared filters is ongoing. By photomodifying the films we can create windows of transparency in the wide absorption band of the film. We are currently working to increase the selectivity of these filters through controlled photomodification and by the surface-enhanced infrared absorption of molecular layers. The photomodification step, which was previously a rapid process involving relatively high powered $CO_2$ laser pulses, has been optimized using a tunable mid-IR laser system and lower pulse powers, yielding increased control in the overall photomodification of the semicontinuous films.

We continue our work on near-field superlens research using metal-dielectric composite films. Our current designs call for a large number of very

thin composite layers (of alternating metal and dielectric layers). These designs show promise for applications such as noncontact sensing and near-field lithography. By combining a nanoantenna array with a composite superlens, we hope to be able to transfer areas of locally high field strength in the nanoantennas to the other side of the composite lens. This would then allow the detection of analytes via enhanced scattering processes without actually exposing the analytes to the metal surface. Through appropriate tailoring, these systems could operate at any of a wide range of frequencies, which imparts more flexibility than traditional continuous metal film superlenses.

We constantly search for better ways to reliably produce semicontinuous metal films for use in several experimental setups. We have recently begun experiments to produce such films using a pulsed laser deposition (PLD) system based on a KrF excimer laser (wavelength = 248 nm). This system may provide greater control over the film deposition process than our usual e-beam evaporation method. The initial results are promising, producing films of similar spectral properties to those of our previous work but in a shorter timeframe and with greater control through the high number of laser pulses used to make the samples. We will continue these studies to determine which method provides optimal films.

### Significance

Control of the photomodification process for tunable windows of transparency in semicontinous films has been demonstrated. This has applications in infrared obscurrants and filter design. We are also applying our photomodification understanding to optical limiting studies.

Near-field superlens designs using composite metal-dieletric films will have potential applications in near-field lithography and remote sensing via surface-enhanced processes such as surface-enhanced Raman scattering.

Leadership and project management skills have been developed through the mentoring of an undergraduate researcher in a related project (pulsed laser deposition of semicontinuous metal films). The experience in designing and directing experiments as well as project management will prove very beneficial for future research work.

### *Other Communications*

V.P. Drachev, U.K. Chettiar, H.-K. Yuan, W. Cai, M.D. Thoreson, A.V. Kildishev, and V.M. Shalaev, "Real Metamaterials," presented at International Conference on Coherent and Nonlinear Optics (ICONO) (invited), Minsk, Belarus, May 2007.

P. Nyga, M.D. Thoreson, V. de Silva, H.-K. Yuan, V.P. Drachev, and V.M. Shalaev, "Infrared Filters Based on Photomodification of Semicontinuous Metal Films," presented at Frontiers in Optics, Laser Science, Optical Fabrication and Testing and Organic Photonics and Electronics, Washington, DC, October 2006.

V.P. Drachev, M.D. Thoreson, and V.M. Shalaev, "Sensing Proteins with Adaptive Metal Nanostructures," in *Surface Plasmon Nanophotonics*, M. Brongersma and P. Kik, editors, Dordrecht: Springer, 2007.

## Atomistic Mechanisms of Semiconductor Nanowire Growth

Bethany Simmons
Stanford University

Jonathan Zimmerman (Org. 8776)
Sandia Principal Investigator

### Project Purpose

Our goal was to develop efficient computational models to understand the detailed mechanisms of the nucleation and growth of semi-conductor nanowires (NWs) at the atomistic scale, in collaboration with Stanford University. Directed growth of semiconductor NWs has attracted significant interest in recent years as key enablers of nanotechnology. With their diameters controllable by the size of the catalyst nanoparticles, and with their electronic properties tunable by doping, NWs can be used to construct nanoscale electronic devices, such as field effect transistors, chemical and biological sensors, as well as nano-electromechanical systems (NEMS). While the vapor-liquid-solid (VLS) mechanism of NW growth from catalyst particles was discovered a long time ago, many important questions concerning the detailed mechanisms and the kinetics of nucleation and growth remain unanswered. Through atomistic modeling and simulations, we hoped to achieve better understanding of the fundamental mechanisms, which would enable better control over NW growth and the construction of complex nanoscale architectures.

### Accomplishments

Research was initiated on the nucleation problem of a two-dimensional Ising model using kinetic Monte Carlo (kMC) simulations. A Matlab program was written that can perform kMC simulations of a ferromagnetic Ising model, which has

two ground states: (A) all spins equal to +1, or (B) all spins equal to –1, when the external magnetic field is zero. When an external magnetic field is applied, the spins prefer to align with the magnetic field, so that the state A is lower in energy while state B is metastable. If the system's initial condition is state B, it may take a long time to move to state A, which requires the nucleation of a critical-sized island.

A set of brute-force kMC simulations were performed to determine the domain in the temperature–magnetic field space for which a transition from state B to A can occur within a specified period of time, e.g., 1 million timesteps. The computation is expensive because the nucleation rate of a critical island can be very small. In general, the higher the temperature, the lower the magnetic field required for the transition to occur within a specified period of time. These simulations also predict the size and shape of the critical island given the temperature and magnetic field.

A special algorithm was developed that can sample the size and shape of the critical island that is much more efficient than the kMC simulation, thereby sampling in the spaces of all trajectories that connect state B and state A. In this way, the trajectories that fluctuate within state B will be excluded from the computer simulation. This algorithm works and we have obtained a set of critical island sizes and shapes that are comparable to brute force kMC simulations.

### Significance

The next step would be to predict the nucleation rate from these path-sampling simulations and compare them with brute-force simulations. After that, we would like to predict the nucleation rate as a function of temperature, magnetic field, and interaction parameters of the Ising model. While the Ising model has been solved analytically for its thermodynamic properties, its kinetic properties remain an open question. It is our hope that the algorithms developed in this project can be used to efficiently study the kinetics of nanostructure formation and growth processes using computation.

This project ties to DOE's goals and strategies to advance nanoscale science and to advance scientific simulation and computation through the development of sophisticated models for complex physical phenomena. These capabilities are useful toward the understanding of nanosystems and the design of nano-electronic devices for defense and energy applications.

## Application of Advanced Laser Diagnostics to Hypersonic Wind Tunnels and Combustion Systems

Andrea Hsu
Texas A&M University

Jonathan Frank (Org. 8351)
Sandia Principal Investigator

### Project Purpose

In hypersonic flight conditions, gas molecules are in a state of nonthermochemical equilibrium (NTE). The purpose of this project, a collaboration with Texas A&M University (TAMU), is to study the interactions of nonequilibrium gas molecules with turbulence properties. The project provides the opportunity for a TAMU graduate student to conduct experimental research on nonequilibrium pehnomena in hypersonic flows, at TAMU and at Sandia. The experimental results from this project will be coupled with computational fluid dynamics simulations to develop a novel hypersonic flow model that can bridge the gap between Lattice-Boltzmann and conventional Navier-Stokes methods, while accommodating NTE.

The experiments will use laser-based imaging diagnostics to study nonreacting hypersonic flows. Planar laser-induced fluorescence (PLIF) imaging of NO (nitric oxide) seeded into the flows will be used to measure rotational and vibrational temperatures as well as pressure. Nonequilibrium conditions will be introduced into the flows, and the subsequent equilibration of the gases will be measured. Two approaches for producing nonequilibrium conditions will be investigated. One approach uses a capacitively coupled radio frequency (CCRF) system to produce plasma with primarily vibrational nonequilibrium. The second approach uses photodissociation of $NO_2$ to produce vibrationally excited NO molecules. For both approaches, the timescale for vibrational energy transfer is expected to be comparable to the hypersonic flow timescales.

### Accomplishments

The calibration of NO PLIF experiments was completed at TAMU using a static test cell and an underexpanded jet flow with single shot relative temperature errors of ~2% at 300 K, using rotational lines R1(3.5) and R1(19.5).

The radiofrequency (RF) plasma system is operational, and emission spectra of the plasma were measured. Kinetics simulations modeling the vibrational relaxation of NO(v=1) show that the prediction of $O_2$ and $N_2$ vibrational temperature

($T_{vib}$) by probing NO(v=1) may be possible. The simulations rely on vibrational-vibrational and vibrational-translational energy exchange between the main species, vibrationally excited and ground state $O_2$, $N_2$, and NO. The energy exchange rate constants show that the vibrational energy "pools" through the NO(v=1) to NO(v=0) since the rate constants for the flow of vibrational energy from NO to $O_2$ and $N_2$ are very slow. Therefore, the vibrational relaxation rate of NO depends on the amount of vibrational energy contained in $O_2$ and $N_2$, and by probing the NO(v=1) vibrational relaxation, one can calculate the starting $TvibO_2$ and $T_{vib}N_2$ produced by the plasma.

PLIF experiments were conducted at the Combustion Research Facility (CRF) using a ~100-ps pulsed dye laser for excitation and a fast-gated intensified charge-coupled device (CCD) camera for detection. The intensifier gate widths were calibrated using a femtosecond laser. NO PLIF measurements in a two-channel flow of NO with different quenching environments demonstrated that significant improvements in quantitative LIF measurements are feasible using detector gate widths of 200 ps to reduce errors due to variations in collisional quenching rates.

A SPEX triple slit Raman spectrometer is operational. The resolution of the spectrometer (~0.02 nm) should be sufficient to resolve the vibrational Stokes spectra of both $O_2$ and $N_2$ on a single CCD and to obtain an accurate measurement of the plasma rotational temperature $T_{rot}$ by fitting the $N_2$(C-B) transitions.

### Significance

This collaboration between TAMU and Sandia will address significant technical challenges in understanding hypersonic nonthermochemical equilibrium turbulence. The accomplishments of FY 2007 constitute foundational work leading up to data collection in both the subsonic and hypersonic flowfields.

The calibration cell results demonstrate the use of NO PLIF in instantaneous temperature profiling, while maintaining relative errors lower than the expected temperature fluctuations caused by turbulence. The PLIF measurements will provide on the order of 5000 single-shot sets of images. A statistical analysis of these data sets will be used for a comparison with theoretical turbulence models.

The operation of the RF plasma will address the particular issue of the effect of nonthermochemical equilibrium on turbulence. Nonthermochemical equilibrium is an issue commonly encountered in hypersonic flows, and its effect on turbulence is not well understood. Kinetic modeling of the RF plasma provides insight into the methods of energy transfer within the plasma and the degree of nonthermochemical equilibrium induced by the plasma. Characterization of the plasma is important in order to compare the nonthermochemical equilibrium against realistic hypersonic flow conditions. The Raman scattering spectra of $N_2$ and $O_2$ provide an accurate measurement of the vibrational temperatures of these two species to compare against the RF plasma kinetic models. By fitting the emission spectra of the plasma, the rotational temperature within the plasma can be found.

The results from these experiments are expected to provide new insight into practical design issues in aeroheating, aerodynamics, and propulsion. The development of improved high-speed propulsion systems will lead to more advanced defense systems and lay the foundations for future hypersonic vehicle design.

### *Other Communications*

A. Hsu, C. Dean, S. North, T. Fuller, J. Garcia, M. Semper, R. Srinivasan, S. Girimaji, and R. Bowersox, "Characterization of Nonequilibrium Thermochemistry in Hypersonic Turbulent Flows," presented at Industry-University Cooperative Chemistry Program, College Station, TX, October 2006.

J.H. Frank, R.J. Sigurdsson, S.A. Kaiser, T.B. Settersten, A. Hsu, and C.C. Hayden, "Time-Resolved Planar Laser-Induced Fluorescence Imaging with Picosecond Excitation and Detection," presented at Gordon Research Conference, Oxford, UK, August 2007.

## Precise Distributed Control and State/Parameter Estimation for Multi-body Satellites and Satellite Formations

James Fisher
Texas A&M University

Jeff Spooner (Org. 5338)
Sandia Principal Investigator

### Project Purpose

Reconnaissance and surveillance satellites use sensor payloads that require accurate pointing and extremely low line-of-sight residual jitter. These sensor payloads are usually not the primary payload of the spacecraft, requiring them to point accurately despite unknown maneuvers of the primary spacecraft

bus. Maintaining pointing accuracy in the face of unknown main body maneuvers, despite incomplete knowledge of the spacecraft dynamics, and under the influence of unknown disturbances, is a very challenging and important problem. The more precise the knowledge of the parameters of a system, the better will be the performance of the control algorithms that govern it. Higher performance can also be achieved by modeling disturbances due to sudden changes in disturbance forces and thermal expansion effects that occur when the satellite passes in and out of the Earth's shadow. The control problem is further complicated by the fact that solar panels of such satellites must continuously track the sun with the help of gimbals. This requirement is often in conflict with the primary goal of payload pointing and ensuring the stability of the satellite. This project will develop novel control and estimation methods for multibody satellites, as well as formations involving multiple, dissimilar satellites.

The key elements of this research are accurate modeling of the vehicle dynamics, space environment, and the associated uncertainty in attitude and orbit. Multibody satellites require stability/partial stability analysis using multiple measures. The limits of performance, propagation of uncertainty, and parameter/state estimation must be addressed. Methods for formation orbit control, collision avoidance, as well as attitude control of the individual satellites will be developed.

Research scope:

1. Stability analysis of multibody systems in the presence of distributed uncertainty in dynamics, sensors, and environment
2. Providing Lyapunov certificates for distributed heterogeneous space systems accounting for uncertainty
3. Reconfigurable formations with collision avoidance and performance guarantees

## Accomplishments

Year 1 Milestones and status:

1. Develop a multibody spacecraft model to include a set of low-order flex modes and two gimbal degrees of freedom

   This milestone was completed. The rigid-body model was completed and the model for the system with low-order flex modes was completed. In addition, a more simplified planar model was developed for concept development as a means to test control strategies before incorporation into the full system. The planar model is easier to analyze and is, therefore, more useful in control development.

2. Integrate attitude and orbit dynamics models and include the effect of solar radiation and diurnal variations; include thermal snapping effects

   Effects of solar radiation were completed in the rigid-body simulation. Furthermore, the effects of the spacecraft passing into and out of the Earth's shadow were also included in the original model. Further modeling of thermal snap required the inclusion of the low-order flex body modes.

3. Stability and performance analysis for distributed control architecture using multiple Lyapunov functions

   Stability analysis of rigid-body control law using multiple Lyapunov functions was completed. Development of analysis tools for stability analysis of interconnected systems was completed.

4. Synthesize adaptive controllers based on multiple Lyapunov functions and parameter estimation

   A framework has been developed for converting linear systems with unknown stochastic parameters into deterministic systems. This allows for the design of control laws and stability analysis of such systems.

5. Develop a simulation package that includes orbit and attitude dynamics and evaluate the control performance with and without adaptation using constraints and performance specifications from a proposed imaging mission

   This milestone has been partially completed. Simulations have been developed for the simplified system with vibrational modes as well as for the multi-body system without vibration modes. Work is under way to include these modes in the system.

## Significance

This year, a flexible body satellite model with two gimbal degrees of freedom was developed for a system in a space environment that includes environmental effects such as solar radiation. A control strategy was developed to control both the motion of the base and the motion of the second body given the motion of the base. This strategy was developed for the rigid-body case. The goal for this initiative is to develop a baseline control for comparison of future control laws that will actively isolate the line of sight (LOS) of the gimbaled instrument from the mechanical environment. To reduce the amount of instrumentation required to perform the control, an estimator to determine attitude and angular velocities was also created. The goal was to formulate a control law that could accomplish objectives based on limited knowledge of the system. Additional work has been accomplished in improving

upon this control strategy to maintain improved line-of-sight accuracy in the presence of host and instrument vibration, uncertain dynamics, and uncertain host motion. To this end, theory has been developed that allows for analysis of interconnected systems and presents new conditions for the stability and performance of these systems. To have better performance and improved ability to maintain accurate and precise sensing, new theory is being developed that allows the control to maintain performance in complex and changing environments.

The significance of this year's work is its benefit to nuclear nonproliferation. Past satellite work has shown the benefits of a stable pointing platform for intelligence and scientific data collection when coupled to a host satellite. The latest technologies allow for higher-fidelity sensing, which increases the demands for a more precise and stable platform. The results of this project can affect the ability of a sensor to point with the desired accuracy and jitter.

## Atmospheric Aerosols

Crystal Reed
Texas A&M University

Bernie Zak (Org 6338)
Sandia Principal Investigator

### Project Purpose

Atmospheric aerosols impact climate, both directly through scattering and absorption of radiation and indirectly through cloud processes. Because of the complex composition and spatial and temporal distribution of the atmospheric aerosol, understanding such impacts is challenging. To better understand the effects of aerosols, we study the processes that transform aerosols, such as new particle formation, condensation/dissolution, coagulation, and cloud processing. Numerous studies have utilized laboratory smog chambers to help predict the behavior of the atmospheric aerosol. Using the results of such laboratory experiments to predict the behavior of the ambient aerosol, however, is difficult given the complexity of the atmosphere and the inability to replicate such conditions. Recently, we designed, tested, and deployed a new type of chamber in order to study the evolution of an initially monodisperse aerosol in ambient conditions over intervals of one or more days. The work is being performed in collaboration with Texas A&M University (TAMU).

The ambient aerosol chamber for evolution studies (AACES) is a cubic chamber consisting of a rigid Acrylite OP-4 acrylic outer shell, which transmits ultraviolet radiation both in the UV-B (280-215nm) and UV-A (315-400nm) ranges. Fluorinated ethylene propylene (FEP) Teflon lines the inside of the chamber on all sides and the top, while expanded-polytetrafluoroethylene (ePTFE) Teflon is used on the bottom of the chamber. The fibrous structure of the ePTFE acts as a barrier to particulates, while allowing gas molecules to move virtually unimpeded from one side of the membrane to the other, creating an initial environment inside the chamber that is free of particles and continuously mimics the ambient air.

### Accomplishments

Numerous tests were conducted to determine the ability of AACES to mimic ambient conditions:

- Monodisperse particles were injected into the reaction chamber and the decay in concentration monitored over time. Since FEP Teflon carries a high static charge, it was determined that the particle loss rate was a direct result of particles being charged over time and depositing on the Teflon surface. To abate this effect, an alpha source static eliminator was used to pass ionized air between the outer shell of the chamber and the inner Teflon lining.

- Chamber response time was tested by injecting high ozone concentrations below the PTFE membrane and monitoring the concentration in the upper portion of the chamber over time. A subsonic mixing system was developed to ensure proper mixing. Chamber response time was determined to be 1.1 hours.

- The penetration efficiency of ozone, ethanol, acetic acid, toluene, NO, and $SO_2$ across the PTFE membrane were tested using a similar setup as described above. Ozone exhibited the lowest penetration efficiency at 92% of original concentration entering the upper reaction chamber, while each of the remaining gas species tested resulted in a near-100% penetration efficiency.

- In order to ensure proper chamber operation prior to field deployment, AACES was placed outdoors and experiments were conducted to monitor the growth rate of ammonium sulfate both with zero and ambient air being supplied to the bottom portion of the chamber. During the time in which zero air was being supplied, the aerosol species exhibited little or no growth. However, when ambient air was passed through the bottom chamber, steady growth rates were observed.

AACES was deployed at the DOE Atmospheric Radiation Measurement (ARM) Climate Research Facility Southern Great Plains location June 22, 2007 to July 9, 2007, and data will be available shortly.

### Significance

The results indicate that the approach represented by the ambient aerosol chamber for evolution studies (AACES)—namely, that of using a chamber into which ambient air can pass, but which contains only the aerosol intentionally injected—in fact works, and is viable for further research studies. Those studies have just begun at TAMU, and at other locations around the country. The AACES will be used to study the behavior of energy-related aerosols important to Sandia's mission.

## A Nutrient Cycle Model for the Middle Rio Grande, New Mexico

Gretchen Oelsner
University of Arizona

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

### Project Purpose

Water quality often limits the potential uses of scarce water resources in semiarid and arid regions. Consequently, changing water quality, particularly nutrient levels, is often an important concern with many water resource decisions. Chronically elevated nutrient loads may result in eutrophication of reservoirs and changes in riparian vegetation. To best manage water quality, one must understand the sources and sinks of both solutes and water to the river system. Therefore, modeling efforts will need to include biogeochemical processes both within the river and within the shallow alluvial aquifers of the riparian corridor. Incorporating these processes and feedback is paramount to modeling and evaluating the water quality dynamics that may result from changing land use practices, waste water treatment policies, watershed/range management, and reservoir operations.

This work will be pursued cooperatively with the University of Arizona and the NSF Science and Technology Center for the Sustainability of Semiarid Hydrology and Riparian Areas (SAHRA). SAHRA is a multi-institutional, multi-disciplinary research program to improve understanding of the hydrologic cycle, provide improved tools for decision-makers, and raise the level of hydrology literacy.

### Accomplishments

Water quality often limits the potential uses of scarce water resources in semiarid and arid regions. To best manage water quality, one must understand the sources and sinks of both solutes and water to the river system. Nutrient concentration patterns can identify source and sink locations, but cannot always determine biotic processes that affect nutrient concentrations. Modeling is a tool that can provide insights into large-scale processes. To address questions about large-scale nitrogen removal in the Middle Rio Grande, NM, we created a system dynamics nitrate model using existing integrated surface water/groundwater model of the region to evaluate uptake and denitrification as nitrate removal mechanisms.

We modeled denitrification in groundwater as a first-order process dependent only on concentration and used a 5% denitrification rate. Uptake was assumed to be proportional to transpiration and was modeled as a percentage of the evapotranspiration calculated within the model multiplied by the nitrate concentration in the water being transpired. We modeled riparian uptake as 90% and agricultural uptake as 50% of the respective evapotranspiration rates. Using these removal rates, our model results suggest that riparian uptake, agricultural uptake and denitrification in groundwater are all needed to produce the observed nitrate concentrations in the groundwater, conveyance channels, and river, as well as to account for the seasonal concentration patterns. The model results indicate that a total of 497 metric tons nitrate-N is removed from the Middle Rio Grande. Where river nitrate concentrations are low and there are no large nitrate sources, nitrate behaves nearly conservatively and riparian and agricultural uptakes are the most important removal mechanisms. Downstream of a large wastewater nitrate source, denitrification and agricultural uptake were responsible for approximately 90% of the nitrogen removal.

### Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries as well as the distribution of water among irrigators, urban developers, and environmentalists. This work focuses on developing tools to better manage our limited resources; specifically, quantifying nutrient cycling processes and their impact on water quality. Nutrients represent the leading anthropogenic source of pollution in surface and groundwater supplies. Nutrients are contributed to the environment through agricultural

chemicals, urban storm and wastewater streams, atmospheric deposition, and natural pathways. The chemistry and ultimate fate of these nutrients undergoes a complicated process of transformation, dispersion, and uptake in the environment. Because of this complexity in the nutrient cycle, tools are needed to understand how changes in the natural and anthropogenic environment impact nutrient loads. In addition, tools are needed to assess how changes in nutrient loads impact the environment, how they may limit water use, and increase treatment costs.

The developed nutrient model of the Middle Rio Grande is novel in its large-scale analysis of nutrient cycling. The developed model provides new insight into the leading causes of nutrient loading to the river. More importantly this work quantifies, for the first time, the role of uptake and denitrification in buffering nutrient levels in the Rio Grande and associated shallow aquifer. These results will contribute to a decision support framework that will allow decision-makers, stakeholders, and the public to explore a wide range of water use scenarios while understanding the downstream consequences in terms of water quality change. Finally, this model represents an important building block in the technical foundation for the Water Resource Decision Support Modeling focus area of Sandia's Water Initiative.

*Refereed Communications*

G.P. Oelsner, P.D. Brooks, and J.F. Hogan, "Nitrogen Sources and Sinks Within the Middle Rio Grande, New Mexico," *Journal of the American Water Resources Association*, vol. 43, pp. 850-863, August 2007.

G.P. Oelsner, "Quantifying Nutrient Sources and Sinks Within the Upper Rio Grande," doctoral dissertation, University of Arizona, Tucson, AZ, August 2007.

## Modeling Nonmarket Value of Water

Matt Weber
University of Arizona

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

### Project Purpose

Fresh water is central to the vitality of our society; however, current demands are increasingly being met through unsustainable practices. As such, improved management of our finite supplies is needed; unfortunately, establishing such practices is complicated by the differing values placed on water by the disparate sectors of our society (industrial, agricultural, environmental). Integrated modeling tools are needed to assist in regional water planning and to facilitate public involvement in the decision process. We take a novel approach to community-mediated water planning, employing a cooperative modeling process formulated within a system dynamics decision framework.

Society values water in many different ways—economic, aesthetic, cultural and instream/environmental. In some cases, these values can be directly quantified, as with economic valuation, while in others, quantifying worth can be difficult. Nevertheless, these diverse value systems are playing an increasing role in establishing management plans that are acceptable both publically and politically. For this reason, valuation methodologies must be developed and implemented within the water planning process.

This work will be pursued cooperatively with the University of Arizona and the NSF Science and Technology Center for the Sustainability of semi-Arid Hydrology and Riparian Areas (SAHRA). SAHRA is a multi-institutional, multi-disciplinary research program to improve understanding of the hydrologic cycle, provide improved tools for decision-makers, and raise the level of hydrology literacy. By leveraging our efforts we gain access to extensive expertise and data from unique studies on social valuation of water conducted in the Rio Grande and San Pedro River basins.

### Accomplishments

An integrated dynamic simulation model for comparing the costs and benefits of alternative riparian restoration and management options was developed. The model is built from original valuation data, regional benefit transfer studies, and extensive stakeholder input. The case study considers the riparian corridor along the Rio Grande in Albuquerque, New Mexico, though the concepts are applicable to other riparian resources in the Southwestern United States. The model includes a forest management module, a process-oriented river restoration module, and a recreation amenity construction and management module as three control variable sectors. These sectors are influenced by human-controlled restoration investment, which in turn, interacts with the natural system and modifies the flow of ecosystem service and recreational amenity benefits to the regional population. Tradeoffs between benefits and costs for particular types of riparian management may be examined individually and the efficacy of various investment possibilities may be tested through comparison of benefit-cost ratios. Fire frequency and nonnative plant infestation rates are subjects of a sensitivity analysis, with radical impacts on restoration strategizing as these key values change. Limitations in current environmental valuation research are found when attempting to build continuous resource demand curves

required for the model, particularly if environmental conditions are predicted to degrade rather than to improve. Over the 100-year planning horizon, and for the range of assumptions tested, the costs of not doing restoration are estimated to accumulate to between one and two billion dollars. With optimized restoration investments on the order of 100 million dollars (approximately $1 million per year), benefit returns accumulate to about one billion dollars, with benefit-cost ratios ranging from 7.7 to 12.5, depending on model assumptions.

### Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries, as well as the distribution of water among irrigators, urban developers, and environmentalists. The completed work focuses on developing tools to better manage our limited resources and engage the public in the water planning process.

All too often, environmental values are overlooked in planning processes aimed at developing equitable water allocation schemes. The developed model provides a novel approach to linking ecosystem response to restoration activities (e.g., change in forest health and diversity due to thinning and revegetation actions) and then evaluating the resulting costs and benefits that accrue over a 100-year time frame. The model is implemented within a decision support framework allowing decision-makers, stakeholders, and the public to explore a wide range of restoration strategies, compare ecosystem response, and quantify resulting benefit-cost ratios. The tool provides resource managers with an integrated and rapid means for planning river restoration projects, which is currently a billion dollar a year industry. Additionally, this model represents a key building block in the technical foundation for the Water Resource Decision Support Modeling focus area under Sandia's Water Initiative.

### *Refereed Publications*

M.A. Weber, "Riparian Valuation in the Southwestern United States," doctoral dissertation, University of Arizona, Tucson, AZ, April 2007.

M.A. Weber and S. Stewart, "Public Valuation of River Restoration Strategies for the Middle Rio Grande," to be published in *Restoration Ecology*.

## Tribological Studies of Microelectromechanical Systems

Shannon Timpe
University of California at Berkeley

Bonnie Antoun (Org. 8776)
Sandia Principal Investigator

### Project Purpose

Polysilicon micromachines have been designed for the purpose of studying the tribological properties of microelectromechanical systems (MEMS). Devices for characterizing interfacial adhesion and for characterizing friction have been developed at the University of California at Berkeley (UCB). In this collaborative project with the UCB, these devices were used to develop an understanding of the physics controlling the interfacial behavior that is critical to the reliability and efficiency of micrometer-scale devices.

### Accomplishments

Two MEMS tribology-testing devices have been successfully designed and implemented—one for testing adhesion alone and a second capable of testing both adhesion and friction. The first experimental phase that examined the adhesion force under a variety of leading and environmental conditions was completed. The second experimental phase utilized the second device and attempted to determine the effect of high adhesive forces on the frictional behavior of the MEMS structures. Experiments were performed on dynamic friction in a variety of environments.

Experiments were also conducted to study the effects of current flow across an interface on the adhesive properties of that interface. This is a particularly important topic for microswitching applications. Recorded data showed a combination of charge trapping in native oxide films and eventual catastrophic failure due to microwelding.

### Significance

This project benefits the general science and technology (S&T) community by developing an understanding of the tribological behavior of MEMS devices under various environments and conditions. This project serves to both develop collaboration with UCB and enable the development of future engineers/scientists that will enter the S&T community and possibly consider employment at Sandia.

### *Refereed Communications*

S.J. Timpe and K. Komvopoulos, "The Effect of Adhesion on the Static Friction Properties of Sidewall Contact Interfaces of Microelectromechanical Devices," *Journal of Microelectromechanical Systems*, vol. 15, pp. 1612-1621, December 2006.

*Other Communications*

S.J. Timpe and K. Komvopoulos, "Electrical Effect on the Adhesion Force at MEMS Contact Interfaces," presented at STLE/ASME International Joint Tribology Conference, San Antonio, TX, October 2006, and published in P*roceedings of the STLE/ASME International Joint Tribology Conference*, October 2006.

## Characterizing and Improving Distributed Intrusion Detection Systems

Elliot Probestel
University at California at Davis

Steve Hurd (Org. 8965)
Sandia Principal Investigator

### Project Purpose

This work with the University of California at Davis was aimed at understanding how well different intrusion detection systems (IDS) work, using network traffic captured on a university campus network. This would allow us to identify which IDS works best with specific types of traffic (e.g. academic, residence halls, etc.). Furthermore, because this captured network traffic represents only a probabilistically sampled fraction of the total network traffic, we also would also be able to identify any shortcomings with traditional IDS when using probabilistically sampled network traffic.

We used existing network traffic capture sources, and applied appropriate sampling rates. One of the two sources used was from a university campus. We completed an analysis regarding the nature of using sampled versus full network captures, as well as identifying whether an individual IDS was more effective for a specific type of traffic.

### Accomplishments

Our FY 2007 accomplishments are primarily in the area of the relationship between packet capture sampling rates and IDS performance. We used network traffic sampled at a wide variety of sampling rates, ranging from 1 packet sampled per 5 packets received (1:5) to 1 packet sampled per 1000 packets received (1:1000), and compared the alerts generated by the IDS using the full packet capture against the alerts generated by the IDS using only the sampled packets. The sampled alerts were categorized into "true positives" when they matched alerts generated by the entire packet capture. Conversely, "false positives" were instances where the sampled packets generated an alert and no corresponding alert was generated by the full packet capture.

Our results showed that IDS performance deteriorated rapidly, even with relatively modest sampling rates. Thus far, we have evaluated the SNORT IDS system using all three "sense level" settings for the sfPortscan preprocessor, namely, low, medium, and high.

At the low sense level, detection rates dropped to no more than 12 percent of the original detection rate at even the most frequent sampling rates (1:5), with false positive rates between 5 and 100 percent.

At the medium sense level, detection rates did not change markedly from those in the low sense level, but the false positive rates improved to below 5%.

At the high sense level, all traffic except "academic" continued to experience poor detection rates. Academic traffic fared better, with a detection rate as high as 50% at 1:5. Again, false positive rates were fairly low.

### Significance

As ever increasing volumes of network traffic and speeds of network links have made it very difficult to successfully conduct full packet captures, packet sampling has become popular, if not necessary. Yet as our work demonstrates, using a packet sampling approach significantly degrades the ability of traditional IDS to adequately identify malicious activity. Accordingly, new techniques are needed for either rapidly filtering full packet captures into more manageable data sets (that retain security-significant traffic), or improving the fidelity of an IDS used to identify malicious activity from sampled network traffic.

## Mobile Agent Abstractions, Methods, and Infrastructure for Efficient Sensor Network Tasking Over Heterogeneous Networks

Leo Szumel
University of California at Davis

Nina Berry (Org. 8961)
Sandia Principal Investigator

### Project Purpose

This research with PhD candidate Leo Szumel at the University of California at Davis (UC Davis) addresses the programming of efficient, scalable, fault-tolerant networks of wireless sensor nodes. These networks are made up of several nodes: elements characterized by a sensor suite, a power source, processing capability,

and a radio. There are several challenges in programming these networks.

First, because no single node has complete knowledge of the world environment, nodes of the network must collaborate with each other in order to solve problems with sufficient fidelity and scalability. Second, a network's full potential is only attainable by multiplexing several users or applications; doing so decreases the effective deployment cost of the network. A third challenge is that limited power means that nodes must spend most of their time sleeping and must perform rapid and efficient collaboration to accommodate that need.

This work integrates the former two challenges into that of "programming," and the latter into that of "communication." This work develops a mobile agent-programming model to solve the first challenge and a pheromone-inspired smart flooding communication primitive to solve the second problem.

This research will be demonstrated in a real, physical sensor network deployment. The network will be deployed at the McLaughlin Reserve (at the UC Davis Natural Reserve System) to enhance traditional plant ecology studies with new data that would not be attainable through human sampling of ecosystem parameters. The network will measure air, surface, and soil temperatures and soil moisture content.

This deployment has interesting network properties that distinguish it from many experimental networks. First, the network is not in range of wired or wireless data communications. Second, the nodes are placed according to existing experimental sites and cannot be moved to improve radio frequency (RF) connectivity. Third, the terrain and the RF landscape will change considerably as plants grow from foot-high to waist-high. Lastly, a mobile node will visit the site every 1–2 weeks.

## Accomplishments

1. We designed, implemented, and tested a system using the DISCERN hardware. In summary, this work involves applying the agent programming and pheromone communication primitives to the DISCERN hardware (imaging-capable sensor nodes). We used this system to study event detection algorithms implemented as mobile agents, and are currently analyzing the datasets created in these experiments.

2. We designed, implemented, and tested a system for general delay-tolerant data collection from sensor networks using the agent programming and pheromone communication primitives. This system is based on Crossbow's Mica2 hardware, which was acquired for a previous research project implemented using basic TinyOS coding. The objective of this effort is to examine the relative advantages and disadvantages of using our primitives as compared to as-written TinyOS programming.

Initial results are positive, indicating that a functional application can be developed using our primitives in less time, and with similar efficiency.

## Significance

This research focuses on the challenges posed by the programming of large sensor networks. The interest in such networks is quite easy to understand—the more measurements we can collect from our environment, the better we can understand and control it. This argument applies across many fields, including environmental monitoring, physical security, and basic science research. What has become clear over the last few years, however, is that we are approaching a time when these large networks are affordable from an equipment standpoint, yet they remain a huge logistical challenge, largely because of software development difficulty. These difficulties arise from the need to handle heterogeneous nodes, the spatial and temporal decoupling of nodes, and scaling challenges, among others.

This research is addressing these issues by providing a framework for the tasking of, and communication between, sensor nodes in large-scale deployments. This framework is scalable, efficient, and can support multiple applications on a single network. The application(s) can be updated independently and/or concurrently.

A specific example of how this research can be applied to Sandia's mission objectives is being demonstrated as a case study. The DISCERN nodes have the ability to detect objects and share their information with neighboring nodes—this is a scalable and efficient design. However, the network is of limited use if all decision synthesis occurs outside the network because doing so limits scalability and increases latency. This agent framework will be used to program the DISCERN nodes, allowing synthesis to occur inside the network.

## Fourier Analysis and Synthesis Tomography

Dan Feldkhun
University of Colorado at Boulder

Michael Sinclair (Org. 1824)
Sandia Principal Investigator

### Project Purpose

Fourier Analysis and Synthesis Tomography (FAST) is a full-field "synthetic aperture" microscopy technique that does not require a lens to form an image. Instead, FAST samples the spatial frequencies and phases of an object by sequentially illuminating it with interfering pairs of pulsed laser beams at different angles, detecting the response with a fast nonresolving detector, and using a novel optical processor to perform Fourier synthesis to reconstruct the object. FAST can be used in fluorescence mode for studying biological samples, or in coherent scattering mode for measuring synthetic objects such as microelectromechanical systems (MEMS). FAST can also be used to form a 3D reconstruction of an object by rotating the illumination axis.

By performing Fourier analysis sequentially, FAST makes possible full-field imaging with millimeters of depth of field, inches of working distance, and submicron resolution. By replacing mechanics with optoelectronics it is possible to acquire a frequency sample every 100 ns, achieving KHz imaging rates. FAST can also be used to detect object motion with very high spatial (nm) and temporal (ns) resolution by tracking the phase of its Fourier components. These capabilities are important for biological applications, such as real-time imaging of signals propagating through neurons and rapid screening of cellular and DNA microarrays, as well as for full-field imaging and motion characterization of microstructures such as MEMS. This project will thus both contribute to and benefit from current Sandia work in biological and MEMS imaging and microfabrication, as well as the imaging systems and optical information processing research at University of Colorado's Optoelectronics Computing Systems Center (OCSC).

FAST is an unconventional and novel approach to imaging and needs to be developed from the ground up. The project will require theory development, simulations, algorithm design, optical and mechanical system implementation, and electronic hardware and control software development.

### Accomplishments

The focus of the first year's work was the construction of a proof-of-concept Fourier analysis and synthesis tomography (PC-FAST) system in order to demonstrate the basic principles and algorithms of FAST. PC-FAST employs a 100-mW 532-nm continuous-wave (CW) laser, an acousto-optic Bragg cell, and a right-angle prism image rotator in order to rapidly generate moving interference patterns with electronically programmable amplitude, frequency, phase, and direction. The interference pattern generator is optically coupled with a conventional stereo microscope and a 0.4 NA (numerical aperture) objective in order to project the interference patterns onto the sample under study and to direct light scattered or fluoresced by the sample onto a fast single-element detector. The entire optoelectronic system fits on a ~1 ft x 2 ft optical breadboard and is capable of generating a different interference pattern every ~10 µs over a spatial frequency range spanning nearly three orders of magnitude. A fast rotation stage allows the system to measure slices through the object's 2D Fourier space over the full angular span of 180 degrees in ~40 ms, enabling the system to acquire 2D images at video rates.

We designed a custom differential detector with an automatic noise-cancellation feedback loop allowing us to make shot-noise-limited measurements over a 40 MHz bandwidth. By illuminating a reflective resolution target with chirped interference fringes and using Fourier-domain post processing, we were able to reconstruct one-dimensional image projections of the target and demonstrate a depth of focus in excess of 1 mm at full system resolution. We also developed a model of the FAST optical transfer function and formulated an image-reconstruction algorithm based on tomographic filtered back projection.

### Significance

FAST is a general-purpose image synthesis technique that unlike lens-based approaches can maintain very large depth of field and working distance at submicron resolution and can be used to detect nanometer-scale motions. As a result, FAST benefits a number of biological science applications such as imaging and tracking of neuron signals, as well as defense and environmental science applications such as characterization of MEMS actuators and sensors used to detect chemical and biological agents.

### *Other Communications*

D. Feldkhun and K. Wagner, " Fourier Analysis and Synthesis Tomography: A Structured Illumination Approach to Computational Imaging," in *Adaptive Optics: Analysis and Methods/ Computational Optical Sensing and Imaging/Information Photonics/ Signal Recovery and Synthesis Topical Meetings on CD-ROM*, 2007, paper CTuB4.

## Modeling and Design of Microstructures with Tailored Adhesive Properties

Kevin Sylves
University of Colorado at Boulder

Dave Reedy, Jr. (Org. 1526)
Sandia Principal Investigator

### Project Purpose

This project is concerned with the analysis and design of micro and nanostructures whose response is dominated by adhesive forces. A multiscale adhesion model will be developed that takes into account van der Waals, friction, capillary and electrostatic force mechanisms at the micro and nanoscale. This model will be implemented into a finite element analysis framework through nonlinear constitutive laws that accurately capture adhesive effects between surfaces. The constitutive model will incorporate internal parameters that capture hysteresis effects and rate dependencies. Additionally, a contact model based on the Lagrange multiplier approach will be adopted to prevent surface penetration. Microbeam/plate example problems incorporating tailored force-displacement characteristics will be constructed that can be verified experimentally. When implemented in a design optimization framework, this tool will allow designers to create devices that integrate tailored surface properties in novel ways including robust microdevices that are insensitive to detrimental adhesive behavior, multiphysics problems such as behavior of soft particles immersed in flow, and self-assembling micro and nanosystems. Gradient-based optimization algorithms already integrated into our finite element code will be employed for shape and topology optimization of adhesive characteristics of surfaces. The nonlinear program will include various objective formulations such as a specific force-displacement characteristic in adhesion/decohesion and constraints such as maximum surface adhesion energy. Both adjoint and direct sensitivity analyses will be implemented for computational efficiency, thus enabling the efficient solution of problems with large numbers of optimization variables and/or criteria. This work will be conducted with the Center for Aerospace Structures at the University of Colorado at Boulder.

### Accomplishments

Over the past year, we have developed and implemented a suite of two- and three-dimensional interface elements in our finite element code. These elements enforce contact penetration prevention through a penalty method implemented as a material nonlinearity. Additionally, these elements incorporate several interfacial interaction force laws including electrostatic forcing and the Lennard-Jones and Dugdale models of van der Waals adhesion. The framework is easily extensible to include additional surface interaction forces to the entire suite of elements. We verified the accuracy of this implementation of adhesive contact by duplicating published examples in the literature including a prior Sandia microbeam stiction study, and a cylindrical variant on the classical Hertz and JKR (fracture mechanics analysis of Johnson, Kendall, and Roberts) spherical adhesive contact problems.

These elements are compatible with the design optimization algorithms already implemented in our code. We implemented and verified gradients through sensitivity analysis for the suite of elements by comparing analytical gradients to numerical finite differencing results. We then formulated and solved optimization problems based on the microbeam delamination and cylinder adhesion examples. The objective of these problems was to match a prescribed force-displacement characteristic at a certain point in the structure. The optimization variables included adhesive energy distribution along the contact interface and the shape of the surfaces in adhesive contact. Adhesive distributions were found that optimized the given objectives for both cases that had analytical solutions and those for which the optimal adhesive pattern was unknown beforehand. These examples validated the original hypothesis that design optimization can be used to find adhesive patterns or surface designs that optimize novel structural objectives in regimes where interfacial forces dominate.

### Significance

This work relates to ongoing research in microsurface adhesion at Sandia and has applications that coincide with and complement the research mission of the Department of Energy. Applications include self-assembled materials, objects with highly tailored surface adhesion properties and reduction of detrimental adhesive properties in microsystems.

## Design, Analysis, and Control of MEMS Devices for Micromanipulation Tasks

Jessica Bronson
University of Florida

James J. Allen (Org. 1769)
Sandia Principal Investigator

### Project Purpose

The objective of this research with the University of Florida is to develop advanced microelectromechanical systems (MEMS) micromirror arrays for use in adaptive optics applications such as optical communications and imaging systems. In order to realize the full capabilities of MEMS optical systems for the demands of next generation technologies, MEMS micromirror components must be robust and agile to the changing needs of performance and environment, and maintain precise and accurate positioning. Micromirror arrays are one of the most successful and versatile MEMS applications, including optical switches for telecommunications, scanning and imaging for projection displays, diffraction gratings for spectroscopy, and adaptive optics for wave front correction. Many of these devices require large arrays of micromirrors and it is desirable to ensure accurate positioning capabilities for each mirror in the array despite the presence of outside disturbances or variations arising from fabrication processes, for example small deviations in dimensional or material properties across the array. Many of today's emerging technologies require true analog positioning capabilities, and in order to guarantee precision and accuracy of the mirror position for analog operation, closed-loop feedback control techniques are required. Feedback control has long been used in many macroscale systems to correct for such factors, yet limited work has been done to apply these techniques to MEMS systems. This research is focused on the development of micromirrors with closed-loop control to ensure accurate position tracking across an array of devices in the presence of parametric uncertainties and external disturbances. This goal will be achieved through considering both optimized design of the actuators as well as developing closed-loop control schemes to meet the unique needs of MEMS systems.

### Accomplishments

This research is focused on the development of MEMS micromirrors with closed-loop control to ensure accurate position tracking across an array of devices in the presence of parametric uncertainties and external disturbances. This goal will be achieved through considering both optimized design of the actuators as well as developing closed-loop control schemes to meet the unique needs of MEMS systems. To achieve this goal the following steps were performed:

- Designed a MEMS micromirror device that can be used to experimentally access the effect of closed-loop control on a MEMS device
- In order to understand the mechanics of the MEMS micromirror, extensive finite element modeling of the MEMS micromirror components was performed
- Micromirror structure
- Electrostatic actuation
- Piezoresistive sensing
- Many simulations were performed with this model to understand the uncertainties and sensitivities of the MEMS mirror device
- Performance measurements of the MEMS micromirror device were used to understand the modeling and system uncertainties
- Control designs were performed; these required input from the model, test data, and an understanding of the system uncertainties
- Simulations of the performance and stability of the closed-loop micromirror control system were performed to access the control design technique
- The control design methodologies of PID (proportional – integral – derivative) and LQR (linear quadratic regulator) were accessed in this work
- Investigated the use of nonlinear elastic springs to counteract the nonlinear electrostatic actuation force and thus enable a more stable system. This activity resulted in a patent application.

This work has provided the fundamental modeling as well as the design and fabrication of an experimental MEMS device that enabled a viable demonstration of the passive and active control methodologies developed as a result of this project.

### Significance

The above accomplishments have provided the fundamental modeling as well as the design and fabrication of an experimental module that will enable viable demonstration of this project's passive and active control methodologies. The full impact of microsystem technology has thus far been limited by a lack of reliable, accurate and high-precision MEMS devices. The successful realization of this project will lead to new capabilities for MEMS optical systems and provide a means for strengthening Sandia's national security capabilities by integrating more reliable and precise microsystems into next generation communication and imaging technologies. The objectives set forth in this research are intended to achieve micromirror arrays with

precise and accurate positioning enabled by use of robust, optimized design and control techniques. The successful completion of this work will allow micromirrors for adaptive optics applications that are robust to parametric uncertainties that commonly arise through microfabrication processes, as well as to disturbance rejection and plant instabilities. The application of optimal design methods and closed-loop control techniques will enable both cost reduction—because the devices will no longer require extensive calibration for open-loop performance—as well as improved performance and reliability. Further, the incorporation of on-chip sensing mechanisms into the device will allow for compact realization of complete microsystems. The method for using piezoresistive methods within SUMMiT V™ (Sandia ultraplanar multilevel MEMS Technology V) fabrication is novel and its success will open up new areas of device applications.

*Refereed Communications*

J.R. Bronson and G.J. Wiens, "Stability Analysis for an Electrostatic MEMS Vertical Comb Drive Actuator," to be published in *ASME Journal of Computational and Nonlinear Dynamics.*

J.R. Bronson, "Modeling and Control of MEMS Micromirror Arrays with Nonlinearities and Parametric Uncertainties," doctoral dissertation, University of Florida, 2007.

## Capture and Utilization of Prosody in Disambiguating Spoken Speech

Laura Matzen
University of Illinois at Urbana-Champaign

Travis Bauer (Org. 6341)
Sandia Principal Investigator

### Project Purpose

The purpose of this project with the University of Illinois at Urbana-Champaign is to investigate the ways in which different types of contextual cues influence how people process and remember linguistic information. Specifically, we are investigating cues that are based on the prosody, syntax, semantics, and visual features of words and sentences to learn more about how people who are reading or comprehending auditory language process information, and what they are later able to remember about that information. This research will be used to develop models of how people create representations of language in memory and how those representations affect later attempts at retrieving the information from memory.

### Accomplishments

We conducted experiments on the following topics:

1. The effects of study time on item memory and source memory for linguistic stimuli
2. The effects of different linguistic study contexts on the prevalence of different types of false memories
3. The effects of prosodic stress on memory for verbal instructions
4. The effects of syntactic ambiguity pragmatic information on sentence processing
5. Hemispheric differences in how the forms and meanings of words are processed in the brain

We also developed a model of item and source memory and submitted a paper on context effects for publication in a leading psychology journal.

### Significance

These experiments have led to new insights into contextual effects that are of great interest in the fields of psychology and neuroscience. Our results have led to the creation of a new model of human memory and have provided an explanation for a discrepancy in the existing literature on false memory. The information provided by these experiments can also benefit Sandia's work in the areas of knowledge preservation and intelligence analysis by enhancing models based on the speech and text of specific individuals.

## Multi-Mode Energy Scavenging from the Environment

Tzeno Galchev
University of Michigan

Chris Apblett (Org. 1723)
Sandia Principal Investigator

### Project Purpose

This project is developing a low-frequency micropower generator that can efficiently scavenge energy from ambient vibrations. We are also exploring a new technique called frequency up-conversion, which can increase the mechanical efficiency of this generator at low frequencies. The basic operation is that energy is coupled from the environment to a

low frequency, sensitive resonator, which then passes a portion of this energy to a second resonant element that, operating at a higher frequency, is used for conversion. Three ways of implementing this technique have been identified. One way of transferring this energy is through a collision between the two devices. This technique has been analyzed in more detail. Simulations show that using two devices with a specific mass ratio can lead to a 37% improvement in energy density when using frequency up-conversion over other approaches. We have shown that an arrayed implementation can potentially provide a 180% improvement in energy density. A micro-implementation of this system is currently being fabricated in order to prove the up-conversion concept. A new high-aspect micromachining technology has been developed, necessitated by the challenges in fabricating some of the geometries in these devices. The work is being performed in collaboration with the University of Michigan.

### Accomplishments

Simulations of the frequency up-converting device have been performed, and first generation devices have been fabricated using a new silicon-on-silicon technology. An optimal mass ratio is reached where a 36% increase in energy density can be attained using frequency up-conversion when compared to direct conversion of low-frequency energy. These simulated results are attained assuming that both the up-conversion device and a single degree of freedom device have the same electrical damping (same coil properties) for a one-to-one comparison. This is also true for the system being fabricated. Further analysis has shown that an arrayed approach, where the up-conversion mass is split into multiple devices can potentially lead to an over 180% increase in power density.

As we continue work to attain test results from the fabricated impact driven system, we expect to reach a point at which the up-conversion principle is proven, and the next step will be to ascertain which of the three implementations of up-conversion is the most favorable. We have begun modeling the scheme using electrostatic actuation. This system is significantly more complicated than the impact driven generator because of the dynamic forces which act on both devices. In order to better understand the generator's operation, a dynamic model has been built using SIMULINK and MATLAB.

A provisional patent application has been filed.

### Significance

This device represents the first practical implementation of a frequency up-conversion mechanical harvesting device. Since this device takes the driving force and converts it to a specific frequency for piezoelectric conversion to electricity, the drive frequency does not have to be matched to the piezoelectric frequency. This allows for transformation and subsequent harvesting of mechanical to electrical energy from a much wider range of mechanical vibration sources than previously achievable. Practical applications of this development include new unattended ground sensor power sources that do not require a battery and never need to be charged, and other small sensor devices that can be remotely placed and then powered by such a device.

### *Other Communications*

T.V. Galchev, W.C. Welch III, and K. Najafi, "Low-Temperature MEMS Process Using Plasma Activated Silicon-On-Silicon (SOS) Bonding," presented at IEEE MEMS, Kobe, Japan, January 2007.

## Diffusion-Based Sensing of Membrane Proteins in Solid Support Platforms

Jason Cox
University of New Mexico

Susan Brozik (Org. 1714)
Sandia Principal Investigator

### Project Purpose

The potential for using naturally occurring membrane proteins as nanomaterials has long been recognized due to the important functions these proteins carry out in biological systems. Membrane proteins are responsible for the regulation of cellular metabolism, signal transduction, and the transport of ions and nutrients in and out of the cell. Despite the fundamental role these proteins play in biological systems, their characterization by experimental techniques remains a considerable hurdle due to the inherent complexity of the membranes and the proteins themselves. Specifically, the expression, detergent solubilization, purification, and reconstitution of functional, multimeric proteins are significant challenges and probing the structure and function of these molecules is nontrivial.

In hopes of unlocking some of the fundamental biophysical questions in membrane bound protein systems, we are developing new ways to study representative proteins in synthetic platforms that aid in probing these molecules. These biophysical questions include the basic thermodynamic properties such as binding states and the dynamics of the protein in native and synthetic membranes. The protein we are studying in detail is the ligand-gated ion channel, serotonin type 3 receptor (5-HT3 R), incorporated into small unilamellar

vesicles (SUVs) that are deposited on planar substrates. The tools we are utilizing to discern these phenomena include the optical techniques of single molecule fluorescence microscopy and fluorescence correlation spectroscopy. We are also using atomic force microscopy to study the topography of the protein in native and synthetic environments. Each of these techniques is capable of single molecule sensitivity and providing high-resolution structural detail that is difficult to retrieve through other methods. The work is performed in collaboration with the University of New Mexico.

### Accomplishments

In the past year, our group has been working toward the characterization of the ligand-gated, ion channel, serotonin human type-3 receptor, (5-HT3 R). Specifically, we are interested in answering some of the fundamental biophysical questions that pertain to this protein in native and synthetic environments. In pursuit of these questions, we have successfully incorporated 5-HT3 R into self-assembled, supported, lipid bilayers on planar substrates and nanoporous silica beads. These synthetic platforms greatly simplify the characterization of membrane proteins and have led to the following achievements in our group:

1. Electrochemical and optical assays for assessment of function for the ligand-gated ion channel, (5-HT3 R)
2. Measurement of membrane fluidity using fluorescence correlation spectroscopy

Additionally, we are interested in studying the binding events that lead to the ion channel opening and closing. To this end, we have developed a general synthetic scheme that allows us to conjugate virtually any amine reactive fluorescent dye molecule to the receptor agonist, serotonin.

3. Synthesis of widely adaptable 5-HT3 R agonists for single molecule studies, fluorescence correlation, and two-photon excitation experiments

### Significance

Over the last several decades, membrane-bound proteins have become recognized as a major target for therapeutic and biosensing technologies. Interfacing these biological structures with synthetic materials thus offers an important challenge for the realization of future innovations. In order to overcome commonly observed artifacts resulting from the secondary interaction of transmembrane proteins with their synthetic substrates, supported phosphocholine bilayers on nanoporous silica microbeads were investigated at a range of sizes common to biological cells. Additionally, two methods of functional protein incorporation were demonstrated for comparison in vivo.

The results of these experiments provide a basis for ionic and fluorescent dye-based compartmentalization assays as well as high-resolution optical and electrochemical interrogation such as laser trapping and patch clamp. The structural stability added to the bilayer as a result of the porous substrate allows proteins to be incorporated using traditional nonionic detergent-based methods. Additionally, the availability of uniformly sized beads with uniform pore structure allows the bilayer diameter and surface area to be directly controlled. These findings demonstrate that bilayer-coated porous silica beads offer a stable, size selective, and convenient platform for the study and incorporation of purified transmembrane-bound proteins with minimal unfavorable protein-substrate interaction due to high surface porosity with less than 10 nm scale surface structures.

### *Refereed Communications*

R.W. Davis, A. Flores, T.A. Barrick, J.M. Cox, S.M. Brozik, G.P. Lopez, and J.A. Brozik, "Nanoporous Microbead Supported Bilayers: Stability, Physical Characterization, and Incorporation of Functional Transmembrane Proteins," *Langmuir,* vol. 23, pp. 3864-3872, February 2007.

## Nanostructured Electrocatalyst for Fuel Cells: Silica Templated Synthesis of Pt/C Composites

Elize Switzer
University of New Mexico

Chris Cornelius (Org. 6338)
Sandia Principal Investigator

### Project Purpose

The essential balance of kinetic and transport properties of the methanol oxidation electrocatalysts are due, in part, to the hierarchical structure that combines distinct structural considerations across length scales. The result of this type of structure is a relatively low surface area for catalysis, which results in inefficient mass transport within the fuel cell catalytic layer. This work will assist in understanding these properties as well as pursue synthesis of enhanced materials through investigation of novel bimetallic Pt-Ru nanowire networks.

The general accomplishment of this project year is an expansion of last year's work that includes the exploration of the synthesis processes and electrochemical activity of nanostructured Pt-Ru nanowire and particle networks. Because the ability to alter and fine-tune the Pt-Ru microstructure exists, fundamental studies of the local structures can be undertaken in the upcoming research period. By controlling the morphology of the Pt-Ru catalyst on the nanoscale, the effects of the local structure on electrochemical activity can be studied, and a new class of catalysts will be developed. Fuel cells testing with hydrogen, methanol, and ethanol have also been added to this year's efforts to examine the performance of these catalysts within real operating fuel cells. This fuel cell testing is necessary to relate electrochemical catalysts characterization efforts via rotating disk electrode to a functional fuel cell as planned for this research project.

The University of New Mexico will continue its effort in the development of synthesis methods for high surface area methanol electrooxidation catalysts. The UNM team will also explore mesoporous materials templating as another method for nanophase stabilization as well as for the development of alkaline fuel cells, in collaboration with the Sandia team. Finally, we will develop a phenomenological model of catalysis in open frame structured materials.

## Accomplishments

An innovative aerosol-based synthesis approach was employed that involves using silica to template Pt and Ru precursors, followed by silica removal for structured electrocatalysts. The structuring of the electrocatalyst on the nanoscale creates advantages in the local mass transfer properties. These improvements result in an advantageous balance of kinetic and transport properties of the electrocatalysts due, in part, to the hierarchical structure that combines distinct structural considerations across length scales. The catalyst precursor solution consists of colloidal silica particles with an average diameter of 20 nm, and metallic-amine platinum and ruthenium complexes. In this method of synthesis, all phases are in intimate contact during synthesis, which promotes the production of a homogeneous material with a higher degree of alloying.

A provisional patent application was submitted for this work.

## Significance

One aspect that is necessary for realizing methanol fuel cells is the development of highly functional electrochemical catalysts. In order to realize this challenge, an understanding of mass transport in the direct methanol fuel cell anode in its entirety (flow fields, gas diffusion layer and catalytic layer) for this extremely complicated system must be elucidated. The primary reason for this technical challenge is the existence of two-phase liquid (reactant methanol solution) and gas (product carbon dioxide) flow.

While the majority of published papers in the scientific literature has focused on the diffusion layer and flow field geometry, there is a conspicuous absence of studies that focus solely on the active layer morphology. It is logical that in this layer, the complex transport of methanol is affected by the gaseous $CO_2$ flow behavior, $CO_2$ production rate and catalyst geometry. It is also reasonable that the morphology of the active layer becomes even more important in smaller fuel cells. The influence of catalytic layer morphology can be examined by a thorough comparison of polarization curves of membrane electrode assemblies with synthesized nanostructured electrocatalysts and conventional electrocatalysts. The mass transport properties of synthesized nanostructured electrocatalysts can be studied based on this relationship. We hypothesize that an open frame structured electrocatalyst will exhibit higher mass transport limited currents for a given inlet concentration and flow rate than will a traditional electrocatalyst.

The mass transport limited current increases with methanol flow rate as qualitatively predicted by theory; and the methodology and experimental parameters have been established. Thus, this work will take studies to the next step by creating fuel cells incorporating these new nanostructured electrocatalysts and test them. Consequently, the effect of local structure of the templated catalysts can now be evaluated based on a comparison of the mass-transport limited performance between the two cells.

### *Refereed Communications*

E. Switzer, P. Atanassov, and A.K. Datye, "Nanostructured Anode Pt-Ru Electrocatalysts for Direct Methanol Fuel Cells," to be published in *Topics in Catalysis - Special Issue on Fuel Cells.*

### *Other Communications*

E. Switzer, P. Atanassov, and A.K. Datye, "Nanostructured Anode Pt-Ru Electrocatalysts for Direct Methanol Fuel Cells," presented at 20th North American Catalysis Society Conference, Houston, TX, June 2007.

T. Olson, P. Atanassov, E. Switzer, M. Hibbs, and C. Cornelius, "Alkaline Fuel Cell Employing Novel Anion Exchange Membrane," presented at 211th Meeting of the Electrochemical Society, Chicago, IL, May 2007.

E. Switzer, A. Datye, and P. Atanassov, "Templated Pt-Ru Electrocatalyst for Electro-Oxidation of Methanol," presented at 211th Meeting of the Electrochemical Society, Chicago, IL, May 2007.

## Advanced Materials for Water Treatment Membranes: Enhanced Rejection Performance and Surface Properties

Elizabeth Van Wagner
University of Texas at Austin

Susan Altman (Org. 6338)
Sandia Principal Investigator

### Project Purpose

This project aims to create a teaming relationship between the University of Texas at Austin (UT) and Sandia to leverage the biofouling testing capabilities of Sandia and the capabilities in membranes, transport measurements, and water purification technologies at UT. The purpose of this work is to create new polymer membranes that have high flux for pure water, but are able to reject salt and have good fouling resistance. We plan to fabricate dense layers of functionalized poly(phenylene) and poly(aniline) on porous supports and test these membrane concepts for their performance in water purification bench-scale experiments.

### Accomplishments

During the past year at UT, we have focused on two main areas of research with reverse osmosis (RO) membranes. The first area is baseline characterization of the commercial (unmodified) RO membranes. We worked to find crucial, but often overlooked, variables that must be controlled during crossflow testing in order to obtain the performance parameters specified by the manufacturer. Reverse osmosis membranes have been optimized for high flux and salt rejection properties, making them much more sensitive to testing conditions than less selective membranes such as ultrafiltration and nanofiltration membranes.

The second area of research focus has been the surface modification of commercial RO membranes. Dip coating and spin coating have been explored as two alternative methods for grafting the hydrophilic molecule poly(ethylene glycol) diglycidyl ether (PEG diepoxide) to the RO membrane surface. Dead end tests determined the pure water flux, or extent of PEG diepoxide grafting (lower flux indicates more PEG diepoxide on the membrane surface), of membranes grafted with various concentrations and molecular weights of PEG diepoxide. Other variables studied for their effect on extent of PEG diepoxide grafting included reaction time and temperature. Crossflow tests will be done to determine the salt rejection properties and oil-fouling behavior of these surface modified RO membranes.

### Significance

Membranes are the technology of choice for water purification. Reverse osmosis processes produce high purity water from saline water, but polyamide membranes, the state of the art, do not have good fouling resistance and their fundamental properties are poorly understood in terms of the mechanisms of salt rejection.

This project supports technology and materials testing capability development in the area of water purification which is of strategic interest to Sandia and may provide future opportunities for programmatic work. Additionally, creating opportunities for graduate student training and opening future avenues for UT students at Sandia is of key importance in this university collaboration.

## Dynamics of Propagating Shock Waves and Phase Fronts

Johnathan Niemczura
University of Texas at Austin

Jim Redmond (Org. 1526)
Sandia Principal Investigator

### Project Purpose

This research—to be performed at the University of Texas at Austin—will focus on an examination of the dynamics associated with the generation and propagation of shock waves and phase fronts in solids. Such phase transformations and shocks are developed in many high-energy impact and explosion problems; understanding the physics of these phenomena in a wide range of materials permits their use in structures designed to mitigate the effects of blast or impact events. This research will involve a combination of experimental observations, analytical modeling, and numerical simulations of models. The research involves special purpose equipment that will trigger phase transformations and shocks in these classes of materials, application of experimental diagnostic techniques for time resolving the response of the material to short duration loading, and interpretation of the physical mechanisms that govern the development of transformations and shocks.

The balance momentum equations used to describe stress wave propagation in single-phase materials cannot be used alone to describe the response of a material that undergoes a phase transformation because the number of phase fronts and speed of these fronts are left underdetermined. In order to complete the formulation of the impact problem, a kinetic relation describing the relationship between the driving force and the speed of propagation of a phase front must be added to the momentum balance equations. However, the experiments permit direct evaluation of the kinetic relation; this relation permits numerical simulation of such events. It is the goal of this work to determine the kinetic relation for both rubber and shape memory alloys and to develop an experimental method that can be applied to other exotic materials that exhibit discontinuities in constitutive relationship.

### Accomplishments

- Conducted numerous tests on the 2-D dynamic fracture of rubber. Crack speeds approaching or exceeding the unstretched speed of sound in the rubber have been recorded. This was an attempt to determine whether phase transformations and shock waves could be triggered in this 2-D strain field.
- Parametric studies of the influence of a crack parallel to the stretch on crack speeds have been conducted
- Conducted a series of experiments examining the response of 2-D radially symmetric rubber specimen to transverse impact
- Improved the efficiency of the tensile impact experimental setup so as to allow higher velocities to be achieved using the same delivery pressure. These higher velocities are in the range needed to create a tensile shock wave in the rubber specimens and phase transformation fronts in shape memory alloys.

### Significance

This research aims to develop the mechanics of shock propagation for materials exhibiting phase transformation. While this research is of great interest for the enduring stockpile, more importantly, it may also enable the future insertion of tailored materials for shock and vibration mitigation.

### *Other Communications*

J. Niemczura, "On the Propagation of Finite Deformation Waves in Rubber," presented at ASME Applied Mechanics and Materials Conference, Austin, TX, June 2007.

## Process and Infrastructure Development for Integrated Three-Dimensional Mesomanufacturing

Contract Research
University of Texas at El Paso

Jeremy Palmer (Org. 1413-2)
Sandia Principal Investigator

### Project Purpose

The purpose of this collaborative research project with the University of Texas at El Paso (UTEP) is to investigate novel functionally integrated layered manufacturing (FILM). Research activities focus on the innovative UTEP multimaterial stereolithography apparatus (MMSLA), and include integrated stereolithography (SL) and direct write media dispensing (DW), SL and selective electroplating, and composite material systems. The anticipated outcomes from these thrust areas are value-added product demonstrations, such as an SL/DW radio frequency (RF) antenna array interconnect, secure electronic packaging, and rapidly manufactured body armor. In these products, the integrated MMSLA system offers the benefit of reduced cycle time and labor cost through collocation and automation of these operations. Moreover, it enables multifunctional smart structures that are unattainable with current technology.

### Accomplishments

Strategies were explored for improving fabrication of complex 3D circuitry with embedded electronics using the Sandia/UTEP integrated stereolithography (SL) and direct write (DW) system. We demonstrated improvements by developing a wireless motion sensor with global positioning system (GPS) capabilities and comparing performance of the 3D circuit with a traditionally manufactured printed circuit board (PCB). The integrated SL/DW system benefited the sensor relative to PCB manufacturing by: (1) reducing the size of the sensor due to the 3D locations of components and circuitry; (2) allowing the shape of the sensor to change according to the environment in which it was fielded (so that it acquired the form of the local terrain, for example); and, (3) providing a natural resistance to reverse engineering through 3D circuitry and component embedding. We explored resistance-inductance-capacitance (RLC) performance measurements for various DW inks and discovered that the E1660 ink from Ercon, Inc. provided the best performance of the four inks tested. In addition, we investigated strategies for improving performance of SL resins. We used a design of experiments approach to investigate the effects of SL build orientation on dimension accuracy and mechanical strength. Mechanical performance was shown to be statistically significantly impacted at a 95% level of confidence by the orientation of the layer-to-layer interfaces on fabricated parts.

Investigations are continuing with a focus on removing the layering effects on mechanical performance so that SL can be used in rapid manufacturing applications (such as rapidly manufactured conformal body armor and satellite subsystems). We also explored alternative strategies for improving SL resin performance, focusing primarily on electroless and electroplating of Ni and Cu coatings on SL-manufactured parts. A significant study is in progress that is examining the effects of different thickness coatings on the mechanical performance of three state-of-the-art SL resins.

### Significance

This work represents the first significant effort to integrate solid freeform fabrication (SFF) with direct write (DW) to rapidly manufacture 3D mechatronic products in a system known as functional integrated layered manufacturing (FILM). It advances the science and technology community a step closer to the goal of practical desktop "printing" of complete products. In the near term, the research demonstrates the potential for FILM in mechatronic products by providing the following advantages:

1. Reducing manufacturing cycle time and direct labor costs in selected high-volume applications by automating manual wiring and consolidating parts

2. Reducing product volume and enabling unique, unprecedented package geometry

### *Other Communications*

M. Navarrete, A. Lopes, J. Acuna, R. Estrada, E. MacDonald, J.A. Palmer, and R.B. Wicker, "Integrated Layered Manufacturing of a Novel Wireless Motion Sensor System with GPS," presented at Solid Freeform Fabrication Symposium, Austin, TX, August 2007, and published in *Proceedings of the Solid Freeform Fabrication Symposium*, August 2007.

## Active Control of Periodic Disturbances

Scott Pigg
University of Utah

Gene Hertel, Jr. (Org. 1516)
Sandia Principal Investigator

### Project Purpose

The objective of this research with the University of Utah is to investigate algorithms for the rejection of unknown disturbances, with a particular interest in active noise and vibration control applications (ANC, AVC, or ANVC). Disturbances are assumed to be the sum of periodic signals with time-varying magnitudes, frequencies, and phases. The control algorithms are of the pure feedback type, where no reference sensor is assumed to be available to give a preview of the disturbance. These problems are more difficult to solve and less well understood. The algorithms are also able to handle systems with unknown dynamics that may change significantly over time.

Specifically, this work will involve the development of new algorithms for adaptive disturbance rejection, with particular emphasis on the cancellation of periodic noise disturbances. In the development and implementation of these algorithms, multichannel active noise control (ANC) experiments will be used to explore issues related to more globalized disturbance rejection. The stability and parameter convergence of all algorithms considered will be examined through averaging theory.

A key emphasis of this project is to treat unknown disturbances as well as unknown systems. Periodic disturbances with unknown frequencies may vary over a wide range. In adaptive feedback control, the rejection of such disturbances can be accomplished by using frequency estimation techniques or by deriving controller structures that obtain this estimate implicitly. Additionally, methods involving adaptive identification can be derived for identifying plant parameters online. Investigation of these methods will be used for the development and analysis of simple and efficient algorithms for systems where both disturbance frequency and system dynamics are unknown and, possibly, time varying. Specifically, plant identification will be added to algorithms for unknown frequency and frequency estimation will be added to algorithms for unknown systems.

### Accomplishments

New algorithms for the rejection of periodic disturbances continue to be developed at the University of Utah. The focus on disturbances that are known to be periodic in nature makes this research relevant to many applications involving rotating equipment. Specifically, attention has

been paid to narrowband adaptive feedback control, in which knowledge of the disturbance frequency and plant dynamics allows for perfect cancellation of periodic disturbances. Algorithms which identify and adapt to variations in either disturbance or plant parameters have been considered. By assuming that the system dynamics have reached steady state with respect to parameter update, simple and meaningful algorithms with established convergence properties have been derived.

Since many applications, such as those concerning rotorcraft, involve unknown and time-varying dynamics due to variations in environmental factors, methods continue to be developed for identifying plant parameters online. Several such methods have been implemented and investigated on an active noise control testbed at the University of Utah. A commonly employed technique involves the use of gradient or conventional least-squares identifiers to continuously update an estimate of plant dynamics. By deriving linear expressions describing the output of the plant, an estimate of the disturbance as well as the plant frequency response is obtained. This estimate is then used in determining the control input that exactly cancels the disturbance. Estimation of the parameters occurs continuously and without the need for any added excitation, whereas previous methods have required the collection of batches of data as well as an externally applied excitation signal. Averaging theory has been used to gain insight into the stability properties of the algorithm and has shown that parameter convergence obeys certain constraints. Averaging theory enables a much simpler time-invariant system to be considered, and ANC experiments have been used to verify results of the averaging analysis.

Previously studied techniques used phase-locked loop based frequency estimation to reject unknown disturbances when system dynamics were known. The effect of adding such frequency estimation to algorithms for unknown systems has achieved up to 97% attenuation in ANC experiments. Due to the interaction of the various components, adding frequency estimation leads to additional complication of the dynamic response of the algorithm, and techniques based on averaging theory are being used to obtain meaningful stability properties. The goal in this work is to obtain solutions that are viable in engineering practice.

### Significance

Examples of applications where disturbance rejection is a primary control objective include the reduction of optical jitter in laser communication systems, isolation in space structures of vibrations produced by control moment gyroscopes, and cryogenic coolers. In several of the aforementioned applications, the tracking of time-varying parameters is essential. In applications involved with space exploration, repair is very costly, and it is preferable to have systems which can adapt to changes caused by aging or harsh environmental conditions. The objective of this research is to derive simple and efficient algorithms for the rejection of unknown periodic disturbances, with an emphasis on unknown and time-varying systems. While existing techniques enable one to tackle known systems, few methods are able to deal with time-varying systems and, typically, they assume the existence of a reference sensor.

Of particular interest are feedback structures that require no reference sensor to provide a preview of the disturbance. This problem has been seriously investigated at the University of Utah. Several techniques have been studied, and methods have been found that continuously estimate system dynamics without the need to collect batches of data. By assuming the disturbance is sinusoidal, the number of parameters is much smaller than the one required to describe the transfer function in ANC systems. The disturbance frequency must either be known or an estimate must be obtained online. From techniques being developed in this project, an online estimate of both plant and disturbance parameters can be obtained. This estimate can then be used to exactly cancel the disturbance. The ability to track both rapidly and slowly time-varying systems demonstrates the practicality and robustness of this approach. Similar algorithms can be used for active vibration control and active noise control, and this research is, in particular, validated experimentally on an active noise control testbed.

## Reliability of Materials in MEMS: Residual Stress and Adhesion in a Micro Power Generation System

Molly Kennedy
Washington State University

Neville Moody (Org. 8759)
Sandia Principal Investigator

### Project Purpose

This project supports a PhD student at Washington State University, collaborating with mentors at Sandia, to determine a self-consistent method to quantify interfacial fracture toughness of thin film systems. During this project, experimental

measurements of adhesion were coupled with analytical solutions to determine interfacial fracture toughness. These results can provide computational model validation and design parameters and lifetime analysis for microelectromechanical systems (MEMS) structures and thin films in microelectronics. This project was finalized by providing direct comparisons between two independent interfacial adhesion tests, compressed over-layer buckling and four-point bend testing. Both Pt films used in MEMS and Au films used in Sandia microelectronics systems have been tested experimentally. This past year, the project has focused on directly comparing these test methods and demonstrating methods to improve the reproducibility of the four-point bend testing. Additionally, these tests have been adopted for other materials systems for nuclear weapons projects, demonstrating their usefulness to a broad range of Sandia materials systems.

## Accomplishments

Previous work using stressed overlayers to determine the toughness of Pt/Ti/SiO2 films suggests a transition occurs from island to uniform film coverage with increasing film thickness. The stressed overlayers triggered buckle formation from which toughness values were determined. However, these tests lead to fracture under strong shear stresses. Four-point bending tests were therefore carried out on sandwich specimens to evaluate the toughness using this technique, which causes delamination under approximately equal contributions from normal and shear stresses.
As part of this study, a new sample fabrication procedure was developed using ethylenediamine pyrocatechol (EDP) etching and photolithography to define the precracks and a hydrofluoric acid/nitric acid/acetic acid (HNA) etching process to remove surface. The result was a marked improvement in reproducibility. Comparison of test results for a range of Ti adhesion layer thicknesses shows that the difference between results from these two test methods is likely due to the differences in applied stress states.

## Significance

This study demonstrates that the two test methods are appropriate for quantifying interfacial fracture toughness. The benefit of the four-point bend test is that the applied stress state is well controlled and provides a more accurate value of toughness than values determined using stressed overlayers. However, with limitations imposed by many sample configurations (for instance in many MEMS samples or with samples from the field), the overlayer tests provide a reasonable measurement of toughness as the trends in measuring toughness track between the two methods. If two material conditions are to be evaluated (i.e., exposure to different hydrogen exposures), the test method most appropriate for the sample geometry can be used with confidence to predict trends in changes in adhesion in thin film systems.

The development of rapid, robust, and verifiable testing techniques enhances our ability to evaluate a wide range of critical materials and technologies that currently exist in the stockpile, as well as to evaluate future stockpile devices and materials. Results from this study and from the use of these techniques will provide computational model validation and design parameters and lifetime analysis for MEMS structures and thin films in microelectronics and with relevance to the nation's stockpile.

### *Refereed Communications*

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "The Effect of Nonuniform Chemistry on Interfacial Fracture Toughness," *Metallurgical and Materials*, vol. 38, pp. 2256-2262, September 2007.

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "The Aging of Metallic Thin Films: Delamination, Strain Relaxation, and Diffusion," *Journal of Materials*, vol. 59, pp. 50-53, September 2007.

### *Other Communications*

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "Environmental Impacts on Fracture of Thin Films," presented at 2007 The Minerals, Metals, and Materials Society Annual Meeting, Orlando, FL, February 2007.

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "Development of Adhesion Layer Chemistry for Metal Ceramic Interfaces," presented at Gordon Conference on Thin Film and Small Volume Mechanical Behavior, Waterville, ME, July 2006.

M.S. Kennedy, D.F. Bahr, D.P. Adams, and N.R. Moody, "Aging of Transition Metal Interfaces and Evolution of Interfacial Fracture Energies," presented at 2006 Materials Science and Technology Conference, Cincinnati, OH, October 2006.

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "Confinement of Plasticity During Interfacial Fracture," presented at 2006 Materials Research Society Fall Meeting, Boston, MA, November 2006.

# PRESIDENTIAL EARLY CAREER AWARDS FOR SCIENTISTS AND ENGINEERS

DOE/NNSA Defense Programs (DP) identifies nominees for the Presidential Early Career Awards for Scientists and Engineers (PECASE) from the most meritorious recipients of the DOE/NNSA-DP Early Career Scientist and Engineer Award. Candidates for this award are researchers employed by academic institutions who are in the first five years of their independent research careers. Individuals are nominated by directors of DP laboratories based on the candidate's contribution to the DP mission. Up to six winners are selected annually by the Office of Defense Programs from the nominations provided by the laboratory directors. Up to three of the winners of the DP Early Career Scientist and Engineer Award may also be designated annually by the laboratory directors as DP nominees for the PECASE. The nominating laboratory is responsible for funding the PECASE awardee for the next five years.

The PECASE embodies the high priority placed by the government on maintaining the leadership position of the United States in science by producing outstanding scientists and engineers and nurturing their continued development. The awards identify a cadre of outstanding scientists and engineers who will broadly advance science and the mission. Further, the awards foster innovative and far-reaching developments in science and technology, increase awareness of careers in science and engineering, give recognition to the scientific missions of participating agencies, enhance connections between fundamental research and national goals, and highlight the importance of science and technology for the nation's future.

The award is $250,000, given to the awardees through a $50,000 per year research contract funded through the Laboratory Directed Research and Development (LDRD) Program. This provides the awardee an opportunity to continue research in the area for which he/she was nominated and for Sandia to benefit from the results of the developments.

## Discontinuous Galerkin Methods for Generalized Continuum Models for Inelasticity

Krishna Garikipati
University of Michigan

Jay Foulk (Org. 8776)
Sandia Principal Investigator

### Project Purpose

This project involves the development of a class of new finite element methods, based on the discontinuous Galerkin (DG) Method, which makes possible the numerical solution of complex, strain gradient continuum models with standard, C0 finite elements. These strain gradient continuum models of plasticity and damage typically involve high-order (usually fourth-order) spatial derivatives, which prevent their numerical solution via standard, C0 finite element methods.

This work is in collaboration with Krishna Garikipati, recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE) award, at the University of Michigan.

### Accomplishments

1. A class of discontinuous Galerkin finite element methods has been formulated for strain gradient plasticity models which are based on geometrically necessary dislocations.

2. The above DG finite element method has been implemented in an open-source C++ coding environment, the FENICS code (www.fenics.org). This makes possible its portability and eventual dissemination.

3. Preliminary computational results have been obtained, which are the first ones for complex loading conditions with this class (geometrically-necessary dislocation-based) of strain gradient plasticity models.

### Significance

The field of plasticity, and particularly computational plasticity is in very early stages of the development of finite element methods for strain gradient continua. This project is at the forefront of these efforts. Strain gradient continuum models of plasticity and damage provide a means to link length scale effects (which originate at the grain and subgrain scale in metals) to macroscopic models of mechanics.

These methodologies are of particular interest to Sandia. From designing microsystems to modeling component failure in abnormal environments, the numerical methods developed in this effort may provide a means to include the requisite physics and obtain regularized (mesh-independent) solutions.

### *Refereed Communications*

R.A. Regueiro, P. Dixit and K. Garikipati, "On Standard and Vector Finite Element Analysis of a Strict Anti-Plane Shear Model with Elastic Curvature," to be published in *Computer Methods in Applied Mechanics and Engineering*.

L. Molari, G.N. Wells, K. Garikipati and F. Ubertini, "A Discontinuous Galerkin Method for Strain Gradient-Dependent Damage: Study of Interpolations and Convergence," *Computer Methods in Applied Mechanics and Engineering*, vol. 195, pp. 1480-1498, 2006.

### *Other Communications*

K. Garikipati and J. Ostien, "Discontinuous Galerkin Method for an Incompatibility-Based Strain Gradient Plasticity Model," presented at COMPLAS 2007, Barcelona, Spain, September 2007.

## Developing Novel Scaffolds for Biological Molecules by Solving the I-QSAR Problem Using the Signature Molecular Descriptor

Donald Visco
Tennessee Technological University

Jean-Loup Faulon (Org. 8333)
Sandia Principal Investigator

### Project Purpose

This project is aimed at designing molecular compounds having specific biological activities and properties. This goal is accomplished in two steps. First, one creates a quantitative structure-activity relationship (QSAR) between a set of known compound structures and their experimentally measured activities. In this step, named "forward QSAR," molecular structures are described using the signature molecular descriptor, which has previously been shown to give good accuracies in property and activity predictions. The second step consists of finding the structural elements (i.e., the signatures) that best match a given target activity and enumerating all the compounds matching these structural elements, this step is named "inverse QSAR." The inverse QSAR step comprises a set of Diophantine equations that are solved to find the signatures that match the targeted activities, and an algorithm that

enumerates all molecular structures corresponding to a given signature. In this fiscal year, the technique has been refined and the use of the molecular descriptor, called Signature, which quantifies a molecule's two-dimensional (2-D) structure, has been explored in other areas. This work is in collaboration with Donald Visco, recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE) award, at Tennessee Technological University.

### Accomplishments

Year three of this work was spent both refining the inverse QSAR approach as well as exploring the use of Signature in other areas. In particular, we have determined the best mapping of the BLOSUM62 matrix elements using Signature occurs when we employ the Soergel coefficient at height-2 (optimized), one of 160 models examined. Also, we have used support vector machine learning to classify bioassays found on PubChem and found this technique more discriminating than multiple linear regression. Working with the University of Texas (UT)-Medical Branch, we have performed an inverse-design study on trypsin inhibitors and have suggested novel inhibitors that are currently being synthesized by our collaborators. "Best candidates" were filtered for selection by, among other techniques, an energetic screen based on a molecular mechanics force field that we have incorporated into our overall protocol. Additional inverse-QSAR technique refinement has occurred in exploring height-2 constraint equation development as well as advanced post-processing screening filters based on aromatic ring requirements.

### Significance

The concept of designing compounds matching targeted properties and activities is novel, and has not been successfully developed and applied prior to this work. Continued exploration is needed, however, to improve the quality of solutions obtained and efficiency of the technique from both a computational speed and storage standpoint. Additionally, the use of Signature outside of the inverse QSAR process opens it up to use in high-throughput screening applications. This is an emerging area of research for this descriptor, especially relative to the problems associated with promiscuous inhibitors.

### *Other Communications*

D. Visco, D. Weis, and J. Faulon, "Design of New Cox-2 Inhibitors Using the Signature Molecular Descriptor," presented at AIChE Annual Meeting, San Francisco, CA, November 2006.

D. Visco, D. Weis, and J. Faulon, "Inverse-QSAR for Inhibitors of Phosphate Cdc25b," presented at AIChE Annual Meeting, San Francisco, CA, November 2006.

## Fundamentals of Embossing Nanoimprint Lithography in Polymer Substrates

William King
University of Illinois at Urbana-Champaign

Blake Simmons (Org. 8759)
Sandia Principal Investigator

### Project Purpose

This project is a collaboration with Prof. William King, a Presidential Early Career Awards for Scientists and Engineers (PECASE) recipient at the University of Illinois at Urbana-Champaign. Nanoimprint lithography (NIL) is a nanomanufacturing technique that uses a nanostructured master template to form features in a substrate with best resolution near 1 nm and areas as large as 100 cm2. In embossing-based NIL, a nanostructured master is heated and pressed into a thermoplastic polymer film, forming a negative relief replica in the polymer film. Nearly all previous research on NIL has been for the purpose of nanoelectronics fabrication in which the polymer film acts as a mask layer. This project seeks to enhance the state-of-the-art in the development of embossed, nanostructured polymer films as an actual functional surface, rather than a mask layer.

The goals of the project are to develop a first-principles understanding of polymer transport during thermal embossing such that any polymeric material could be employed for embossing-based NIL. The need for this research is particularly acute when polymer nanostructures are of size comparable to the polymer molecule radius of gyration, and when the nanoscale heat and mass transport properties of the polymer are not known. The lack of fundamental materials science knowledge is the major limit to rational design of nanofabrication methods to produce specific feature sizes and shapes. This work aims to model and measure polymer properties during NIL for a large number of thermoplastic polymers. This link between material properties and processing parameters will enable rational NIL process design.

### Accomplishments

In FY07, we have investigated nanoscale polymer heat and mass transport during embossing-based nanoimprint lithography and direct-write atomic force microscopy (AFM) nanoindentation. We have fabricated several master templates with features in the range 2 μm–10 nm. These

masters have been manufactured in silicon and subsequently electroplated into nickel metal. These metal stamps are robust enough to accommodate several hundred embossing trials with minimal feature degradation. We have selected and tested a number of thermoplastic polymers (e.g., polymethylmethacrylate and polyimide) with molecular weights in the range 104–107 kDa. These molecular weights were selected to produce characteristic molecular length scales in the range of 3–50 nm. After embossing, we have utilized atomic force microscopy (AFM) to characterize the embossed substrates and correlate embossing conditions, polymer molecular properties, and manufactured feature sizes. Continuum and subcontinuum models of polymer transport and template deformation have been developed and utilized to aid in this analysis.

### Significance

Nanoimprint lithography is the ultraminiaturized version of the decades-old embossing process in which a master tool — or a mold — is pressed into a soft material to create detailed patterns. Using a broad range of polymer materials, nanoimprint lithography produces structures on the micrometer or nanometer size scales, offering the potential for lowering production costs.

However, quality issues caused by unpredictable polymer flow into the nonuniform features of embossing tools pose a major stumbling block. Earlier research into this complex process has produced often conflicting recommendations, forcing manufacturers to pursue costly trial and error.

Using the results of experimental work, we are examining every variable involved in the nanoimprinting process, recording the outcome of each incremental change through the design space. We are studying such variables as shear deformation of the polymer, elastic stress release, capillary flow and viscous flow during the filling of imprinting tool cavities that had varying sizes and shapes.

The results apply to any polymeric material that follows standard viscous flow rules and produces feature sizes larger than 50 nm. The next step in this research will be to modify the simulation software to account for physics changes that occur on smaller size scales.

These results will have applications in semiconductor manufacturing, where nanoimprinting offers a potential alternative to increasingly expensive lithography processes to produce circuitry. It could also help make high-volume production of nanoscale structures more economically feasible for optoelectronic, biomedical and other applications.

### *Refereed Communications*

M.T. Eliason, J.L. Charest, B.A. Simmons, A.J. Garcia, and W.P. King, "Nanoimprint Fabrication of Polymer Cell Substrates With Combined Microscale and Nanoscale Topography," *Journal of Vacuum Science & Technology, B: Microelectronics and Nanometer Structures--Processing, Measurement, and Phenomena,* vol. 25(4), pp. L31-34, 2007.

## Fabrication and Device Applications of Aligned Mesoporous Architectures

Yunfeng Lu
University of California at Los Angeles

Jeff Brinker (Org. 1002)
Sandia Principal Investigator

### Project Purpose

During the last decade, mesoporous materials with tunable periodic pores have been synthesized using surfactant liquid crystalline as templates, opening a new avenue for a wide spectrum of applications. However, their applications are somewhat limited by their unfavorable pore orientation. Although a great effort has been devoted to align the pore channels, fabrication of mesoporous materials with perpendicular pore channels remains challenging. This project, with Presidential Early Career Award for Scientist and Engineers (PECASE) recipient Dr. Yunfeng Lu at the University of California, Los Angeles, will fabricate mesoporous materials with perpendicularly aligned pore channels.

Our previous work in this project has demonstrated that the mesoporous channels can be aligned using capillary force. More specifically, we contacted a lytropic liquid crystalline fluid that contains inorganic or organic building blocks (e.g., silicate) and surfactant molecules with anodized porous alumina membranes. Capillary force generated by the curvature of the fluid meniscus created capillary rise of the complex fluid and filled the alumina pore channels with aligned liquid crystalline templates. Subsequent removal of the templates creates mesoporous silica membranes with perpendicular pore channels.

Success of this work may provide a new technique to fabricate controlled structure materials and devices for water purification, separation, sensors, templated synthesis, microelectronics, optics, controlled release, highly selective catalysts, and other applications. For example, such aligned mesoporous materials can be further functionalized with responsive or recognizable components, leading to the fabrication of smart devices, such as intelligent artificial membranes and highly sensitive sensors.

### Accomplishments

During the last year's research, we have demonstrated the alignment of hexagonal pore channels within porous anodize alumina membranes using capillary forces, as follows:

1. Optimized the synthesis condition to achieved highly aligned mesostructure,
2. Conducted preliminary calculation to understand the aligning mechanism, and
3. Investigated alignment of the mesostructure within different size alumina pore channels.

### Significance

Self-assembled, oriented nanoporous channels are ideal model systems in which to understand molecular and ionic transport. When the pore size becomes comparable to the Debye length, a rich diversity of transport phenomena is expected. Self-assembled, oriented pore channel systems are also of immense importance in solving challenging engineering problems like water purification, where oriented carbon nanotubes (CNTs) were recently reported to support ballistic transport of water. This work will specifically impact two Sandia projects: a DOE/ Basic Energy Sciences (BES) molecular nanocomposites project and a new LDRD project on engineered membranes for water purification. In both cases the oriented silica channels will be constructed into membranes and silane coupling chemistry and new plasma-assisted atomic layer deposition (ALD) procedures will be used to carefully modify the pore size and pore surface chemistry. By varying the pore size with respect to the Debye length, this work contributes to a fundamental understanding of nanoconfinement on both water transport and selectivity.

### *Refereed Communications*

H. Li, Z. Bian, J. Zhu, D. Zhang, G. Li, Y. Huo, H. Li, and Y. Lu, "Mesoporous Titania Spheres with Tunable Chamber Structure and Enhanced Photocatalytic Activity," *Journal of the American Chemical Society*, vol. 127, pp. 8406-8407, 2007.

Q. Hi, R. Kou, J. Pang, T.L. Ward, M. Cai, Z. Yang, Y. Lu and J. Tang, "Mesoporous Carbon/Silica Nanocomposite Through Multi-component Assembly," *Chemical Communications*, vol. 6, pp. 601-603, 2007.

### *Other Communications*

Y. Lu, "Hierarchical Assembly," presented at Rice University (invited), Houston, TX, 2007.

Y. Lu, "Hierarchical Assembly," presented at the University of Kentucky (invited), Lexington, KY, 2007.

## On the Role of Numerical Error in Turbulence Simulations

Christopher Roy
Virginia Technical University

Matthew Barone (Org. 1515)
Sandia Principal Investigator

### Project Purpose

Because of the difficulties in isolating numerical and modeling errors in turbulence simulations, new approaches are needed to assess numerical errors. One promising approach is the method of nearby problems (MNP) developed by Presidential Early Career Awards for Scientists and Engineers (PECASE) recipient Chris Roy at Virginia Technical University, where exact solutions are generated through spline fitting of highly resolved numerical solutions. These exact solutions can then be operated on by the governing equations in order to generate small, distributed source terms. In the first year of this collaboration with Dr. Roy, MNP was successfully extended from 1D to multiple dimensions with a general approach which can be extended to 3D and 4D problems in a straightforward manner. Successful implementation of multidimensional MNP will facilitate the development of a unique test bed of realistic flow problems for evaluating different numerical discretization schemes used in unsteady turbulence simulations. Furthermore, multidimensional MNP also has important applications in code and solution verification for the broader area of computational science and engineering. Year two will focus on generating realistic, two-dimensional, exact solutions for the diffusion, Euler, and Navier-Stokes equations with small source terms. This second year will also include the extension of the spline-fitting

procedure to higher dimensions. Year three will focus on 3D and 4D (3D + time) solutions to the Euler and Navier-Stokes equations.

## Accomplishments

In FY 2007 the work focused on the extension of the MNP from one dimension to two dimensions. Initial work focused on two-dimensional problems such as heat conduction and unsteady Burgers equation, for which a number of exact solutions exist. Only general approaches were investigated, which can be extended to three- and four-dimensional problems in a straightforward manner. The chief difficulty that had to be overcome was the development of spline fits that are continuous up to an arbitrary number of derivatives over the boundaries of each spline zone. MNP has been successfully applied to one-dimensional problems, and extensions to multiple dimensions were successful, building on the prior work of others.

## Significance

This research addresses fundamental issues related to the DOE mission of providing verified and validated predictive simulation capabilities for nuclear weapon stockpile systems. Accurate unsteady turbulence simulations play an essential role in predicting delivery vehicle aerodynamics, pool fire environments, and other key system behavior. This research will attack the unresolved issue of solution verification of such simulations.

Successful implementation of multidimensional MNP will facilitate the development of a unique test bed of realistic flow problems for evaluating different numerical discretization schemes used in unsteady turbulence simulations for cases where exact solutions exist (i.e., where the numerical errors can be evaluated exactly and do not have to be estimated). Furthermore, multidimensional MNP also has important applications in code and solution verification for the broader area of computational science and engineering, including, grid adaptation, evaluation of error estimators, assessment of grid quality, and algorithm robustness studies.

### *Refereed Communications*

C.J. Roy, A. Raju, and M.M. Hopkins, "Estimation of Discretization Errors Using the Method of Nearby Problems," *AIAA Journal*, vol. 45, pp. 1232-1243, June 2007.

## President Harry S. Truman Fellowship in National Security Science and Engineering

University Research, in partnership with Human Resources, established the President Harry S. Truman Fellowship in National Security Science and Engineering (Truman Fellowship Program) in 2004. This program provides an opportunity each year for exceptional scholars to join Sandia National Laboratories (Sandia) in the continuation of Sandia's tradition of excellence. The Fellowship is named for President Harry S. Truman who, in 1949, asked AT&T to accept managerial responsibility of Sandia and challenged us to provide "an exceptional service in the national interest"—a motto that leads us to excel to this day.

The Truman Fellowship seeks to attract the best nationally recognized, new PhD scientists and engineers. It provides the opportunity for recipients to pursue independent research of their own choosing that supports Sandia's mission. The appointees are expected to foster creativity and to stimulate exploration of forefront science and technology and high-risk, potentially high-value R&D. Fellowships are for three years and are funded through the Laboratory Directed Research and Development (LDRD) Program.

Truman Fellowship candidates are expected to have solved a major scientific or engineering problem in their thesis work or have provided a new approach or insight to a major problem, as evidenced by a recognized impact in their field.

In 2007, two additional Fellows were selected. They came to Sandia from Oxford University and the University of Colorado at Boulder. They joined four Fellows who had previously competed for the Truman Fellowship. Progress reports on all six independent research projects follow.

### 2007 TRUMAN FELLOWS

Dr. Whitney Colella has a BS (ME, minor in public policy) from Princeton and the Woodrow Wilson School, MS (Science and Public Policy, Sussex), MS (ME, Stanford), MBA (Oxford), and DPhil (Engineering Science, Oxford). She has been recognized with British Marshall, Fulbright, NSF, T.J. Watson, Gilbreath, and ORS scholarships and fellowships. She plans to develop and employ computer simulations of alternative energy systems so as to maximize their positive impacts on the environment, national security, and costs. Models will be used to examine alternative designs for stationary tri-generative fuel cell power plants tuned to the electricity, heating, and cooling demand curves for the buildings they could serve. The model analyses will enable evaluation of the energy supply by fuel cell systems and distributed energy devices relative to the energy demand. She joined Sandia in January 2007 and is conducting her research in the Hydrogen and Combustion Technology Department (8367). She collaborates with the Fuels and Energy Transitions Department (6338).

Dr. Hung (Jacques) Loui has a PhD in electrical engineering from the University of Colorado at Boulder. He double-majored in electrical engineering and piano performance and won a number of prestigious piano competitions before focusing on engineering research. He was the recipient of a number of scholarships and fellowships including a Department of Education Graduate Assistance in Areas of National Need (GAANN) Fellowship. In his PhD work, Dr. Loui tackled an unsolved problem in quantitively describing the Radio Frequency (RF) characteristics of thick metal surfaces with arbitrary inclusions. His analysis capabilities and expertise will immediately benefit Synthetic Aperture Radar (SAR) applications for nuclear weapons and the intelligence community. Dr. Loui works in the SAR Sensor Technologies Department (5345) where he employs his analysis methods on the design of thin metal, frequency selective surfaces for SAR. His goals are to extend his analysis methods and develop new RF MEMS devices. Jacques began work in October 2006.

## Bayesian Inference for Inverse Problems, Model Structure, and Uncertainties

Youssef Marzouk (Org. 8351)
Truman Fellow

### Project Purpose

Inverse problems are of great relevance to science and engineering. While progress in detailed, first-principles modeling of physical systems has been enormous, this progress has exposed a challenging and complementary task — inferring unknown model parameters, spatiotemporal fields, and structures from data in realistic problems. Several factors render these problems difficult to solve. Real-world observations are inevitably limited in number and corrupted by measurement error. Inversion is typically ill conditioned; small errors in measurement can lead to enormous changes in the estimated model or model parameters. Moreover, multiple models may match a given data set, or no model may match the data.

This work develops a probabilistic setting for inverse problems, based on Bayesian inference. Bayesian statistics provides a rigorous foundation for inference from limited and noisy data, a natural mechanism for incorporating disparate prior sources of information, and a quantitative assessment of uncertainty in the inferred results. We also seek to develop efficient computational tools that surmount the cost of evaluating high-dimensional Bayesian integrals and exploring posterior distributions, particularly for complex forward problems accessible only through expensive computational simulations.

We consider two key applications, contaminant source inversion and chemical reaction network construction. Statistical algorithms for source inversion are critical to environmental applications (e.g., subsurface plumes and transport) and to homeland security (e.g., in response to risks of bioagent/toxin release in public spaces). Efficient Bayesian inference from sparse and noisy data provides rigorous estimates of confidence in threat characterizations, enabling targeted and effective responses. Robust inference of chemical reaction networks has fundamental applications in both energy conversion and in biology — in the former case, by elucidating the kinetics of utilization of new fuels, and in the latter case, by revealing crucial aspects of cellular function, such as signaling pathways and innate response to pathogens.

### Accomplishments

Work in much of FY 2007 built on previous years' efforts in stochastic spectral reformulations of the Bayesian approach to inverse problems, by developing new algorithms for larger-scale problems:

- Inference of spatiotemporal fields: We demonstrated Bayesian inference for inverse problems in which the unknown quantity is an inhomogeneous field (e.g., a spatially-varying material/transport property) and the forward model is computationally intensive. We introduced statistical regularization via hierarchical Gaussian process priors, and designed Markov chain Monte Carlo (MCMC) algorithms to achieve efficient posterior sampling.
- Dimensionality reduction: We demonstrated dimensionality reduction in inverse problems, using the Karhunen-Loève expansion of the prior stochastic process. After benchmarking speedup and convergence, we explored the impact of data resolution (length and time scales) on the posterior, and found that taking advantage of data scarcity allowed further dimensionality reductions and gains in computational efficiency.
- Sparsity in forward uncertainty quantification (UQ): We explored the use of "sparse truncation" in order to mitigate the size of the polynomial chaos basis used to solve stochastic forward problems. We demonstrated the use of sparse polynomial chaos bases in the solution of inverse problems, with excellent accuracy. These truncations hold promise both in Bayesian inversion and forward UQ.
- Advection-diffusion problems: We applied the Bayesian approach to source inversion problems involving convective transport, identifying key physical time scales that control the ill-conditioning of the problem and the degree of uncertainty in the inverse solution.

We spent the latter part of FY 2007 developing more advanced Bayesian methodologies for parameter inference in stochastic models, such as stochastic chemical reaction networks. Further, we formulated MCMC algorithms to treat model uncertainty and inference of model structure. These algorithms include reversible-jump and trans-dimensional MCMC, and comprise a common framework for structural inference in reaction networks and the construction of polynomial chaos representations from inaccurate data.

### Significance

New algorithms for Bayesian inference in complex inverse problems, developed here, have growing impact on both the inverse problems and the statistics communities. By introducing efficient spectral methods for uncertainty propagation into the

realm of inverse problems, we have rendered Bayesian inference with detailed physical models far more computationally tractable. We expect that this will facilitate the adoption of Bayesian approaches, with their rigorous treatment of uncertainties, in large-scale inverse problem applications.

Impact on potential application areas:
- *Atmospheric and subsurface transport of contaminants:* The prototypical source inversion problems we have solved are at the heart of pressing problems in homeland security, e.g., responding to toxic releases in public spaces. The inverse estimation of fields also has impact on geophysical applications, e.g., characterizing subsurface properties from indirect measurements.

- *Energy conversion and molecular biology:* Statistical methods for constructing kinetic models from indirect and noisy data are of growing importance in energy applications, where reaction mechanisms for the utilization of biofuels and complex hydrocarbons are replete with uncertainties and difficult to characterize. Similar challenges pervade molecular biology; techniques developed here will take advantage of emerging time- and cell-resolved kinetic data.

Bayesian methods developed here have led to the PI's sustained involvement in additional Sandia efforts:

(1) "Practical Reliability and Uncertainty Quantification for Complex Hierarchical Systems." This LDRD project (105814) uses Bayesian techniques to estimate and extrapolate the reliability of engineered systems from test data, with quantifiable credibility bounds.

(2) "Distributed Microreleases of Bioterror Pathogens." This LDRD project (93505) uses Bayesian inference to characterize bioterror attacks from patient data, in the earliest phases of an outbreak.

(3) Analysis of laser-diagnostic data in combustion chemistry, using Bayesian computation to construct uncertain kinetic models (funded by DOE Basic Energy Sciences program).

(4) Collaboration with Sandians at the Computer Science Research Institute (CSRI) to implement Bayesian inversion methodologies in flexible high-performance simulation frameworks designed for end users.

*Refereed Communications*

Y.M. Marzouk, H.N. Najm, and L.A. Rahn, "Stochastic Spectral Methods for Efficient Bayesian Solution of Inverse Problems," *Journal of Computational Physics*, vol. 224, pp. 560-586, 2007.

Y.M. Marzouk and A.F. Ghoniem, "Vorticity Structure and Evolution in a Transverse Jet," *Journal of Fluid Mechanics,* vol. 575, pp. 267-305, 2007.

*Other Communications*

Y.M. Marzouk and H.N. Najm, "A Bayesian Approach to Inverse Problems in Scalar Transport," presented at APS Division of Fluid Dynamics, Tampa, FL, November 2006.

Y.M. Marzouk, "Uncertainty and Bayesian Inference in Inverse Problems," presented at Pacific Northwest National Laboratories (invited), Richland, WA, February 2007.

Y.M. Marzouk and H.N. Najm, "Dimensionality Reduction and Polynomial Chaos Acceleration of Bayesian Inference in Inverse Problems," presented at SIAM Conference on Computational Science and Engineering, Costa Mesa, CA, February 2007.

Y.M. Marzouk, "Computationally Efficient Bayesian Inference for Inverse Problems," presented at UC-Berkeley Applied Mathematics Seminar (invited), Berkeley, CA, April 2007.

Y.M. Marzouk and H.N. Najm, "Dimensionality Reduction and Polynomial Chaos Acceleration of Bayesian Inference for Inverse Problems," presented at ICOSAHOM (International Conference on Spectral and High Order Methods) 2007 (invited), Beijing, China, June 2007.

Y.M. Marzouk and H. N. Najm, "Dimensionality Reduction in Bayesian Inverse Problems," presented at Applied Inverse Problems 2007, Vancouver, Canada, June 2007.

Y.M. Marzouk and H.N. Najm, "Efficient Bayesian Estimation of Random Fields with Gaussian Process Priors," presented at 9th US National Congress on Computational Mechanics, San Francisco, CA, July 2007.

Y.M. Marzouk, "Computationally Efficient Bayesian Inference for Inverse Problems," presented at Sandia CSRI Workshop on Large-Scale Inverse Problems and Quantification of Uncertainty (invited), Santa Fe, NM, September 2007.

J. Ray, Y.M. Marzouk, M. Kraus, and P. Fast, "A Bayesian Method for Characterizing Distributed Microreleases: Inference Under Model Uncertainty with Short Time Series Data," SAND2006-7568, Sandia National Laboratories, Livermore, CA, January 2007.

P.T. Boggs, Y.M. Marzouk, P.P. Pebay, J. Red-Horse, K. Diegert, and R. Zurn, "Bayesian Methods for Estimating the Reliability in Complex Hierarchical Networks," SAND2007-2758, Sandia National Laboratories, Livermore, CA, May 2007.

## Ultrafast Low-Voltage MEMS Switches for Optics and RF Applications

Gregory Nielson (Org. 1749-2)
Truman Fellow

### Project Purpose

The purpose of this project is to explore the use of dynamic behavior of microelectromechanical system (MEMS) switches for increasing switch performance. Performance improvements from this approach can include increased switching speed, decreased power required, and decreased voltage required.

MEMS switches of nearly all sorts have been limited to fairly slow switching speeds as well as high operating voltages (or, in the case of thermal or magnetic switches, high operating power). This has limited the applications that can be addressed by MEMS switches. We anticipate that the results of this work will be new levels of performance for MEMS switches that open new application areas to MEMS switching.

Secondary benefits of the dynamic switching techniques include possible improvements in reliability. This advantage derives from slower contact speeds and lower voltages, which, in turn, lead to less dielectric charging.

In FY 2007, the focus of this project has been to demonstrate improved switching performance in optical MEMS switches.

### Accomplishments

The focus of the work this year has been on MEMS optical switches. The primary accomplishments have occurred in demonstrating a MEMS micromirror device with world record performance and in the development of a fabrication process that allows the integration of a MEMS structure with an integrated waveguide for switching applications.

The MEMS micromirror devices were designed to specifications that were developed for ion-trap quantum computing applications. The primary driver that had not been previously achieved with a MEMS micromirror was achievement of switching speeds faster than a microsecond. With the devices we designed, fabricated, and tested, we achieved switching speeds of 225 ns. This is approximately an order of magnitude improvement over any other MEMS micromirror device that has appeared in the literature to date. This level of performance puts this device very nearly in league with acousto-optic modulator switching speeds. It is likely that with some additional refinements, switching speeds of 100 ns could be possible.

The second significant accomplishment is the development of a process flow and the fabrication of a MEMS device that incorporates an optical waveguide into the structure. This device is designed such that optical switching can be achieved by utilizing evanescent coupling. Evanescent coupling allows a switching mechanism that can be completely lossless. We have developed a process and have released structures that have combined MEMS and waveguide components. Preliminary tests of comparable MEMS structures without attached waveguides demonstrated switching times of less than 500 ns. These devices were tested with both standard as well as with high-permittivity dielectrics. The high dielectric materials have the potential to significantly decrease the hold voltage of MEMS switches (i.e., the operating voltage of dynamically operated MEMS switches).

### Significance

Through this project, we have significantly advanced the state of the art in switching speeds for MEMS devices. While the FY 2007 work was directed primarily toward optical applications, the results and concepts can be applied to any MEMS switch that can be operated in a manner that does not remove significant energy from the mechanical domain. For example, these switching concepts would be excellent for electrical relays, RF MEMS switches, and free-space and integrated optical MEMS switches, but would be inappropriate for microfluidic valves.

With respect to optical applications, the MEMS micromirrors would be ideal for scaling-up ion-trap based quantum computers (QCs). It is our understanding that such QCs require a unique set of parameters for optical switching that only this micromirror device can provide. In addition, the MEMS micromirror device we demonstrated could potentially replace acousto-optic modulators in all the various applications in which they currently operate.

The integrated optical MEMS switch has a variety of applications. This device could be used in any system that is fiber based such as telecommunications, computing, lasers, avionics, and many others. This switch has the unique ability to handle high powers since it is does not require optically lossy electro-optic materials. It also is readily applied to devices involving CMOS (complementary metal-oxide semiconductor) processing, given that the materials employed are all CMOS-compatible.

*Other Communications*

G.N. Nielson, R.H. Olsson III, P.R. Resnick, and O.B. Spahn, "High-Speed MEMS Micromirror Switching," presented at Conference on Lasers and Electro-Optics (CLEO) (invited), Baltimore, MD, May 2007, and published in *Proceedings of the Conference on Lasers and Electro-Optics (CLEO)*, p. CMP2, May 2007.

G.N. Nielson, R.H. Olsson III, G.R. Bogart, P.R. Resnick, O.B. Spahn, C. Tigges, G. Grossetete, and G. Barbastathis, "Dynamic Pull-In and Switching for Sub-Pull-In Voltage Electrostatic Actuation," presented at International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers), Lyon, France, June 2007, and published in *Proceedings of the International Conference on Solid-state Sensors, Actuators and Microsystems (Transducers)*, pp. 455-459, June 2007.

G. Barbastathis, K. Tian, W.J. Arora, A. Nichol, S. Takahashi, G.N. Nielson, and J. Hong, "Three-Dimensional Nanophotonics for Computational Imaging," presented at OSA Annual Meeting: Frontiers in Optics (OSA FiO 2006) (invited), Rochester, NY, October 2006, and published in *Proceedings of the OSA Annual Meeting: Frontiers in Optics (OSA FiO 2006)*, October 2006.

## Three-Dimensional Analysis for Nanoscale Materials Science

Ilke Arslan (Org. 8756)
Truman Fellow

### Project Purpose

The purpose of this project is to study the structure-property relationships of nanomaterials and thin films through the development and application of state-of-the-art techniques in electron microscopy. These techniques include scanning transmission electron microscope (STEM) tomography for 3-D imaging, aberration-corrected STEM for the highest spatial resolution available today, and monochromation for the highest-energy resolution spectroscopy for bonding/chemical information. The main materials systems that this project is characterizing are gallium nitride (GaN)-based nanowires and thin films in order to understand how the structure and geometry impact the functionality of these semiconductor materials.

For the thin film GaN work, we would like to understand why this solid-state lighting semiconductor can be made into devices that function despite the high density of threading dislocations. To gain some understanding of this question, we need to characterize the dislocation on the atomic scale using imaging and spectroscopic techniques. Through a combination of experimental and theoretical work, we are beginning to come to the conclusion that all of the dislocations are controlled by impurity segregation. Not all of the dislocations are deleterious, but if impurities have segregated to a particular dislocation, then the material's properties appear to be altered.

In the nanowire work, we are trying to understand the effect of constraining GaN and its alloys to one dimension, and studying the quantum effects. The material will now be dominated by surface effects, because the surface-to-bulk ratio is high. We would like to understand what these effects are, and how they impact device functionality. We will employ a combination of atomic, electronic, and 3-D measurements in the electron microscope, as well as conductivity measurements and theoretical calculations.

### Accomplishments

During FY 2007, significant progress has been made toward the project's goals and milestones. Namely, all necessary hardware and software is now installed and operational, and we have accomplished the following:

- successfully obtained three-dimensional data from GaN/AlN core/shell nanowires;
- made progress on the investigation of electronic structure at dislocation cores in GaN using electron energy loss spectroscopy (EELS);
- made progress in studying three different surfaces of GaN nanowires using monochromated low loss EELS;
- begun exploratory studies to correlate electron tomography with atom probe tomography.

From the 3-D tomography of GaN/AlN core/shell nanowires, we have been able to observe that, depending on the position of the catalyst particle (post-growth), the morphology of the nanowire is different, with the introduction of an extra facet and surface notches on the nanowires during nonideal growth. This is important because these surface defects will certainly affect the conductivity of the nanowires, and hence affect device performance. By studying

dislocations with atomic resolution sensitivity together with theoretical work, we have been able to show that the dislocations become problematic only when impurities have segregated to them. The impurity segregation causes nitrogen bonds to distort, and this distortion causes a change in the density of states that we measure using EELS. Finally, using a newly obtained holder, we have taken the first steps in correlating electron tomography with atom probe tomography on a test specimen of Ag precipitates in an Al matrix. We have prepared the tips and put them into the electron microscope for imaging, and we are now at the stage of doing tomography on these materials with both instruments. The ultimate goal will be to do this for the GaN nanowires in year three of this project.

### Significance

GaN is a direct, wide band gap semiconductor, and is the central material upon which most solid-state lighting is being developed. This is a tremendously important endeavor because the US releases approximately 130 million tons of carbon into the atmosphere yearly due to inefficient artificial lighting, and we are consuming 22 percent of the nation's electrical energy in the process. GaN and its alloys are one set of materials that present us with the opportunity to make (nearly) 100 percent efficient light, and they are therefore extremely important to understand on a fundamental level.

## Piezoelectric Properties of Arrayed Nanostructures of Zinc Oxide for Sensor Applications

David Scrymgeour (Org. 1114)
Truman Fellow

### Project Purpose

The drive toward smaller and more sensitive sensors for hazardous gas, explosive material, and biological agent detection is naturally leading toward the utilization of nanostructured materials and devices. The advantage of nanostructured sensors is that the small size leads to enhanced surface-to-volume ratios ideal for ultrasensitivity. Using piezoelectric nanostructured zinc oxide (ZnO), one can create electrically addressable nanoscale mechanical devices. Such structures can provide both actuation and sensing capabilities through the converse and direct piezoelectric responses, respectively.

The piezoelectric and electrical properties of ZnO in nanoscale geometries will be characterized using scanning force microscopy techniques and nanoscale electrical impedance measurements. The basic research will provide the groundwork for creating ultrahigh sensitivity sensors, which use the piezoelectric effect and resistive and capacitive properties. Piezoelectric sensors operate by measuring the frequency shift and resonant impedance change of the piezoelectrically generated acoustic waves. The propagation of these waves is strongly dependent upon the material/environment interface and can be shifted by surface adsorbed species. Additionally, the resistive and capacitive properties of nanostructures are profoundly affected by interaction of the surface with gaseous species. The extremely high surface-to-volume ratio, the inherently high resonant frequencies, and the surface sensitive nature of the electrical properties of these nanostructures will enable the creation of small, accurate, sensors to target specific agents (gas, explosive, biological). By using piezoelectric materials such as ZnO instead of silicon, an additional dimension of functionality and control will now be available in creating resonators and transducers for nanoscale electrical timing circuits, force measurements, filters, and sensors. Project goals include measuring both the static and high frequency piezoelectric properties of nanostructured ZnO, and exploit these properties in conjunction with studies of surface functionalization to make high sensitivity and increased selectivity sensors.

### Accomplishments

Techniques were developed to deposit ZnO nanorods controllably onto electrode patterns using dielectrophoresis. Zinc oxide nanorods are grown through solution techniques to be ~2.5 µm in length and 50–150 nm in diameter on silicon substrates. They are released from the substrates by sonication in either ethanol or water solutions and are then dielectrophoretically deposited on to the gaps in interdigitated electrodes and waveguide structures by applying an AC bias to the electrode arrays. The optimal conditions are used to controllably assemble the nanorods for resistive sensor applications and high-frequency characterization where developed.

Zinc oxide nanorods are assembled onto interdigitated electrodes in either random or aligned arrays. These structures form resistive arrays that are biased and the small current (0.1–100 nA range) is monitored as a function of environmental exposure. Initial testing of random arrays show zinc oxide to have strong interactions with volatile organic compounds

like acetone, ethanol, and dimethyl methanephosphonate (DMMP), a sarin nerve gas simulant. Nanostructured sensors showed good selectivity between the polarities of solvents, showing high sensitivity to ethanol (polar) and no sensitivity to toluene (nonpolar).

The high frequency (HF) response of ZnO rods was examined by assembling the rods across the gaps between the center conductor and the ground planes of a microwave coplanar waveguide (CPW) so that the rods are aligned with the electric field of the propagating mode of the CPW. The transmission and reflection scattering parameters of arrays of ZnO nanorods have been measured from 0.01 to 50 GHz at room temperature using a network analyzer. These measurements allow for the independent determination of the contact resistance and the nanorod resistance, from which the carrier concentration can be determined. The ZnO nanorods have charge carrier concentrations of about $10^{18}$ per $cm^3$, verifying earlier estimates from scanning force microscopy techniques.

### Significance

Previous studies of metal oxide nanowires chemically modified by surface functionalization have shown improved sensor selectivity to specific analyte species and improved contacts between nanorods and metal electrodes. However, the exact mechanism responsible for this finding is unclear because the behavior could be attributed to modification of the nanorod surface, the nanorod-metal contact, or a combination of both. The ability to measure and separate the contact resistance from the nanowire resistance through the high-frequency microwave measurement is a key research accomplishment that enables in-depth studies of metal oxide nanowire surface functionalization by separating contact resistance and nanowire resistance. Combining this high-frequency measurement technique with complementary investigations, using dielectrophoretic trapping of individual nanowires studied with scanning force microscopy techniques and nanowire sensor responses to analytes, will enable the study of surface modification by looking at contact and nanowire resistance changes, work function modification, and sensor selectivity modification. This research will make possible a more systemic approach to surface modification that will be an enabling technology for next generation nanostructured sensors.

### *Refereed Communications*

D.A. Scrymgeour, T.L. Sounart, N.C. Simmons, and J.W.P. Hsu, "Polarity and Piezoelectric Response of Solution Grown Zinc Oxide Nanocrystals on Silver," *Journal of Applied Physics,* vol. 101, pp. 014316 1-6, January 2007.

### *Other Communications*

D.A. Scrymgeour, C. Highstrete, Y. Lee, S. Howell, M. Lee, and J.W.P. Hsu, "Aligned ZnO Nanorod Arrays for Sensor Applications," presented at Material Research Society Spring Meeting, San Francisco, CA, April 2007.

D. Scrymgeour, D. Olson, and J.W.P. Hsu, "Electrical Properties of Solution Grown Piezoelectric ZnO Nanorods," presented at Material Research Society Fall Meeting, Boston, MA, December 2006.

## Passive and Active Electromagnetic Frequency Selective Surfaces for High-Power Beam Applications

Hung (Jacques) Loui (Org. 5345)
Truman Fellow

### Project Purpose

The primary goal of this research is to produce novel, reconfigurable, metal/dielectric surfaces/volumes for adaptive control over electromagnetic (EM) scattering. The idea is to embed tunable devices into the periodic unit cells of a thick metal plate, so that, collectively, the structure can affect EM beam propagation based on electrical configuration.

When configured as a shutter, the plate would deflect an incoming beam and provide EM shielding; as a lens, the plate would focus or redirect the beam; finally, as an absorber, the plate would reduce its visibility to radar detection. This and more, such as frequency filtering and beam steering, are the cutting-edge science and technology in this research.

The secondary goal of this research is to investigate EM scattering from a new class of compound frequency selective surfaces (FSS) with multiple perforations per periodic unit-cell. The objectives are to understand the physics behind the scattering processes and to develop the engineering principles for creating novel volume/surface FSS topologies.

Frequency selective surfaces have potential application in DOE Defense Programs and national security missions where low-observable antenna radomes are needed. This technology is also relevant to covert radio frequency (RF) systems and low-observable weapon systems and can

be applied to the DoD Missile Defense Agency Targets programs, providing tailored radar response. The potential of a chameleon-like surface supporting synthetic-aperture radar, stealth, and covert applications are the anticipated benefits of this project.

## Accomplishments

1. Science/Physics — We discovered that the width of phase resonances in compound transmissive structures with subwavelength slits can be controlled by making at least one slit different (dielectric filling or thickness) from the rest within a compound unit cell. Furthermore, the frequencies and occurrences of these resonances change with incidence angle and polarization.

2. Metamaterials — We showed that a cubic array of layered nonmagnetic spherical particles permits adjustment of electric and magnetic dipole resonances and produces a low-loss isotropic negative refractive index.

3. Engineering — We designed, fabricated, and characterized large-scan-angle, thick-metal FSSs comprised of a periodic array of dielectric-filled tapered holes. We demonstrated that hole tapering enhances the transmission bandwidth of a thick metal FSS plate by reducing the pass-band ripple.

4. Numerical Modeling — We developed an arbitrary order 2D finite element Eigen-mode solver, incorporating an in-house mesher to handle FSS unit-cell perforations of arbitrary cross section filled with inhomogeneous, anisotropic and gyrotropic materials.

5. Experimental Setup — We built a Gaussian beam apparatus to measure electromagnetic transmission/reflection responses from FSS/material samples.

6. Manufacturing — We utilized the wire-electrical-discharge machining (EDM) process to produce thick-metal FSSs with subwavelength slits having large depth-to-width aspect ratios.

7. Simulations — We designed antireflective surfaces in the mid-infrared using both mode-matching and method-of-moment codes. Simulations of shapes etched in silicon and coated in gold predicted over 90 percent transmission in the mid-infrared.

8. Technical Advance — Based on an understanding of gyrotropic materials and passive thick-metal FSSs, the concept of ferrite-based multipurpose FSS was developed and a technical advance has been filed.

9. Transformative Research — An extensive study of available ferrite-based devices led to a new FY 2008 LDRD project to pursue miniaturized magnetic phasers for electronic beam steering of synthetic-aperture radar.

## Significance

Significance matching each accomplishment (by number) listed above is given below:

1. Recent numerical predictions reveal that compound gratings with subwavelength slits exhibit anomalous transmission, i.e., sharp stop bands appear in the pass band. These resonances appear and shift in frequency depending on incidence angle and polarization. Accomplishment 1 provides engineering means to alter the resonance response of spatial filters.

2. Metamaterials with negative refractive index have been largely realized using variants of periodic split-ring resonators and metal rods that exhibit high loss and anisotropy. Low-loss isotropic metamaterials of Accomplishment 2 make practical the design of unconventional lenses and wave-guiding structures.

3. Thick-metal FSSs are known to exhibit angle and polarization-dependent transmission responses if external dielectric matching layers are not present. Accomplishment 3 provides an alternative way of response improvement via hole tapering for radome applications.

4. Analysis of EM scattering from thick-metal surfaces containing complex geometries requires determination of eigenvectors (large domain basis) representing EM modes of various substructures. Accomplishment 4 enables this capability and facilitates integration with future in-house scattering codes.

5. Accurate characterization of EM scattering from finite FSS samples requires a focused beam system. Accomplishment 5 provides the initial capability of measuring FSSs/metamaterials in X, K and Ka bands, and can be scaled up to subterahertz frequencies with available sources.

6. The wire-EDM process produces thick-metal FSSs with highly complex unit-cell structures. Accomplishment 6 facilitates the experimental validation of anomalous transmission.

7. FSSs at mid-infrared frequencies are extremely difficult to model due to material loss. Accomplishment 7 provides general design guidelines for improving FSS performance at these frequencies.

8. Ferrite, a low-loss gyro-magnetic material, exhibits a tunable permeability tensor via magnetic bias. Accomplishment 8 is applicable to low-observable RF antenna systems for defense applications.

9. Broadband electronic beam steering of synthetic aperture radar (SAR) is a formidable challenge. Accomplishment 9 has the potential to significantly expand Sandia's existing SAR capabilities.

*Refereed Communications*

D.C. Skigin and H. Loui, "Bandwidth Control of Forbidden Transmission Gaps in Compound Structures with Subwavelength Slits," *Physical Review E,* vol. 76, p. 016604, July 2007.

*Other Communications*

E.F. Kuester, N. Memic, S. Shen, and H. Loui, "A Double Negative (DNG) Composite Medium Based on a Cubic Array of Layered Nonmagnetic Spherical Particles," presented at North America Radio Science Meeting, United States National Committee of The International Union of Radio Science (URSI - CNC/USNC), Ottawa, Canada, July 2007.

D.W. Peters, L.I. Basilio, and H. Loui, "Plasmonic Antireflection Surfaces for the Mid-Infrared," presented at Society of Photographic Instrumentation Engineers (SPIE) Photonics West Conference, San Jose, CA, January 2007.

N. Ehsan, H. Loui, E.F. Kuester, and Z. Popovic, "Dual-Polarization Large Scan Angle Broadband Thick-Metal FSS," presented at IEEE AP-S International Symposium, Honolulu, HI, June 2007.

L.I. Basilio, D.W. Peters, and H. Loui, "Plasmonic Antireflection Coatings in the Infrared," presented at IEEE AP-S International Symposium (invited), Honolulu, HI, June 2007.

## Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

Whitney Colella (Org. 8367)
Truman Fellow

### Project Purpose

This project involves the modeling of energy systems with the aim of designing them to achieve environmental, infrastructure security, and economic goals. Designs of alternative vehicles, power plants, and building thermal management systems, along with each technology's related energy supply chain, will be evaluated. Assessment criteria for these energy systems and supply chains will include the following:

1) their impact on the environment including, a) greenhouse gas emissions, b) criteria air pollutants, c) solid waste production, d) human health, and e) energy efficiency;
2) their implications for national security including, a) the security of the fuel and energy supplied, b) the diversity of the fuel supply, and c) the dependence on foreign oil; and
3) their costs to consumers, governments, and incumbent energy suppliers.

Both mobile and stationary energy systems, as well as different types of future transportation supply chains, such as those based on biofuels, hydrogen internal combustion engines, batteries, plug-in hybrids, and fuel cells will be examined. Models of distributed energy networks will be constructed that, on the supply side, incorporate the details of fuel cell system operation and, on the demand side, incorporate the differing electricity, heating, and cooling demand patterns of American buildings. Test data for key system components derived from other Sandia programs will be incorporated.

This project will combine Sandia's unique expertise in three main areas: 1) systems engineering applied to complex networks, 2) the design of renewable and efficient energy technologies, and 3) the design of national infrastructure to increase homeland security.

### Accomplishments

We analyzed greenhouse gas emissions from cogenerative and noncogenerative power plants between 1990 and 2004 and identified a significant discrepancy (34 percent on average) between DOE and California Energy Commission (CEC) data series for California's carbon dioxide emissions from the electric power sector. We quantified the sources of the discrepancy, both omissions and inconsistencies, and the impact of the discrepancy on meeting reduction targets. We developed preliminary estimates and visual maps

showing the change in greenhouse gas emissions over time with a switch to electrically networked noncogenerative fuel cell systems.

We critically reviewed literature encompassing alternative vehicle efficiency, alternative power systems, renewable energy in developing countries, and environmental impacts of alternative vehicles

### Significance

This research has strong relevance to Sandia's environmental, energy efficiency, and national security missions. It supports the DOE's Office of Fossil Energy strategy of reducing carbon emissions that contribute to climate change by making emission accounting more precise and fossil energy systems more efficient. It also addresses DOE goals of diversifying energy supplies, modernizing the energy infrastructure, and ensuring the optimal use of energy resources, with limited environmental impacts.

Results will be documented for publication in refereed journal articles, in presentations at conferences, and in educational book chapters.

***Two individuals were selected as Truman Fellows beginning October 2007. Abstracts of their planned research for FY08 follow.***

## Multiscale Schemes for the Predictive Description and Virtual Engineering of Materials

Anatole von Lilienfeld-Toal (Org. 1435)
Truman Fellow

Dr. von Lilienfeld-Toal received his PhD at the Swiss Federal Institute of Technology and has held postdoctoral appointments at University of California at Los Angeles and New York University. His work is in the development of multiple length-scale computational tools that may be used in the molecular material design, using quantum mechanics/MD and the extension to density functional theory (DFT) toward addressing the unsolved problem of predicting crystal structures. He will apply a variational multiscale approach in optimizing material properties at the continuum scale. His vision is to apply these techniques in the development of specialized materials, such as the design of a catalyst that would convert water to hydrogen fuel. His expertise and interests will complement and enhance computational material studies being done at Sandia in areas such as high energy density physics, molecular electronics, explosive materials, energy production/storage, bio-hazards, etc. He joined the Multiscale and Dynamics Material Modeling Department (1435) in April 2007.

### Abstract

The predictive power of computational materials simulation shall be enhanced dramatically by delivering a tool which enables engineers and experimentalists not only to routinely characterize, but also to identify, customize, and subsequently also synthesize from scratch new materials which exhibit valuable and desired properties. Such in silico rational compound design (RCD) efforts are not only hampered by the difficulty of reliably predicting macroscopic properties for any given material but also by the sheer size of chemical space, i.e., the mind-bogglingly large number of all the stable and potentially interesting chemical compositions which define a material. Methods from seemingly different areas and levels of theory, such as physics, chemistry, materials sciences, applied mathematics, and even molecular biology will be combined in order to account in a rigorous way for fluctuations in chemical composition and link them to their macroscopic properties which can then be exploited for a purposefully guided exploration of chemical space. The feasibility and versatility of the underlying theory shall be evidenced by applying the devised RCD algorithms towards a prototypical materials discovery problem, namely the design of photo-catalytic surfaces that exploit sun light energy for the efficient conversion of abundant materials, such as carbon dioxide, water, or nitrogen, into energetically rich material such as methanol, methane, molecular hydrogen, or ammonia, for subsequent fuel storage, distribution, and combustion. While the potential benefit of such a tool, for science, engineering, and eventually society can hardly be overestimated, the technological and technical barriers on the way to its assembly appear immense, for the involved research fields are only now on the edge of making such a project conceivable.

## Cosmic Ray Hydrometrologic Imaging of Water Fluxes

Darin Desilets (Org. 6316)
Truman Fellow

Dr. Desilets has built a new technical field, "Cosmic Ray Metrology", the quantification of cosmic ray flux attenuation at the Earth's surface and its application to understand such things as water balances in soils, global climate change, and earthquake dynamics. Dr. Desilets also demonstrated a national security application; specifically, how the approach might be used to rapidly track the movement of large numbers of people in urban areas. He received his BS from the University of Vermont and his PhD from the Deptartment of Hydrology and Water Resources at the

University of Arizona. Dr. Desilets will be based in the Geohydrology Department (6316) where he will initially enhance the efforts of Sandia's Water Initiative—in particular basin-scale modeling of water balances in the southwestern US and potentially climinate change modeling. The expectation is that remote sensing/ national security applications of his cosmic-ray work would be pursued as well. These interactions will extend outside of Division 6000 and may involve greater interaction with Division 5000.


## Abstract

Energetic cosmic rays continually bombard Earth, with implications important to humanity. For example, cosmic-ray neutrons interact with earth materials in the upper meter of crust, producing rare radionuclides that are retained in mineral lattices. Measurements of the buildup of these radionuclides (e.g., 10Be and 36Cl) have proved to be invaluable in determining the numerical ages of geologic hazards such as pre-historic earthquakes, volcanic eruptions and landslides. Cosmic rays also produce radionuclides in the atmosphere, providing a valuable tracer for the study of atmospheric transport and mixing processes. Cosmic rays interact with microelectronic components, producing soft errors in advanced computing systems, posing design challenges to electrical engineers.

This work is centered on the novel application of cosmic rays to remote sensing of snow water equivalence and water content, two of the most important parameters in the hydrologic cycle. Surprisingly, the possibility of utilizing cosmic rays as a remote sensing tool on Earth has hardly been explored outside of the work described in this proposal, although a similar method has been employed to remotely sense water on Mars.

## SANDIA-UNIVERSITY RESEARCH PROGRAM (SURP)

Since 1958, Sandia National Laboratories has provided research-funding support to beginning faculty researchers at the University of New Mexico (UNM), the New Mexico Institute of Mining and Technology (NMT), and New Mexico State University (NMSU) through the Sandia-University Research Program (SURP). Each university researcher is partnered with a Sandia collaborator to satisfy the program's primary goals of obtaining needed scientific knowledge and technical expertise while strengthening the university-laboratory technical community in mission-relevant areas. Investment in new faculty development helps create partnerships that build long-term strength in areas deemed critical to support Sandia's Nuclear Weapons mission and its Science and Technology Research Foundations.

Funding for SURP comes from the U.S. Department of Energy/National Nuclear Security Administration's Office of Defense Programs through Sandia's Nuclear Weapons Strategic Business Unit. This program is currently part of the Nuclear Weapons Readiness in Technical Base and Facilities People Readiness workforce development portfolio. In order to ensure a close association between the faculty member and the Sandia technical collaborator, the SURP program has a matching-funds requirement for each funded research project. The Sandia collaborators view these investments as excellent leverage for their program's research dollars. Today, a new award is $40,000 per project, with $15,000 coming from the Sandia collaborator.

The SURP projects are selected for their high relevance to Sandia's research interests and mission needs. The project should complement Sandia's Nuclear Weapons Capabilities as well as its Research Foundations, which include materials and process sciences, computational and information sciences, microelectronics and photonics, engineering, and pulsed power. Projects may also include maturation and/or commercialization research support of technologies under development at Sandia. SURP benefits to Sandia include increased understanding in the subject matter explored by the projects, exposure to unique research areas, cost-effective research, and collaborative relationships between Sandia and New Mexico university faculty.

Universities and individual faculty members benefit from their participation in SURP through increased interaction with Sandia researchers, increases in faculty research production, faculty and student recruitment, grants from other institutions, experience in managing projects and student assistants, and awards, tenure, and fellowships.

While Sandia selects SURP projects based on their value to Sandia's mission-relevant research needs, the Labs also tracks the significance of the SURP projects by their contribution to the broader scientific and technical communities. Two indicators of this significance are the additional funding and follow-on work obtained by the university researchers as a result of the SURP project and the number and breadth of conferences and publications that accept SURP project-related presentations and articles. A broad collection of national and international scientific and technical organizations and journals has accepted submissions related to the SURP projects by the university researchers. The diverse fields of these organizations represent Sandia's far-reaching interests and influence.

## Development and Application of Modern Analysis Techniques to Determine Yields of Nevada Test Site Explosions Using Sandia Seismic Data

Susan Bilek
New Mexico Institute of Mining and Technology

Robert E. Abbott (Org. 1647)
Sandia Principal Investigator

### Abstract

Nuclear test detection is an important task for treaty verification. Many techniques have been developed to discriminate between an explosion and an earthquake and to determine the yield of explosions. Since 1960, Sandia has maintained the Leo Brady Seismic Network (LBSN) to record nuclear tests at the Nevada Test Site (NTS), providing a unique data set for yield determination. The LBSN is comprised of five permanent stations surrounding the NTS at regional distances, and data exists for almost all tests. In this project, we are applying modern seismic data-processing techniques to better determine the seismic yield.

### Accomplishments

The dataset consists of seismic waveforms recorded during tests at the NTS. The waveforms and source information were stored in database software (Seismosaic), which allowed easy extraction for new processing and analysis tools, such as Matlab. We completed a literature search for techniques that are currently used with other datasets or could be applied to the Sandia dataset to refine yield measurements.

To verify accuracy during data conversion to the new format and to gain confidence in choosing amplitudes, we used amplitudes from two events, 8201 (Jornada) and 7912 (Hearts) with known yields (see Table 1), and we computed the yield using the method of Garbin (1989). These two were used because they occurred in the same geographic area, a requirement for this method that compares the measured amplitudes (A):

$$Y_t = ((At/Ar)^b)*Y_r$$

Here, Y denotes yield, b is a regression constant (0.86, *Garbin* [1989]), and subscripts t and r are for test and reference events, respectively. We used Jornada as the reference event and Hearts (yield = 140 Kt) as the test event. Using amplitudes from all stations, the yield was 158 Kt with a standard deviation of 22 Kt.

*Nuttli* [1986] and *Patton* [1988b] developed a magnitude scale, mb(Lg), for explosion data. For our data, Lg amplitudes for mb(Lg) were measured on short-period radial seismograms. For the three events with published yield, this method produced yields that were low for the larger events, Chancellor (published yield 143 Kt, estimated 84 Kt) and Cybar (published 119 Kt, estimated 84 Kt), and high for the smaller event, Glencoe (published 29 Kt, estimated 36 Kt).

Short-period body-waves can be used to calculate the magnitude, mb, of an explosion.

The largest P-amplitude (A) at periods (T) around 1 Hz was measured and mb was calculated: mb = log(A/T) + Q(h,D), where Q(h,D) is an attenuation factor. Using the relation, mb = 0.75logW + 4.45, the seismic yield (W) can be calculated from mb. For three events with published magnitudes, this method produced yields that were high, likely due to the small distances and interference of the Pn and Pg phases.

Spectral modeling (*Fisk* [2006,2007]) was used to compute the corner frequency. The corner frequency (fc) and yield can be related since both scale with the elastic radius. For our events, Chancellor showed the best estimate, 150 Kt, with both Cybar (240 Kt [est.]) and Glencoe (46 Kt [est.]) showing estimates much larger than the actual yield. This could be due to a tradeoff in calculating fc — there are two free parameters that must be solved for, spectral amplitude and fc.

Using these same techniques, we analyzed events other than these three with published yields. However, because most of the yields are classified, we cannot definitively state which yield estimation method is preferred. During October 2007, we provided a table of our analyzed events (109 events) to the Sandia collaborator for review and final decisions about the feasibility of these measurements for yield estimates.

*Mayeda* [1993] presented a method of measuring magnitude using the coda, or later scattered wave energy, in the seismogram that can be used for single-station calculations. This method is useful because it can reduce site effects that can bias the Lg measurements. In addition, this method may perform better than mb and mb(Lg) because only one station is needed for measurement [*Mayeda*, 1993]. We examined the seismic dataset to explore the feasibility of using this technique, and found that several (but not all) of the waveforms in the dataset have sufficient time length to measure the Lg coda. However the technique of *Mayeda* [1993] was not fully explained in their published work, and we will need to explore, in more detail, some of the parameter definitions for the NTS dataset. This will be one focus of Year 2 research efforts.

We applied for, and have received, a second year of funding from the Sandia-University Research Program (SURP). The work for year 2 includes using Lg coda measurements (as previously described) to estimate yield, estimating the seismic energy, developing an energy-yield relationship, and compiling a catalog of synthetic waveforms and spectra to be available for future researchers. The seismic energy calculation is based on measurements from the earliest portion of the seismogram, where the highest amplitudes are located for an explosion. The codes must be ported to the system at New Mexico Institute of Mining and Technology (NMT), but they have been previously used by Dr. Schramm, which should expedite this process. In order to be used in a testing situation, an energy-yield relationship must be developed. It is possible that both the spectra analysis and waveform modeling components of the Year 1 research can be used to create synthetic data representing different explosion yields for comparison with potential new events at NTS and elsewhere.

*Presentation*

K. Schramm and S. Bilek, "Analysis of Modern Techniques for Nuclear-Test Yield Determination of NTS Events Using Data from the Leo Brady Seismic Network," presented at American Geophysical Union meeting, San Francisco, California, December 2007.

*References*

M.D. Fisk, "Source Spectral Modeling of Regional P/S Discriminants at Nuclear Test Sites in China and the Former Soviet Union," *Bull. Seism. Soc. Am.*, 96, 2348-2367, 2006.

M.D. Fisk, "Corner Frequency Scaling of Regional Seismic Phases for Underground Nuclear Explosions at the Nevada Test Site," *Bull. Seism. Soc. Am.*, 97, 977-988, doi: 10.1785/0120060186, 2007.

H.D. Garbin, "Statistical Analysis of Yield Calibration Curves at NTS," Sandia Report SAND88-3327, 1989.

K. Mayeda, "Mb(LgCoda): A Stable Single Station Estimator of Magnitude," *Bull. Seism. Soc. Am.*, 83, 851-861, 1993.

O.W. Nuttli, "Lg Magnitudes of Selected East Kazakhstan Underground Explosions," *Bull. Seism. Soc. Am.*, 76, 1241-1251, 1986.

H.J. Patton, "Application of Nuttli's Method to Estimate Yield of Nevada Test Site Explosions Recorded on Lawrence Livermore National Laboratory's Digital Seismic System," *Bull. Seism. Soc. Am.*, 78, 1759-1772, 1988.

## Nanocharacterization of Gold/Gold Contact Plates Failure in RF-MEMS Switches

Marwan Al-Haik
University of New Mexico

Hartono (Anton) Sumali (Org. 1526)
Sandia Principal Investigator

### Abstract

Mechanical properties of micro/nanoscale structures are needed to design reliable microelectromechanical systems (MEMS). This study presents a basic step toward the understanding of the reliability and failure of the gold film used for MEMS. The mechanical properties of gold film and surface damage under impact were investigated in the normal-force regime of 1–2 mN. Nanomechanical characterization of the gold films was carried out. Hardness, elastic modulus, and resistance against fatigue failure were measured by nanoindentation and nanoimpact tests. The results provide guidelines and assessment of elastic/plastic deformation, and surface impact characteristics of the gold film.

### Accomplishments

An important challenge in the reliability of this radiofrequency (RF)-MEMS is to understand contact failure. In many cases, impacts between contacting surfaces increase the contact resistance to such an extent that the device is rendered out of specifications after only a few thousand cycles. A major cause of contact failure is surface damage due to mechanical impact, asperity welding and ripping off, and chemical reactions on the contacting surfaces. A nanoscale understanding of how contacting surfaces evolve with repeated impacts is, therefore, crucial to understanding how electrical resistance in micro contacts changes with time. Figure1 shows a scanning electron micrograph (ESEM) of the test structure, which is schematically illustrated in Figure 2. The device comprises a plank supported by four folded-beam springs. Each of the springs is supported by an anchor, which is, in turn, fixed to the substrate in a raised position. The springs and the supported plank are from the same fabricated layer about 3.7 µm above the substrate. In its operation, when the device is energized electrostatically, the plank moves down toward the substrate. When the device is de-energized, the springs bring the plank back to its raised position. In this study, the geometry is not as important as the material, since the test was done only on an anchor.

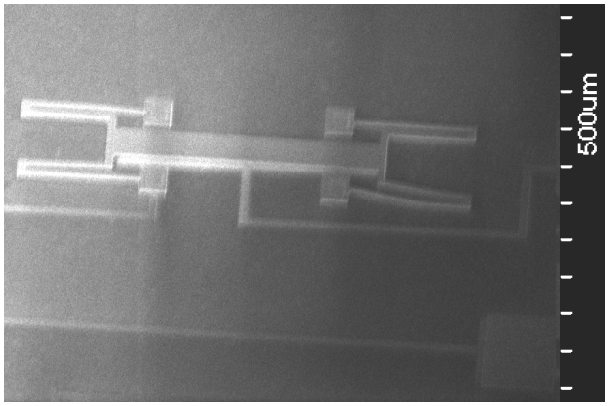



Figure 1: ESEM micrograph of the sample. Film thickness approx 5 µm.

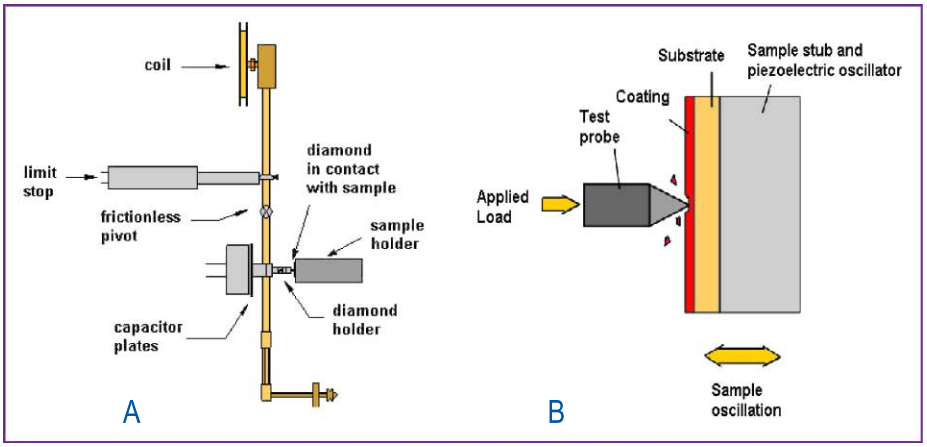



Figure 2: (A) Schematic diagram of the NanoTest system. (B) Operating Principle of the Nano-impact technique.

To test the surface failure of the gold film, it is necessary to produce an alternating contact stress with a relatively high frequency. This is achieved by the pendulum impulse technique. Essentially, for each impact, the pendulum is pushed away from the specimen by means of a small solenoid and then released to allow the probe to accelerate toward the specimen. Since the accelerating force, the distance moved, the pendulum damping, and the pendulum effective mass are known, the impact energy can be calculated. The gold film remains stationary and the pendulum is moved to create individual quantifiable impacts. The gold film damage under fatigue is shown in Figure 3B.
For the first time, nanoimpact testing was utilized to mimic the failure of

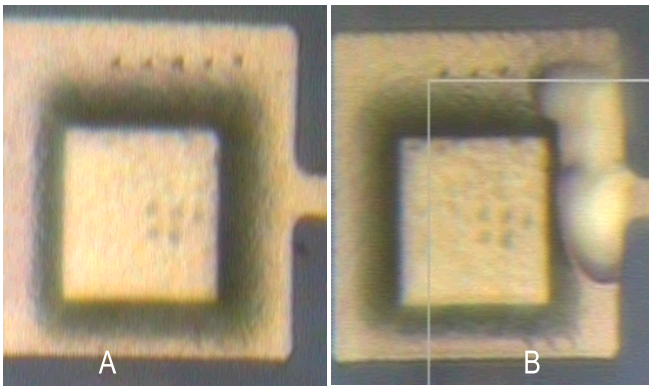



Figure 3: Optical microscope image of the raised post anchor (A) before nanoimpact test and (B) after nanoimpact tests. All images at 800x magnification.

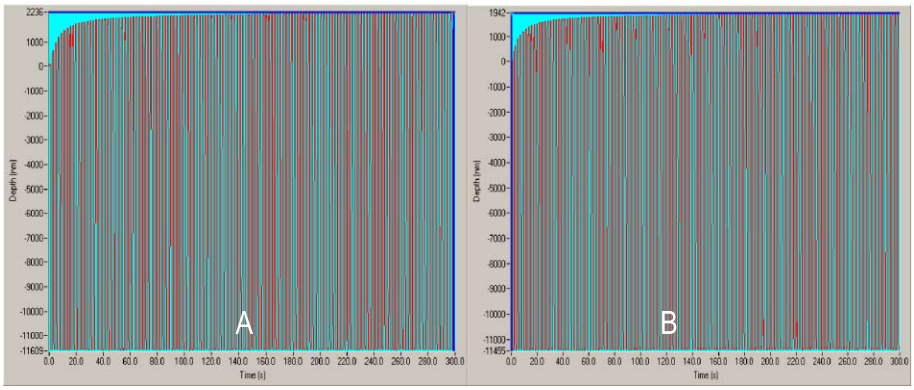



Figure 4: (A) Impact test on the 5-mm gold film. Applied load 2 mN using 25-µm Rockwell diamond probe. (B) Repeating the Impact test over the same spot reduced the depth, indicating work hardening.

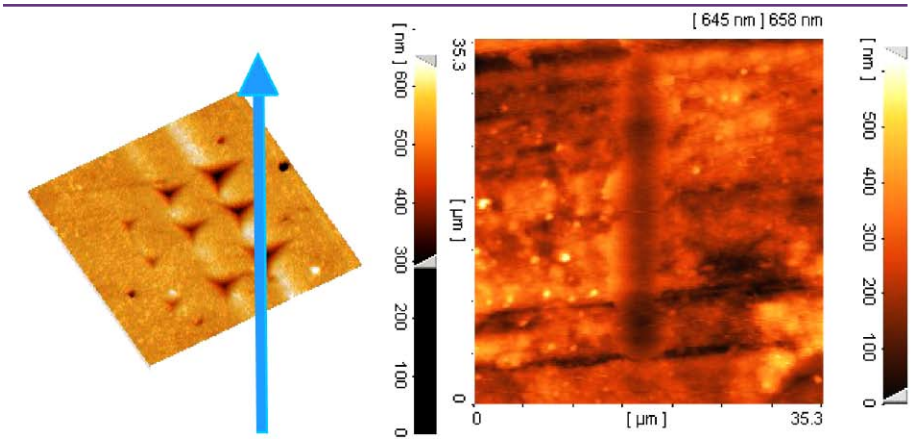



Figure 5: (A). Atomic force microscopy (AFM) scan for series of 2, 6 and 10 mN indentations on the surface of dentine, (B) AFM image for nanoscratch test performed on the surface of the silver amalgam filler. Constant scratch was carried out under 20mN for 33-µm distance.

gold films. Figure 4A shows pendulum impulse test data for the gold films. The curve actually consists of small, juxtaposed constant-depth segments obtained during a short surface dwell period following each impact. A static load of 2mN was applied throughout the test. There was no failure at this load during normal indentation testing. The Rockwell spherical diamond indenter (25 µm in diameter) was used for this test. The indenter impacted the gold surface repetitively, leading to a gradual accumulation of surface damage by a fatigue process. The impact test shows the following qualitative results: plastic deformation was produced by the first few impacts, followed by intervals of relatively slow depth increase. However, unlike the brittle material behavior there was no rapid depth increase. The results indicate ductile behavior without adhesion failure as the probe approaches the gold film. These data can be useful in deriving the work hardening information. Repeating the impact test at 2 mN over the same spot on the gold film, Figure 4B, shows a reduced depth as a consequence of impact repeat, indicating work hardening.

We limited our tests to nanoindentation and impact due to unexpected damage of the RF-MEMS switch upon removing it from ESEM facility.

Due to unexpected unavailability of hot stage, we limited our investigation to room temperature. Further investigation of impact failure of silicon cantilever beam is currently ongoing to determine through de-convolution, the effect of gold film on the beam stiffness, wear resistance, and impact resistance. This extension will be concluded as part of a Master thesis by Shane Trinkle, a graduate student at UNM Mechanical Engineering Department.

Utilizing some of the novel characterization techniques, nanoindentation and nanoscratch were employed for testing both human tooth enamel and dentine, together with two biocompatible dental filling materials; epoxy nanocomposite and silver amalgam. Nanoindentation tests were performed to obtain accurate hardness and reduced modulus values for

the enamel, dentin and two different fillers. We utilized nanoscratch tests to obtain critical load in scratch test and resistance to sliding wear. Tests showed the silver amalgam filling has a higher modulus of elasticity, hardness and wear resistance as compared to the nanocomposite. Atomic force microscopy (AFM) was performed on these samples (Figure 5). These novel mechanical characterization techniques might assist in better understanding the mechanical behavior of the dental fillers, and thus facilitate the design of robust fillers with excellent mechanical properties.

Funding to conduct basic science in the broader area of MEMS Mechanical Failure from NSF is being pursued, in collaboration with Sandia, through a joint proposal to the National Science Foundation (NSF). Independent proposals concerned with testing dental materials at the nano/microscale are under consideration by the National Institutes of Health (NIH) Division of Oral Health.

*Publications*

M. Al-Haik, H. Sumali, S. Trinkle, and J.M. Redmond, "Nanocharacterization of Gold/ Gold Contact Surface Failure in MEMS Contact Switches," in *Experimental Analysis of Nano and Engineering Materials and Structures*, ISBN 978-1-4020-6238-4. pp 621-623, E.E. Gdoutos (editor), Springer, Dordrecht, The Netherlands, 2007.

M. Al-Haik, S. Trinkle, H. Sumali, D. Garcia, U. Martinez, Y. Fang, and S. Miltenberger, "Investigation of the Nano-Mechanical and Tribological Properties of Tooth-Fillings Materials," in *Proceedings of 2007 ASME International Mechanical Engineering Congress and Exposition*, Seattle, WA, November 2007.

*Presentation*

M. Al-Haik, H. Sumali, S. Trinkle, and J.M. Redmond, "Nanocharacterization of Gold/Gold Contact Surface Failure in MEMS Contact Switches," International Conference on Experimental Mechanics Experimental Analysis of Nano and Engineering Materials and Structures, Alexandroupolis, Greece, July 2007.

# Development of a Cell-Based "Smart" Microfluidic Sensor

Heather Canavan
University of New Mexico

Ron Manginell (Org. 1744)
Sandia Principal Investigator

## Abstract

This proposal describes the development of a cell-based sensor utilizing the surface modification with poly(N-isopropyl acrylamide) (pNIPAM) derivatized with a benzo-crown ether (BCE) moiety. The unique cell-release behavior of pNIPAM-BCE, combined with the ease of manufacture of microfluidic channels and plasma polymerizations, will allow the development of regenerable, continuous flow-through sensor/actuators for the rapid detection host/pathogen interactions — the subject of Sandia's Microscale Immune Study Laboratory (MISL) Grand Challenge. The proposed research unites the unique capabilities of the principal investigator (PI) at the University of New Mexico (UNM) (the use of thermoresponsive polymers for the nondestructive harvest of cells) with those of the co-investigators at Sandia (fabrication of microfluidic arrays).

## Accomplishments

***Synthesis and characterization of pNIPAM substrates via plasma polymerization.*** Many methods have been reported to graft pNIPAM on surfaces. Previous investigations demonstrated that plasma polymerization of pNIPAM (ppNIPAM) affords a one-step, solvent-free, vapor-phase method for the deposition of ppNIPAM films that are sterile and pinhole-free, regardless of the surface chemistry or topography of the underlying substrate.

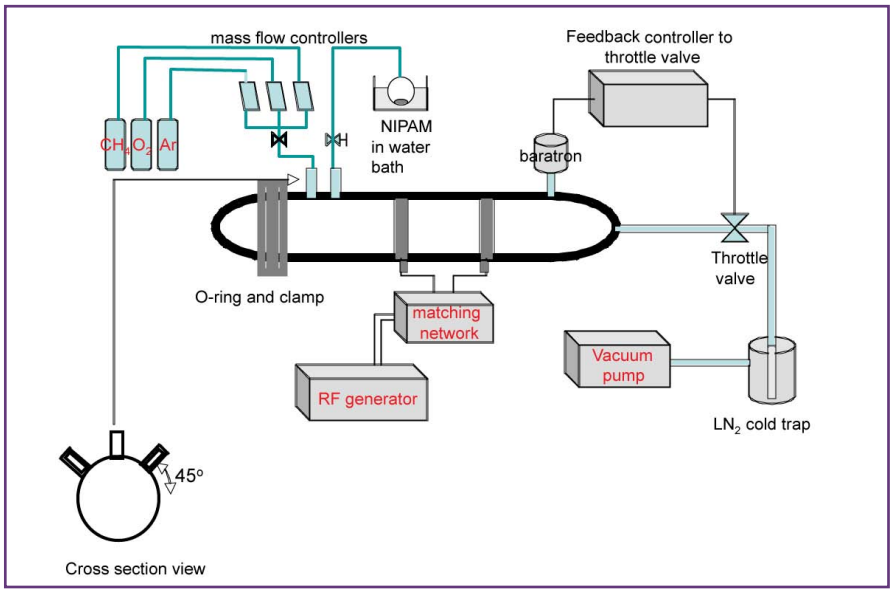



Figure 1. Schematic illustrating the rf plasma reactor constructed at UNM during Year 1 for the deposition of plasma polymerized NIPAM (ppNIPAM) and mixed NIPAM-BCE films.

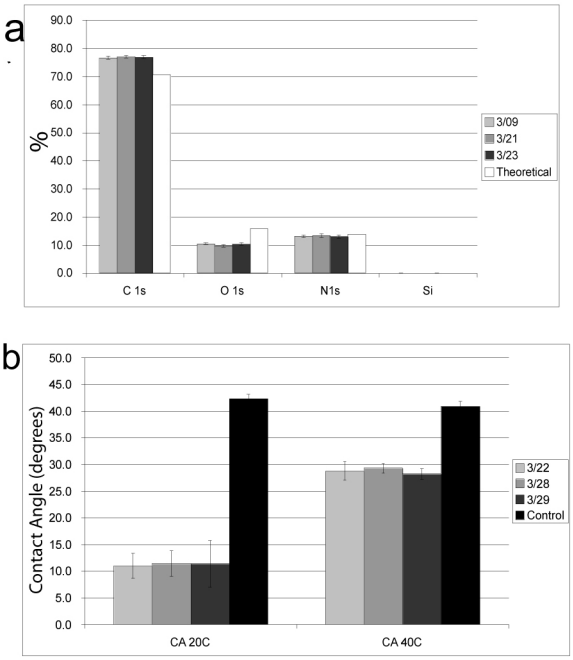



Figure 2. Plasma polymerized NIPAM films deposited at UNM were characterized for surface chemistry by XPS (a) and contact angle analysis (b). XPS indicates that the elemental composition of ppNIPAM surfaces (grey) are comparable with that expected from the stoichiometry of the monomer (white). Contact angles indicate that ppNIPAM surfaces (grey) are thermoresponsive, becoming more hydrophilic below the LCST (20 °C).

In Year 1 of this proposal, the radio-frequency (RF) plasma reactor was fabricated at UNM (see Figure 1), based on a similar plasma chamber previously used by the PI during her postdoctoral fellowship. Briefly, the apparatus consists of a tubular glass reactor capable of operating in both pulsed and continuous-wave mode,

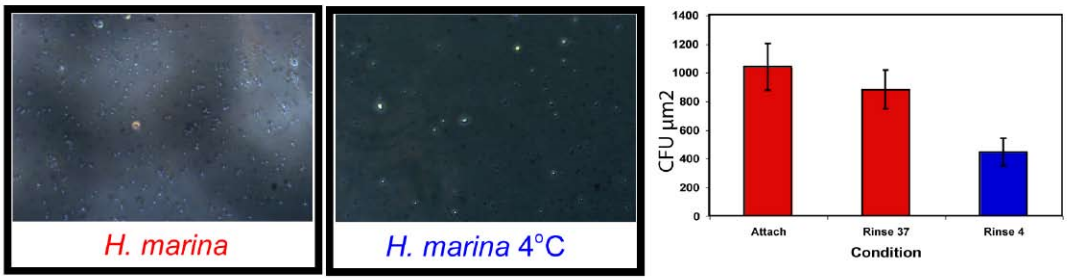



Figure 3. H. marina bacteria adhere to pNIPAM surfaces above the LCST (37 °C, left). When rinsed at below the LCST (4 °C) the bacteria detach (center). The number of bacteria detached from rinsing is shown (right).

base pressure in the low 10-$^{3}$ Torr range, and adjustable applied rf powers from 1–120 W. We have modified the design of this reactor to include multiple monomer inlet ports, thereby making it capable of the deposition of mixed copolymers such as pNIPAM-BCE.

Research has demonstrated that variations of certain key aspects of the process directly impact the mechanical and physical properties of the resulting films. In turn, these mechanical and physical changes can affect the films' biocompatibility. Therefore, the second priority of the work accomplished at UNM was the characterization of the ppNIPAM films using surface characterization tools. Using x-ray photoelectron spectrometry (XPS), the surface chemistry of ppNIPAM films deposited using this reactor were evaluated and compared to films deposited using other techniques, as well as the theoretical composition of the monomer. Using contact angle measurements and atomic force microscopy (AFM), the thermoresponsive behavior of the films was validated. As shown in Figure 2, the ppNIPAM films generated using this reactor demonstrate the proper surface chemistry and thermoresponsive behavior.

***Cell attachment and detachment from ppNIPAM substrates.***
Subsequent to the demonstration of our ability to reproducibly generate thermoresponsive films with the desired characteristics in Year 1, the cell-releasing properties of the ppNIPAM films were evaluated. Because the mammalian cell culture facilities are still under construction, we tested the release of bacterial cell cultures of *Halomonas marina*. Briefly, ppNIPAM surfaces fabricated using the procedure described above were incubated with artificial seawater containing *H. marina* cells for 3 hours at 37 ºC. To test cell release, the culture media was removed and replaced with phosphate buffered saline (PBS) at or below the lower critical solution temperature (LCST) of the polymer. The surfaces were observed using phase contrast microscopy and recorded using a digital camera such that the relative amount of adherent bacteria at each condition could be directly determined. As demonstrated in Figure 3, the ppNIPAM films generated using this reactor demonstrate the expected cell releasing properties.

Extensive construction delays of the two laboratories used for this research (Farris Engineering Center Lab 001: the Biocompatible Surfaces Laboratory, including RF Plasma Reactor; and FEC Lab 045: the Tissue Culture Facility) slowed the progress of research during year one of this proposal.

Therefore, although the plasma reactor was constructed, and the resulting films characterized with regard to surface chemistry, thermo-response, and reversible cell adhesion, we were not able to interface our pNIPAM films with the linear chip assemblies fabricated at Sandia. In the year two renewal of this project, we intend to carry out the remaining objectives, including:

1. Interface SNL's linear chip assembly with ppNIPAM;
2. Implement the thermo-responsive linear microfluidic chip (TL_C); and,
3. Implement the TL_C for the study of host/pathogen interactions.

During year one of this proposal, the research team met on three different occasions to plan experiments and to discuss the progress of the research. In addition, the graduate students supported with SURP funding traveled several times to Sandia to observe the linear array microchip's use by Sandia personnel for other experiments. During year two, such meetings are expected to continue, but with increased frequency.

*Presentations*

A.E. Lucero, X. Wu, S. Candelaria, and H.E. Canavan, "Construction and Characterization of an RF Reactor to Create Plasma Polymerized Thermoresponsive Coatings," presented at the UNM Bioengineering Student Seminar, April 2007

A.E. Lucero, X. Wu, S. Candelaria, and H.E. Canavan, "Construction and Characterization of an RF Reactor to Create Plasma Polymerized Thermoresponsive Coatings," presented at the AVS New Mexico Chapter Symposium and Exhibition, May 2007 (1st place for best student poster).

# Hyperspectral Imaging, Multivariate Curve Resolution Analysis and Multi-Color Single-Particle Quantum Dot Tracking: Elucidating Membrane Protein Dynamics in Living Cells

Diane Lidke
University of New Mexico

David Haaland (Org. 8332)
Sandia Principal Investigator

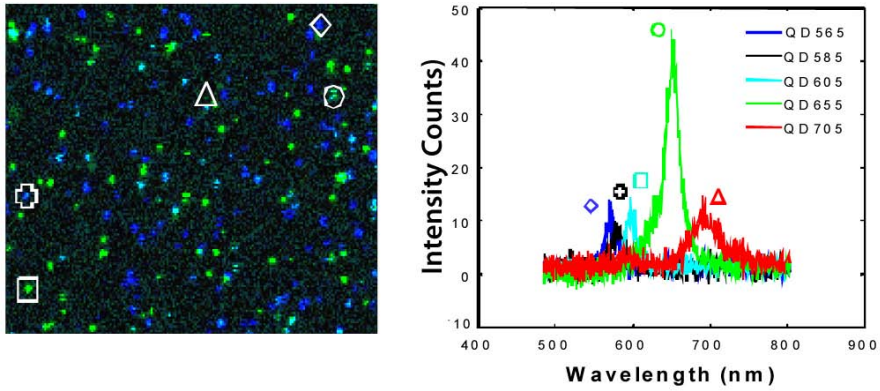



Figure 1 (Left) Image containing a mixture of five spectrally distinct QDs. (Right) Spectra corresponding to the selected points in Left image.

## Abstract

The goal of this collaboration is to characterize quantum dots (QDs) for multiplex imaging using the hyperspectral microscope(HSM) and multivariate curve resolution (MCR) analysis developed at Sandia. The techniques developed in this project will be useful for the study of many different membrane protein dynamics in living cells. In addition, advancing the use of QDs for multiplexing is important to many fields, such as diagnostics and high-throughput screening.

## Accomplishments

This work has resulted in an oral presentation by Diane Lidke at the Society of Photo-Optical Instrumentation Engineers (SPIE) Photonics West Meeting in January 2007, as well as a publication in the *Proceedings of SPIE*.

We had previously generated a QD-tagged immunoglobulin E antibody (IgE) that is capable of binding to its cell-membrane-associated receptor, FceRI, while retaining physiological activity. We have now developed a QD-based multivalent antigen-mimic that is capable of activating RBL-2H3 cells sensitized with DNP-specific IgE. We have reported identification of five spectrally distinct QDs on glass (Figure 1) and recently distinguished six classes of QDs on living cells. The algorithms for distinguishing different color QDs on cover-slip samples have been developed. The next step is to apply these similar techniques to the real-time movies of particle motion on living cells. We have recently acquired such data and analysis is under way. Our recent live-cell experiments have shown us that the microscope cannot acquire data as rapidly as we expected, and we are, therefore, currently limited at 0.25 Hz. Michael Sinclair is working on adjustments that will improve the acquisition speed. In the short term, we can achieve 1Hz, but over the next several months we hope to improve this further.

The exploration of MCR analysis techniques applied to single QDs has revealed the intriguing possibility that there is enough heterogeneity between QDs of the same class for unique identification. The implication is that we may not be limited to separating QDs by distinct color classes but can distinguish every individual QD as unique, opening the possibility for a dramatic increase in the multiplexing capability of QDs. Initial experiments with 655-nm QDs immobilized on glass coverslips confirm that the spectral peak of the QD emission for individual QDs is constant over time. Statistical analyses on the time-resolved emission spectra of individual QDs will be performed to determine if the spectral width of the emission is also invariant with time. If both spectral position and bandwidth were constant over time, it would then be possible that both these parameters could be used to track individual QDs as they migrate on or in cells.

## Significance

We have received a second year of SURP funding to continue this project. The main goals of the second year are to: 1) determine if we can separate QDs of a single class based on the small differences in each individual QD spectrum; 2) achieve faster imaging frame rates; and 3) perform live cell imaging to compare the dynamics of QD-labeled IgE receptors on resting and stimulated cells.

## *Publications*

D. S. Lidke, N.L. Andrews, J.R. Pfeiffer, H.D.T. Jones, M.B. Sinclair, D.M. Haaland, A.R. Burns, B.S. Wilson, J.M. Oliver and K.A. Lidke, "Exploring Membrane Protein Dynamics by Multicolor Single Quantum Dot Imaging Using Wide Field, TIRF, and Hyperspectral Microscopy," *Proceedings of SPIE*. 6448: 64480Y1-8, 2007.

## Application of Molecular Techniques to the Study of Microbial Biofilms

Cristina Takacs-Vesbach
University of New Mexico

Susan Altman (Org. 6313)
Sandia Principal Investigator

### Abstract
The overall objective of the project is to apply molecular microbial techniques to study the formation of laboratory biofilms and to track the integration and persistence of potential pathogens in simulated water distribution systems. The project is of a broader scientific significance because of the increased interest in the formation and persistence of biofilms, especially with respect to homeland security. This work addresses Sandia's mission in two of the five key strategic areas: Energy, Resources and Nonproliferation (ERN) and Homeland Security and Defense. By understanding the formation, persistence, and decontamination of biofilms, this work will aid in the protection and delivery of safe drinking water for our nation.

### Accomplishments
During our first year, we used two approaches to analyze biofilms. The first approach, denaturing gradient gel electrophoresis (DGGE, described below), enabled us to track the development of multispecies biofilms grown in reactors with supplemented drinking water. We determined the limits of our ability to extract DNA from the biofilms, and learned that the biofilms are highly dynamic over the period we sample. This work has made it possible for us to outline future experiments that will test the effect of various treatments on the community. We also cloned and sequenced these samples to gain a better understanding of the organisms the formed the biofilms.

The second approach we used is real-time PCR (QPCR). We developed a QPCR assay that is highly specific and sensitive for *Bacillus Cereus (B. cereus)*. The assay can detect as little as 30 cells/µL and is not affected by the presence of nonspecific template. We have now used this assay to monitor the entrainment of *B. cereus* in a *Pseudomonas* biofilm. *A Pseudomonas* biofilm was grown in an annular reactor and *B. cereus* was introduced for several days. Finally, the biofilm was treated with chlorine, to determine if there was any effect on the *B. cereus*. Our QPCR results showed that *B. cereus* numbers remained very low during the course of the experiment and that cell numbers decreased with the chlorine treatment. Our results were very similar to simultaneous monitoring by the Sandia Biofilm Laboratory using cell counts.

The methods developed are also being used for the third objective of the project, which is being conducted along with Susan Altman and Sandia researchers, Patricia Dolan and W. Graham Yelton. This project, though in its infancy, is highly interdisciplinary in its approach to investigate and detect the onset of biofilm growth in water treatment systems by probing quorum sensing (Dolan) and using microsensors to electronically monitor biofilm growth (Yelton). My role has been the identification and quantification of important organisms in the drinking-water biofilms, which will assist in identifying autoinducer molecules. For this work, we developed an additional QPCR assay to quantify *Pseudomonas* biofilm formation.

### Significance
We developed two QPCR assays that will be useful in monitoring biofilm growth for many applications.

We are currently collecting data for a manuscript to be submitted for publication.

## Quantum Dots for Melanoma Tumor Imaging

Wei Wang
University of New Mexico

Hongyou Fan (Org. 1815)
Sandia Principal Investigator

### Abstract
Malignant melanoma has become a significant public health problem especially in the United States. The development of effective new technologies for early detection and treatment of the disease has become crucial. With Sandia's strong interest and capabilities in the areas of advanced materials and biosensing, the goal of the collaborative research program is to develop clinically useful diagnostic and imaging agents for detection, and tagging for the purpose of localization, staging, tissue biopsy, and fluorescence-directed surgical removal of melanoma tumors.

### Accomplishments
Since the start of the research project on October 1, 2006, we have closely collaborated with Dr. Hongyou Fan and his research team at Sandia and have made significant progress. As proposed, we plan to design and synthesize the potent and selective a-MSH (alpha melanocyte stimulating hormone) peptides MT-I and MT-II (Specific Aim 1). We have synthesized MT-I. Meanwhile, we have synthesized the quantum dots (QDs) and immobilized them on the surface of the

QDs. Currently, we are characterizing the properties of the peptide-conjugate QDs. With the functionalized MT-I QDs, we will determine their binding affinity to the melanocortin receptor 1 (Specific Aim 2) and evaluate selective targeting efficacy of the conjugates using murine melanoma B16/F1 and human TXM13 cell lines.

The significant merit of the SURP program is that it provides a wonderful collaboration opportunity for effective interaction with the Sandia scientists. In the past six months, my research team at the University of New Mexico has actively interacted with Dr. Fan and his team. We have monthly research meetings to discuss the research progress and direction. More significantly, such interaction affords numerous opportunities for exploring new collaborations. This research lies at the interface of chemistry, materials and biology. A long-standing research interest is to develop new materials for biological applications such as disease diagnosis, molecular imaging, and drug delivery. As a synthetic organic chemist with extensive experience in biomedical research areas, the PI is in a unique position for interdisciplinary research and collaboration. The PI's research team can design and synthesize any compounds with desired properties. On the other hand, Dr. Fan and his research team have extensive experience and expertise in the development of new materials. For example, Dr. Fan and his post-doctoral researcher, Dr. Chen, have made several mesoporous nanoparticles and magnetic nanoparticles. Because of undesired properties and intrinsic structural shortcomings, these nanoparticles have poor stability in aqueous solution and tend to aggregate. Moreover, they are difficult for new functionalization. Using our expertise in drug design and organic synthesis, we have helped Dr. Fan and Dr. Chen design and synthesize


Figure 1. Structures of new ligands **A** and **B** for preparation of new functionalized nanoparticles.

new customer designed ligands A and B (Figure 1), which can be used for improving the properties of these nanoparticles and for their surface functionalization. Such functionalized nanoparticles will attract considerable interests in the fields of materials and nanobiotechnology. We also collaborate on the development of new fluorescent imaging probes for the detection of important chemicals. Recently, we have developed a highly sensitive and sensitive fluorescent reagent for the detection of highly toxic and pollutant thiophenols. To our knowledge, this is the first example of a highly selective chemical probe for thiophenols over thioalcohols. The probe will have a great potential for practical application as a useful reagent for the detection of highly toxic chemicals. We have co-authored a paper in Angewandte Chemie International Edition (see *Publication*).

## Significance

The development of highly sensitive and selective detection techniques for the discrimination of biologically active and toxic relevant molecules is of considerable importance in the fields of chemical, biological, and environmental sciences. Thiols are an important class of molecules in biological systems and chemical science. Aliphatic thiols are found in several biologically important molecules including cysteine, homocysteine and glutathione, which are associated with a wide range of biological functions. In contrast, thiophenols, albeit their broad synthetic utility, are a class of highly toxic and pollutant compounds. Symptoms of their exposure include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting by targeting central nervous system, kidney and liver. In a more serious scenario, they can result in death. A variety of methods including sensitive fluorescent probes have been reported. However, the examination of these probes reveals that most of them suffer from poor selectivity toward aliphatic thiols and thiophenols. Accordingly, a fluorescent reagent, which enables selective differentiation between thiophenols and aliphatic thiols is

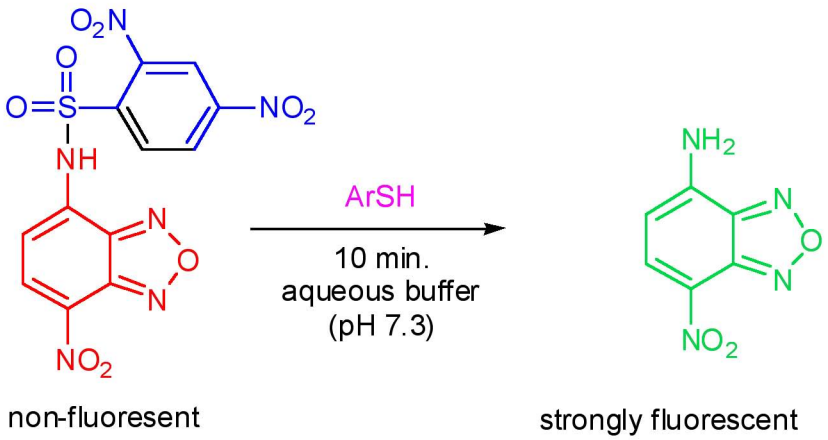



Figure 2. Fluorescent probe for thiolphenols

needed. We are fully aware that the design of such fluorescent reagents is a challenging task because of the similar chemical profiles between aliphatic thiols and thiophenols. To the best of our knowledge, such a probe has not been described. Recently, we have developed a novel sensitive fluorescent probe for highly selective detection of thiophenols (Figure 2). The studies have demonstrated that >50-fold fluorescence intensity enhancement is observed for thiophenols, but no gain for aliphatic thiols under a neutral aqueous condition. This significant finding has been recently published in *Angew. Chem. Int. Ed*.

We are developing a proposal aimed at the development of highly sensitive and selective fluorescent chemosensors for the detection of toxic chemicals and highly explosive material. This proposal will be submitted to the National Science Foundation (NSF) in November 2007.

*Publication*

W. Jiang; Q-Q. Fu, H-Y. Fan; J. Ho, and W. Wang, "A Highly Selective Fluorescent Probe for Facile Detection of Thiophenols," *Angew. Chem. Int. Ed.*, 2007, in press.

*Conference*

W. Jiang; Q-Q. Fu, H-Y. Fan; J. Ho, and W. Wang, "A Highly Selective Fluorescent Probe for Facile Detection of Thiophenols," The 63rd Southwest Regional American Chemical Society Meeting, Lubbock, Texas, November 2007 (both poster and oral presentation).

## A Neurophysiologically Testable Model of Decision Processes

James Kroger
New Mexico State University

Ann Speed (Org. 6341)
Sandia Principal Investigator

### Abstract
We sought to establish a neurally based foundation for computational modeling occurring at Sandia, in order to emulate human decision processes. In particular, our project focused on understanding how the brain enables induction of new knowledge through analogical reasoning. We observed brain activity as study subjects performed analogical reasoning problems. We designed the study with Dr. Speed, wrote protocol programs implementing an established analogical reasoning task, tested fifteen subjects, and analyzed the data over the course of the year-long project. Neural implementations of analogical reasoning to acquire new knowledge will enhance cognitive models under development at Sandia.

### Accomplishments
Our results revealed the recruitment of frontal cortex at different stages in the reasoning process, and that it is recruited to a greater extent for more complex analogical solutions. This provides more accurate goals for modeling efforts at Sandia. This work was presented at the Annual Meeting of the Society for Psychophysiological Research, and is currently being written for publication. Subjects saw an initial stimulus composed of three or four letters. This was followed by a second letter string that was the same as the first string, or had either one or three letters altered. Subjects were asked to calculate the difference between the two and deduce what series of transformations had produced the difference. This constitutes a structured representation of the transformation. The more letters altered, the deeper the depth of processing and complexity of the transformation. Subjects then saw a third, novel letter string, and were to apply the same transformation to it. Finally they saw a fourth letter string and were to indicate whether it matched the third letter string after being so transformed.

We collected both behavioral (reaction time [RT]) and EEG data. The reaction times suggest that the more complex the transformation, the longer subjects had to deliberate. This effect was most apparent in presentations 2 and 3, where RTs were significantly different between depth 0 and 1 and between 1 and 2. In presentation 4 the reaction times for D1 and D2 were longer than D0 but were not significantly different from each other. Thus, the extra demands of increased complexity impacted response time the most during the operations required for presentations 2 and 3.

The findings show that an analogical reasoning task such as the one performed elicits activations over both hemispheres, including over the prefrontal cortex, supporting the findings of previous studies. An EEG negativity around 200 ms, a positivity around 300 ms, and a negativity around 400 ms were present at most frontal and parietal electrodes. A positivity around 200 ms, a negativity around 300 ms, and a positivity around 400 ms were present in most occipital electrodes. Similarities in activity across all presentations might represent top-down control processes induced by the instructions of the task.

In the second presentation, differences across depths start to emerge. The differences across depth are most apparent in this presentation. Electrodes over the frontal pole displayed a positivity (700–1000ms) that was selectively active during presentation 2, which suggests that these processes plays a specific role in the deciphering and encoding of similarities. Likewise, the greater difficulty of more complex transformations elicited distinct activations and modulated processes that were present for all depths. Though depth did not impact reaction time at presentation 4 significantly, event-related potentials (ERPs) revealed a large effect in depth-sensitive activity (DSA).

Discovering the neural substrates for analogical reasoning created a breakthrough in this project.

### Significance
Our follow-up study is focusing on how the frontal lobe processes at work interact with attention. This is not a change, but a logical extension of the work. Executive functioning and the control of attention have been linked in higher cognitive function. This is applicable to many real-world applications. We will better assess the relationship between the two, as well as determine how sensitive our methods are at detecting the interactions between them.

As just described, we are conducting a follow-up SURP project. Dr. Speed and Dr. Kroger joined in a proposal to DARPA this year. Dr. Speed submitted a proposal to NIH.

### *Presentations*
J.K. Kroger, A.E. Speed, J.P. Anderson, E.J. Mikkelsen, D.K. Spring, and A.L. Polsky, "An ERP Study of Analogical Reasoning," Annual Meeting of the Society for Psychophysiological Research, Savannah, GA, 2007.

## The Role of Emotion and Emotion Regulation in Decision Making and Action in Critical Situations

Bruce W. Smith
University of New Mexico

Michael L. Bernard (Org. 6341)
Sandia Principal Investigator

### Abstract
The purpose of this research and development effort is to focus on what is a significant technical gap in existing modeling and simulation capabilities: the representation of trait and state emotion in humans. This proposed effort will provide the empirical data and framework for modeling: (1) the eliciting of strong emotions related to high-consequence events (e.g., terrorism, disasters, epidemics); (2) the effect of emotions on the inhibition or facilitation of decision-making in these situations; and the (3) the effects of emotion regulation strategies on effective decision-making.

### Accomplishments
a. **Review paper.** We wrote a review paper detailing the current state of research and theoretical work on the influence of emotion on decision-making in critical situations. This paper will be revised for submission to a peer-reviewed journal.

b. **Indexed electronic library**. We created an indexed electronic library of published literature relevant to emotion and decision-making, covering the fields of clinical and cognitive psychology, public policy, and economics. This electronic resource currently consists of over 500 peer-reviewed journal articles and chapters. Target literature areas were identified through collaboration with psychology, public policy, and economics researchers at SNL and UNM.

c. **Critical situation experimental scenarios.** Drawing upon the expertise of Dr. Elizabeth Yeater of the UNM Department of Psychology and her Trauma Lab, we developed 12 scenarios depicting emergency and disaster situations which are aimed to simulate situations that may involve strong emotions and call for decision-making. These scenarios depict a variety of situations including response to a flu pandemic, terrorist attack, urban sniper fire, chemical spill, and crowd riot.

d. **The Relationship between Individual Differences, Appraisals, and Emotions in Critical Situations.** Using these scenarios, we examined the correlations between measures of individual differences (neuroticism, resilience, emotional suppression, and mindfulness), appraisals of the situation itself (the ability to predict what will happen, the ability to control the outcome, the effort required to deal with the situation), and the emotional response (assessing several specific emotions) to the situations in 40 first responders (e.g., fire firefighters, police officers, and emergency medical technicians).

With regard to individual differences and appraisals, we found that neuroticism was related to decreased appraisals of prediction and control; resilience was related to increased appraisals of control; and mindfulness was related to increased appraisals of prediction and control. With regard to individual differences and emotions, we found that neuroticism was related to more anger, fear, frustration, and disgust; resilience was related to more pride and less fear and sadness; emotional suppression was related to more disgust, guilt, sadness, anger, and shame; and mindfulness was related to more happiness and less guilt.

Finally, with regard to appraisals and emotions, the ability to predict what will happen was related to hope; the ability to control the outcome was related to less frustration; and the amount of effort required was related to greater challenge, hope, surprise, fear, frustration, anger, and disgust.

e. **The Effects of Emotion and Pain on Decision Making in First Responders.** We tested the influences of induced emotions and pain on first responder decisions in emergency and disaster situations. We examined the effects of anger, fear, happiness, and pain on the ability to generate effective decisions in response to five of the scenarios described above. Showing pictures that have been validated for these emotions induced anger, fear, and happiness. Pain was induced using the cold pressor test. Although the emotion inductions did not appear to affect decision-making, the induction of acute pain was related to decreased decision-making effectiveness.

### Significance
The major breakthroughs are alluded to in the above descriptions, but specifically:

1. We developed realistic scenarios of the kinds of critical situations that first responders face. These scenarios may be useful for future research.

2. We found that neuroticism, resilience, emotional suppression, and mindfulness appear to be important predictors of the appraisals and emotions of first responders in the context of critical situations. The implication is that these individual differences may have important implications for the decisions that first responders make and for their emotional consequences.

3. We found that acute pain was related to less effectiveness in decision-making. The implication is that future research should seek to better understand the effects of pain on decision-making.

There are three major changes in research direction:

1. We plan a more thorough assessment of the individual differences that may affect first responders and their ability to make decisions in the context of critical situations.

2. We plan a follow-up study to examine the effects of pain during decision-making rather than prior to decision-making.

3. We plan to use a time-limited experimental paradigm to examine decision-making when first responders are under pressure to make quick decisions.

We plan to apply for the following grants:

1. National Institutes of Health — "Prevention of Trauma Related Adjustment and Mental Disorders in High-Risk Occupations." This is a special RFA (request for application) with dues dates on 3/24/08 and 11/21/08.

2. National Institutes of Health — "Mental Health Consequences of Violence and Trauma." This is an ongoing program with applications accepted up to 2009.

## Integrating Design and Construction Processes to Reduce Project Delivery Time

Susan Bogus
University of New Mexico

Steve Fattor (Org. 10825)
Sandia Principal Investigator

### Abstract
Development of best practices and technologies to improve the management of General Plant Project (GPP) processes at Sandia can lead to improved project performance, including cost and schedule performance. Conducting a thorough search of current literature in Construction Engineering and Management developed best practices. Building Information Modeling (BIM) technologies were specifically considered for use in the Project Definition stage. The use of BIM can provide better information for decision-making at the early stages. Additionally, it provides better visualization to improve the understanding of the project by the client and other stakeholders.

### Accomplishments
The purpose of the research was to analyze the application of current best practices and technology in the improvement of GPP projects for Sandia. In this initial stage, a focus was placed upon the Project Definition (PD) phases (i.e., project development and pre-design stages in the GPP process). From the analysis of the GPP process map and conversations with Sandia personnel, we observed that more integration and a formal methodology could be used to improve the current execution of the PD phase of the GPP process. From the literature regarding best practices in PD, a methodology was recommended that aims to include all stakeholders and provide solution-neutral specifications that will identify the client requirements.

Also, the use of BIM was suggested as a way to perform early engineering to improve the decision-making and accuracy of the PD phase. Other benefits are also expected from the use of BIM, such as improving the understanding of the project, particularly to people that are not experienced in design and construction; reliable and easily extractable documentation of the design intent; improved communication among stakeholders; and a higher degree of accuracy in the information.

Finally, recommendations on future research to measure the success of the PD improvements were provided. This could take place in the form of multiple case studies that aim to measure the satisfaction of the project stakeholders in the short term; and compare the performance of past and future projects at different stages of the project with quantitative and qualitative measures.

The research direction changed mid-way through the project because of a request from the office of the Sandia collaborator. The Projects Office was interested in potential applications of BIM in the GPP process, so the research was re-directed to focus more on best practices for BIM.

### Significance
As a result of the SURP proposal review process, I was introduced to SNL researchers in other groups. One of these researchers, Cynthia Phillips, Org. 1412, has become a collaborator on a different research project with the University of Colorado and the National Science Foundation. Dr. Phillips introduced expertise in optimization algorithms that we are using to evaluate alternative scenarios for overlapping sequential design activities to reduce project delivery times. The work on which Dr. Phillips is collaborating will likely result in a future journal article and form the foundation for a future proposal to the National Science Foundation.

## Optimal Resource Deployment in a Microgrid

Joydeep Mitra
New Mexico State University

John Boyes (Org. 6251)
Sandia Principal Investigator

### Abstract

A microgrid is an electrical network connecting distributed energy resources to the load centers such that the network can provide reliable service to its customers under both grid-connected and islanded conditions. This project consisted of developing a method to determine strategies for optimally deploying distributed energy resources (DER) within a microgrid so as to meet pre-specified reliability criteria. The research included development of suitable reliability models for different types of DER technologies. This work is part of the research that will enable the realization of reliable and secure power systems. The method was demonstrated on a surety microgrid test system, resembling a military base, provided by Sandia National Laboratories.

### Accomplishments

In this project, a method was developed to determine strategies for optimally deploying distributed energy resources (DER) within a microgrid so as to meet pre-specified reliability criteria. The strategy would specify the optimal location, size and mix of different DER technologies that must be deployed in a microgrid in order to meet pre-specified reliability targets, both system-wide and at specific locations in the system. A deployment strategy determined by the method would be optimal, in that it would meet the reliability targets at minimum cost. For the purpose of demonstrating the method developed, the Sandia team provided the NMSU team with a test system that resembled a military base, and named it 'Base Alpha' (a schematic is shown in the appendix). The system data made available to the NMSU team was also typical of the kind of data generally available for military bases.

The problem for this project was posed as follows: "If a microgrid had to be augmented by different types of DER so as to meet specified reliability targets, what size and mix of such resources should be installed at each candidate location in the system in order to achieve the necessary expansion at minimum cost?"

***Problem formulation:*** Consider a system with $N_B$ nodes, $N_G$ generators, and $N_T$ feeders. It is desired to improve reliability system-wide and, if necessary, at selected locations (such as hospitals, process plants, military installations) by installing DER at suitable locations in the system. The network constraints and the stipulated reliability criteria cause the problem to be one of nonlinear optimization. For this situation, the nonlinear optimization problem consists of minimizing the objective function (total annualized costs) subject to operational constraints and reliability targets.

In general, DER is classified into three categories—intermittent (e.g., photovoltaic —PV—and wind), dispatchable (e.g., gas turbines, diesel generators, microturbines, fuel cells) and storage (e.g. batteries). Some intermittent resources can be combined with storage to behave as dispatchable resources. A PV module in parallel with a battery of appropriate size can be treated as a dispatchable unit[1]. In a military application, it would be feasible to attach sufficient storage to render it almost completely dispatchable. For the purpose of the method presented here, we will consider a framework where every resource is capable of being dispatched, either independently or as a suitable combination of an intermittent resource and a storage resource.

The costs incurred in the deployment, operation and maintenance of the new resources in the system constitute the objective function. This is formulated as shown below.

The total annualized cost can be expressed as follows.

$$Q = Q_1 + Q_2 + Q_3$$

where
$Q1$ = annualized capital cost of deploying the required amount of DER
$Q_2$ = annual O&M cost for the required amount of DER
$Q_3$ = annual cost of fuel consumed by the augmented system

The capital cost component $Q_1$ is formulated as follows. Let $J_1$ be an $N_B$ 2-dimensional matrix of deployment cost. The first column of the $i^{th}$ row of this matrix is the cost of deploying a unit of dispatchable resource at the ith node. Second column is the cost of deploying a unit

[1]PV-battery-inverter combinations have been used in several situations for "limited-dispatchability" applications, such as peak shaving. A laboratory setup with several components—PV, supercapacitors, inverter, signal conditioners—has been built in the Power Systems Laboratory at New Mexico State University by groups of undergraduate students in several capstone projects. This setup is designed to provide considerable flexibility in terms of "dispatchability" and is being improved upon by more students.

of the PV-battery module at the $i^{th}$ node. The solution space Gnew is a selection of the size of each type of DER at every node; Gnew is a vector of size $N_B$ 2. Then the annualized cost Q1 for deploying the resource in such a system is given by

$$Q_1 = r(J_1^T \cdot G^{new})$$

where
$r$ = rate of depreciation per year
$J_1 = N_B$ 2 matrix of deployment cost per unit of DER.

The O&M cost component $Q_2$ is formulated as follows. A cost matrix $J_1$ of size $N_B$ 2 is developed to account for all other annual costs like operation and maintenance per unit capacity, as before. The corresponding cost per year is

where $J_1 = N_B$ 2 matrix of operation and maintenance costs per unit of DER.

The cost of fuel consumption per year will be

$$Q_3 = j_p \left[ l\left(\sum_{i=1}^{N_B} D_i\right) - \left( \sum_{i=1}^{N_B} A^i \cdot G^{new}(i,2) \right) \right] 8760$$

where
$\sum$ = load factor for the system
$D_{-i}$ = the load at bus i.
$A_i$ = availability of the PV module at $i^{th}$ bus
$j_p$ = cost of a unit of power

The optimization problem can be expressed as follows.
Minimize

$$Q = Q_1 + Q_2 + Q_3$$

Subject to:

$$A_n \geq R_0^n$$

where
$An$ = availability at bus $n$
$R_0^n$ = minimum reliability (availability) desired at bus $n$.

The availability [1, 2] is determined from the sum of probabilities of the first and second order contingencies leading to system loss of load. Assuming that in a system of this size the power flows can be represented by a transportation model[2], system loss of load can be determined from the following.

$$\text{Loss of Load} = \text{Min} \left( \sum_{i=1}^{N_{bus}} C_i \right)$$

subject to:

$$\hat{A}^T F + G + C = D$$
$$G \leq G^{max}$$
$$C \leq D$$
$$|F| \leq F_{max}$$

where
$D = N_B$ vector of bus load
$C = N_B$ vector of bus load curtailments (load not met)
$G_{max} = N_B$ vector of available generation at buses
$F_{max} = N_T$ vector of flow capacities of transmission lines
$\hat{A} = N_T \_ N_B$ element-node incidence matrix.

If the minimum curtailment is zero, the contingency does not result in a loss of load, i.e., a feasible dispatch exists. Otherwise, the probability of the contingency contributes to the system unavailability index.

## Significance

The major contribution of this research consisted of developing a solution strategy to solve this computationally intensive nonlinear optimization problem. Traditional analytical methods like dynamic programming tend to take inordinately long times to solve problems of this size. In this research, a method of equivalent injections is developed that linearizes the problem, and makes it amenable to solution by standard linear programming algorithms. This method has a much lower time complexity than traditional nonlinear optimization or even heuristic methods. The results are validated by simulated annealing which is a proven heuristic approach.

*Linearization method:* This section describes the method of equivalent injections, which eliminates the nonlinearity in the constraints, thereby reducing the complexity of the problem. This is achieved by first building a probability distribution of curtailed power for every bus, and thereby determining the capacity augmentation required at every bus to meet the stipulated reliability criteria. This is described below in detail.

*A. Probability distributions of curtailed load:* At every bus in the system, a probability distribution of curtailed power is constructed. For every contingency in the system a power flow is solved to determine the curtailment at the buses. A distribution function is generated with the statistics generated. Figure 1 depicts a typical distribution of curtailed power. The intercept on the probability axis is the availability at that bus. (By definition, the *availability* is the probability of zero curtailment). To increase the availability to meet a stipulated criterion, the corresponding curtailment should be balanced by an equal amount of power injection, which must come from the newly added DER. In other words, this is an additional power injection capacity required at this bus. This process is repeated iteratively until the required reliability criteria are satisfied.

[2]The justification for using a transportation model for the 'Base Alpha' system was discussed in [3].

*B. Linearized optimization problem:* It is now necessary to determine the new power flow solution, subject to network constraints, that will result from additional power injections at all the buses that are necessary to meet the stipulated reliability criteria. The initial nonlinear constraint is eliminated by transforming the reliability target into a capacity augmentation problem. As shown in Figure 1, $C'$ is the deficit capacity which when supplied at bus n can help meet the reliability target [4]. Eliminating the nonlinear reliability constraint, the new optimization problem can be written as shown below.

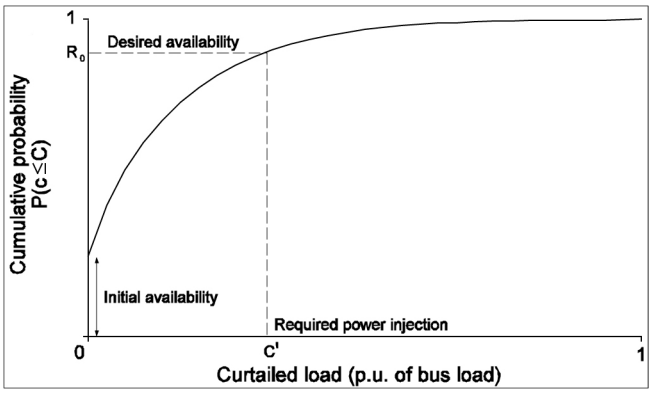



Figure 1. Sample Probability distributions of curtailed load

Minimize Cost =

$$r(J_1^T \cdot G^{new}) + J_2^T \cdot G^{new} + j_p \left[ l\left(\sum_{i=1}^{N_B} D_i\right) - \left( \sum_{i=1}^{N_B} A^i \cdot G^{new}(i,2) \right) \right] 8760$$

Subject to:

$$\hat{A}^T \Delta F + G = C'$$

$$G_i \le \sum G^{new}(i,1) + G^{new}(i,2)$$

$$\left| \Delta F + F^* \right| \le F_{max}$$

where

$F^*$ = feeder power flows computed from the previous iteration.

$\Delta F$ = change in bus power flows in the feeders.

*Simulated annealing optimization:* The results obtained from the method described above were validated using an implementation of the Simulated Annealing (SA) method. SA is a stochastic global optimization technique which has an asymptotic convergence to the global minima [5]. This method can get over the local minima as we not only consider downhill moves but also uphill moves with a probability based on the metropolis criteria. The implementation of simulated annealing based algorithm for the resource optimization problem is described in [6].

The solution space is the continuous space with limits zero and the total deficit capacity in the system. The solution space might have a lot of local minima and few global minima. In the search, if only downhill moves are allowed, the search will get trapped into local minima. So the initial acceptance probability of uphill moves is chosen reasonably high. Every time we sample a random solution in the current neighborhood. Initially the neighborhood is chosen very large and is reduced depending on the current global solution. The solution neighborhood finally gets concentrated around the global minimum.

The Sandia team is now interested in working with the NMSU team in converting the research-grade software developed in this work to a more user-friendly format, and disseminate it through Sandia and DOE web sites. Discussions regarding further research collaboration and additional funding are in progress.

### *Publications*

M. R. Vallem, J. Mitra, and S. J. Ranade, "A Reliability-Based Method for Optimal Deployment of Distributed Generation in Microgrids," in *Proceedings of International Conference on Power Systems,* Bangalore, December 2007.

M. R. Vallem and J. Mitra, "Siting and Sizing of Distributed Generation for Optimal Microgrid Architecture," North American Power Symposium, pp. 611-616, Ames, October 2005.

*References*

*IEEE Tutorial on Electric Delivery System Reliability Evaluation.* IEEE, 2005. Editor: J. Mitra. IEEE Publication No. 05TP175.

C. Singh and R. Billinton, "System Reliability Modeling and Evaluation," Hutchinson of London, 1977.

J. Mitra, "Storage Optimization in a Microgrid," complete report on SURP FY2006 project, submitted to J. D. Boyes and A. Akhil, Sandia National Laboratories, October 2006.

M. R. Vallem, J. Mitra, and S. J. Ranade, "A Reliability-Based Method for Optimal Deployment of Distributed Generation in Microgrids," in *Proceedings of International Conference on Power Systems,* Bangalore, December, 2007.

P. J. Van Larhooven and E. H. Aarts, "Simulated Annealing: Theory and Applications," Springer, 1987.

M. R. Vallem, J. Mitra, "Siting and Sizing of Distributed Generation for Optimal Microgrid Architecture," North American Power Symposium, pp. 611-616, Ames, October, 2005.

Appendix

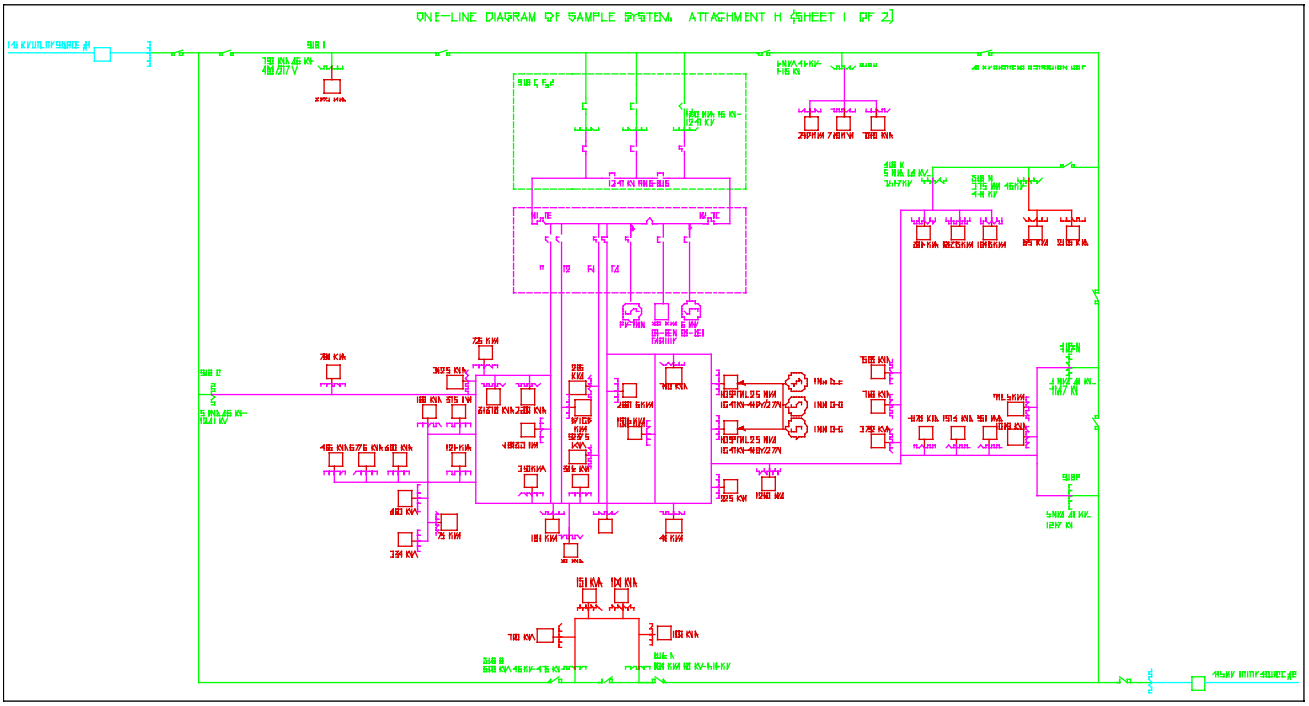



Figure A.1. Original schematic for Base Alpha.

## Self-Sealing Liners for Desalination Evaporation Ponds

Manoj Shukla
New Mexico State University

Patrick V. Brady (Org. 6316)
Sandia Principal Investigator

### Abstract
The disposal of wastes resulting from desalination processes in evaporation ponds lined with clay-based materials is inexpensive. However, an increase in the concentration of saline wastes due to the evaporation reduces the resistance of clay-based lining material to flow, with apparent decrease in the thickness of diffuse double layer and increase in hydraulic conductivity of the lining medium. Consequently, salinity in underlying layers builds up and increases the risk of groundwater pollution. Development of a low-cost, self-healing liner system can minimize the seepage through the bottom of an evaporation pond by precipitating some of the ions and may be a cost-effective solution.

### Accomplishments
The objectives of this research were to: (1) determine the effect of solution electrical conductivity (EC) on the saturated hydraulic conductivity ($K_s$), and (2) identify a lining material of low $K_s$ that could be used to minimize the leaching of saline wastes from evaporation ponds into the groundwater. The materials used in these laboratory experiments were the following: sodium silicate, magnesium hydroxide, and calcium hydroxide as lining materials, and soil from Tularosa Basin and a surrogate soil as the porous medium. A total of 82 columns were packed with either a layer of lining material sandwiched between soil layers or a homogeneous mix of lining material and soil.

The results showed that the $K_s$ of the porous medium was inversely related to the bulk density. The $K_s$ of the surrogate soil without lining material increased with increasing EC likely due to reduction in the diffuse double layer. The change in $K_s$ of the surrogate soil with changing concentration was low, most probably due to the low clay content of the soil. The $K_s$ of the Tularosa soil decreased over time, probably due to the presence of calcium or magnesium elements in the soil that precipitated after reacting with ions present in the solution.

The $K_s$ of the porous medium with the soil and soil-lining material mix showed a divergent response, in some cases increasing with increasing EC, while in some others especially in the layered columns, decreasing with increasing time. We hypothesize that the decrease in $K_s$ through layered columns could be due to the continuous high-density layer that acts as a barrier within the porous medium to the mass flow. Consequently, it can increase the formation of precipitates due to the higher resident time for the chemical reaction between lining material and the ions in solution. Solutions with high EC could further enhance the precipitation process of a material within the pore spaces and decrease the movement of fluids through the pores.

Overall, $K_s$ was lower in the layered than the homogeneous columns and layered columns seemed to inhibit the movement of fluids more effectively than the columns packed with the homogeneous mix. The lining material in the homogeneous mix could be dispersed and unable to fill the pore spaces uniformly with precipitates to retard the flow. The analysis of precipitates is currently ongoing at Sandia.

### Significance
This study showed that the arrangement of the lining material within the porous medium influenced the $K_s$. The $K_s$ was lower in columns with layers than in columns packed with the homogeneous mix. The layer seemed to provide a larger surface area where the insoluble precipitates were formed. In contrast, lining material in the homogeneous mix did not fill the pore spaces uniformly to prevent the water movement.

Increasing bulk density of the porous medium decreased the $K_s$. Columns with low bulk density had a high $K_s$, and $K_s$ was low in columns with high bulk density. The $K_s$ of porous media decreased with time for all ECs ranging from 0.5 to 30 dS/m. The reduction of $K_s$ with time indicated that the amount of precipitate formed between the pore spaces probably increased due to the increased reaction time between ions in the lining material and the ions present in the solution.

Based upon the reduction in $K_s$ values, the layer consisting of magnesium hydroxide and sodium silicate was identified as the best lining material in columns packed with the surrogate soil. However, the layers of calcium hydroxide and magnesium hydroxide were found to work better than the sodium silicate layer for columns packed with the soil from Tularosa basin. Thus, the layer of a lining material would be more effective to reduce the $K_s$ in the evaporation ponds.

A surrogate soil was used in most of the bench experiments to determine the self-sealing capacity of the lining materials. The surrogate soil was included in the study because permission to collect undisturbed and disturbed soil samples from Tularosa Basin Desalination Research Facility was not granted. The study proposed a second bench experiment to test the

behavior of the lining materials in undisturbed rectangular soil blocks to be collected from the Tularosa Basin Desalination Research Facility. The undisturbed rectangular soil blocks could not be collected due to the final stages of construction occurring at the Tularosa Basin Desalination Research Facility. Therefore, loose soil samples were collected from a site located close to the Tularosa Basin Desalination Research Facility and were used to conduct additional bench experiments. The initial results showed that the $K_s$ decreased with time. More replicated bench experiments will be performed with the loose soil and these experiments will be conducted for a much longer duration, for example, one day, three days, one week and two weeks using an antiscalant (Nalco Perma Treat PC-19), a chemical compound used in desalination process that is present in the saline wastes to determine the lowest possible $K_s$ using layers of calcium hydroxide, magnesium hydroxide and sodium silicate. These experiments will be carried out to more closely replicate some of the conditions in the evaporation ponds.

*Presentation*

A.M.González, S.A. León, M.K. Shukla, and P.V. Brady. "Effect of Solute Concentration on Saturated Hydraulic Conductivity," New Mexico Water Research Symposium, New Mexico Water Resources Research Institute, Socorro, NM, 14 August 2007.

## Aquifer Analog Modeling using Ground-Based Lidar Surveys in Support of DOE-BES Proposal — Investigation Into the Relationship between Heterogeneity and Heavy-Tailed Solute Transport

Gary Weissmann
University of New Mexico

Vincent Tidwell (Org. 6313)
Sandia Principal Investigator

### Abstract

When modeling groundwater solute or contaminant transport, we typically assume that heterogeneities below the model resolution average solute movement to produce a Gaussian-shaped solute distribution. Many studies indicate that the Gaussian breakthrough is not the norm, and that most observed breakthrough events display heavy-tailed solute distributions. Thus, our assumptions about the affect of heterogeneities below model resolution require revision. In this work, we used lidar imagery of outcrop-scale heterogeneity to populate highly resolved groundwater models in order to evaluate the influence of small-scale heterogeneity on solute movement. Additionally, we also evaluated the influence of sediment texture on transport behavior.

### Accomplishments

Using terrestrial, backpack portable lidar technology, we are able to efficiently acquire precise high-resolution facies geometries and juxtapositions as well as grain size distributions at the outcrop scale. The lidar scanner at the University of New Mexico uses infrared laser pulses to produce a highly resolved (< 5mm) three-dimensional image. For each point measured, the scanner also records the strength of the return signal (laser reflective intensity) to produce grayscale images that we calibrate to lithology, grain size, and surface roughness, where the latter can also be evaluated within the 3D lidar point cloud data set by examination of data dispersion with respect to a mean surface fit to the data.

In the first year of this study (this work will be continued under a joint DOE-BES [Basic Energy Sciences] grant), we collected lidar scans from numerous outcrop exposures in the Albuquerque, New Mexico, area (Figure 1). We successfully applied segmentation approaches using live wire and threshold segmentation algorithms in order to distinguish various lithologic types from the high-resolution (2 mm) outcrop scans (Figure 2). By applying reasonable hydraulic conductivity values for sand or gravel (0.001 cm/s and 0.1 cm/s, respectively), and populating a groundwater model with conductivities based on the lidar scan, we produce steady-state velocity fields that capture the influence of this fine-scale heterogeneity (Figure 3). Pathline analysis, using MODPATH, shows the strong influence of gravel interbeds, where most of the groundwater flow is focused through these beds (Figure 4). The non-Fickian breakthrough observed from this model is striking (Figure 5) and will be used by collaborators at Colorado School of Mines and Sandia to evaluate transport through this sediment type. Additionally, collaborators at Sandia are planning to construct a scale model of the sedimentary structure in order to validate these modeling results.

Though these models offer an indication of the influence of heterogeneity at small scales, assumptions behind these models must be evaluated more fully. First, these are two-dimensional models, thus, the influences of heterogeneity and

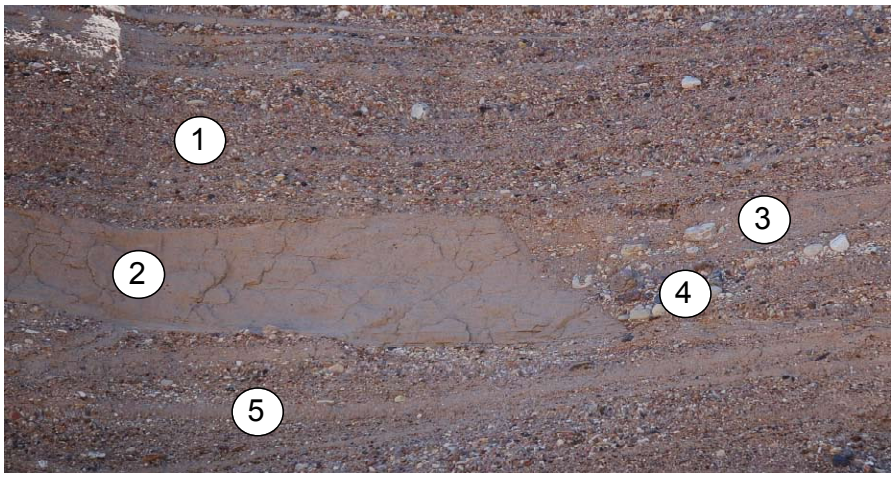
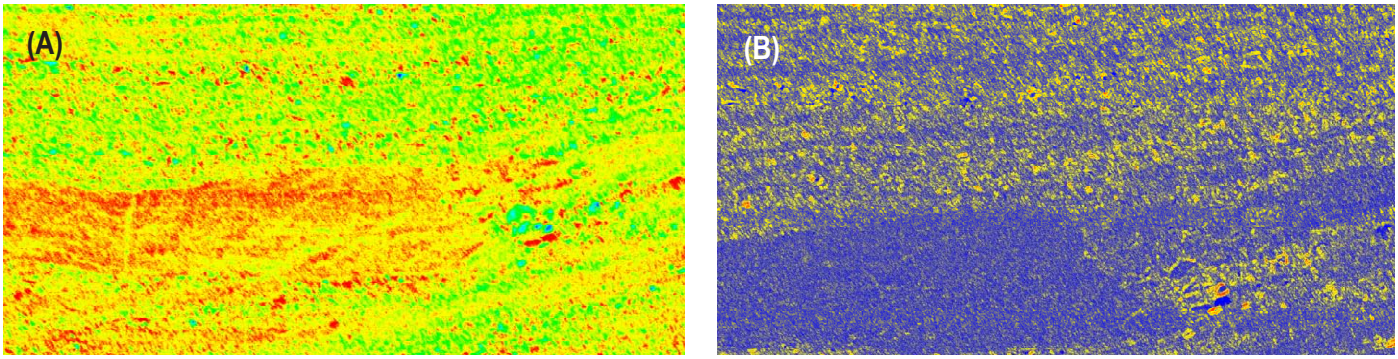



Figure 1: Outcrop exposure of the Arroyo Ojito Formation, located northwest of Albuquerque, NM. Five facies groups are present on this outcrop: (1) cross bedded sand and gravel, (2) horizontally-laminated medium sand, (3) gravelly sand with some cross-bedding, (4) cobble lag deposit, and (5) cross-bedded sand and gravel. This outcrop was scanned at a 2-mm grid resolution.



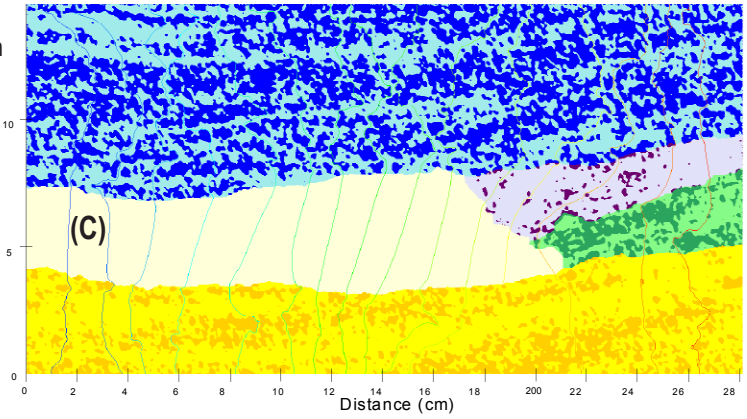




Figure 2: Mean intensity map (A), standard deviation map (B), and segmented facies map (C) of the outcrop exposure from lidar. Mean intensity and standard deviation are calculated by stacking multiple scans of the same outcrop (7 in this case). Segmentation was accomplished using live-wire and threshold approaches.

connections in the third dimension are uncertain. Additionally, the outcrops are not perfectly planar, so some distortion occurs when bringing the 3D outcrop to a 2D image. We also use very few hydraulic conductivity values for the various lithologic types, therefore, we do not consider 'within facies' variability at present. Finally, not all outcrops have been conducive to detailed scans since facies may not provide sufficient contrast for the lidar scanner to capture. We plan to evaluate these aspects of our results over the next two years under the DOE-BES funding. We are still constructing models based on some lidar scans and will complete these in the coming year.

For the evaluation of sedimentary texture on non-Fickian transport, we constructed a specialized permeameter to induce an instantaneous tracer pulse (deuterated water). By collecting samples at the downgradient end of the permeameter, we measured breakthrough characteristics for different sedimentary textures (varying mean grain size and sorting). We are still evaluating the results from this experiment.

## Significance

Two aspects of this work may significantly add to the field of hydrogeology. First, this work shows

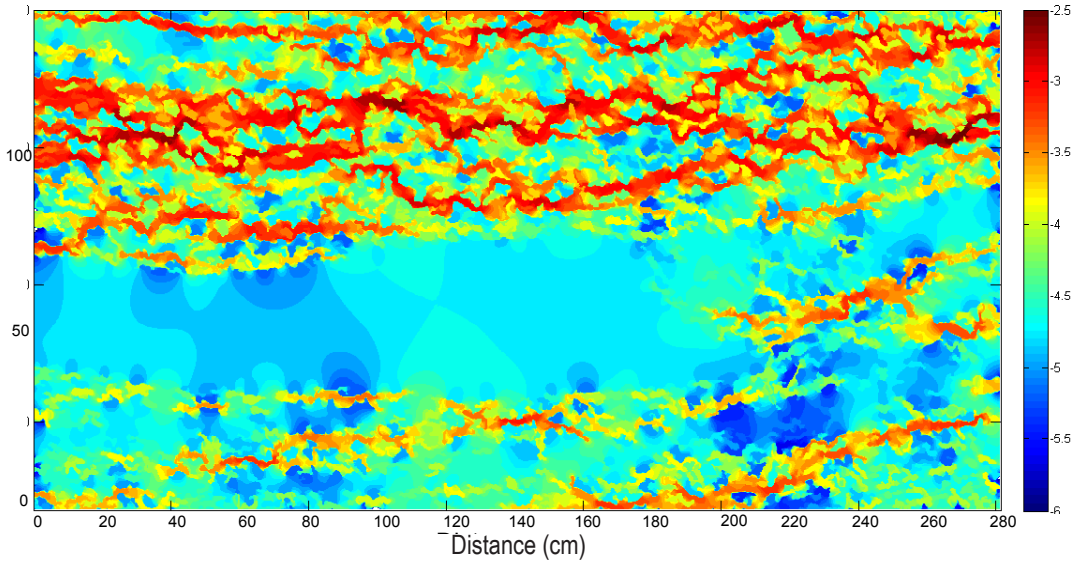



Figure 3: Resultant velocity field from high-resolution model (produced by Katherine Klise, a Sandia collaborator). Scale is log (velocity).

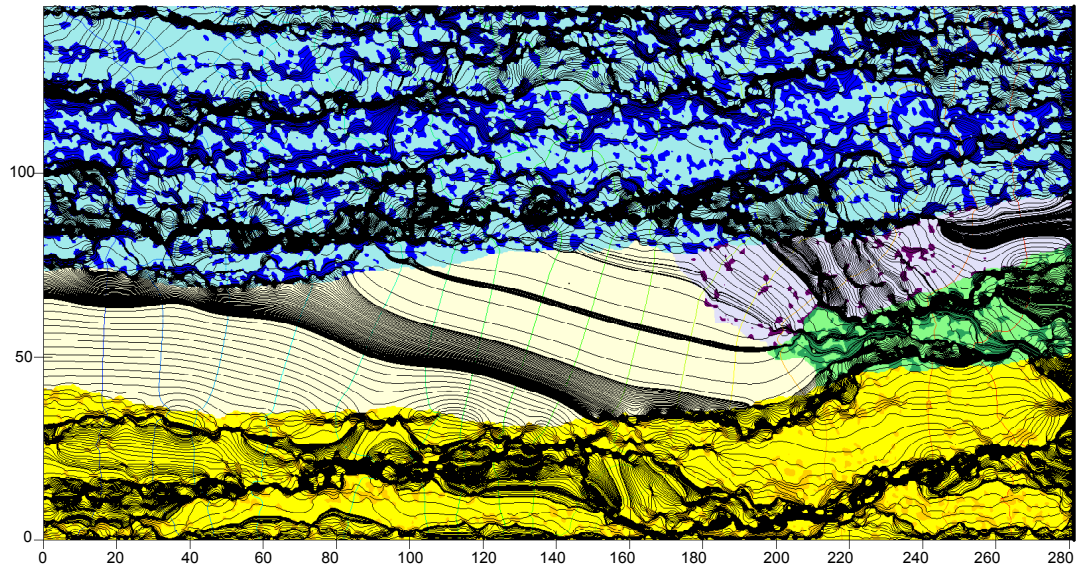



Figure 4: Advective pathlines (shown in black) developed using MODPATH. Notice the strong focusing that occurs along gravel cross-beds.

how the small-scale heterogeneities influence transport to create the observed non-Fickian breakthrough character. Preferential flowpaths are quickly developed within coarse-grained cross-bedded units, and length of time particles remain in lower permeability facies relates to the degree of tailing observed. We are still evaluating the influence of bedding orientation versus groundwater gradient orientation, and we expect these results to inform about ways to parameterize upscaled flow models based on knowledge of sediment structure.

Though we are not surprised by the non-Fickian breakthrough character, the degree of 'focusing' of solute into high-permeability crossbeds (e.g., gravels) and the small extent of flow passing through sands is striking and surprising. Because of this result, our perspective of the significance of this work is taking on new form. These results have strong implications for many concerns in groundwater flow and contaminant transport beyond the non-Fickian transport concepts, including the following:

- What is meant by "pore volumes," considering that much of the flow bypasses a significant portion of the porous media?
- Does this focusing in high-permeability cross-beds help explain incomplete sweeping of contaminants or petroleum in reservoirs?
- Do these flow patterns indicate why we get differential cementation in siliciclastic sediments?

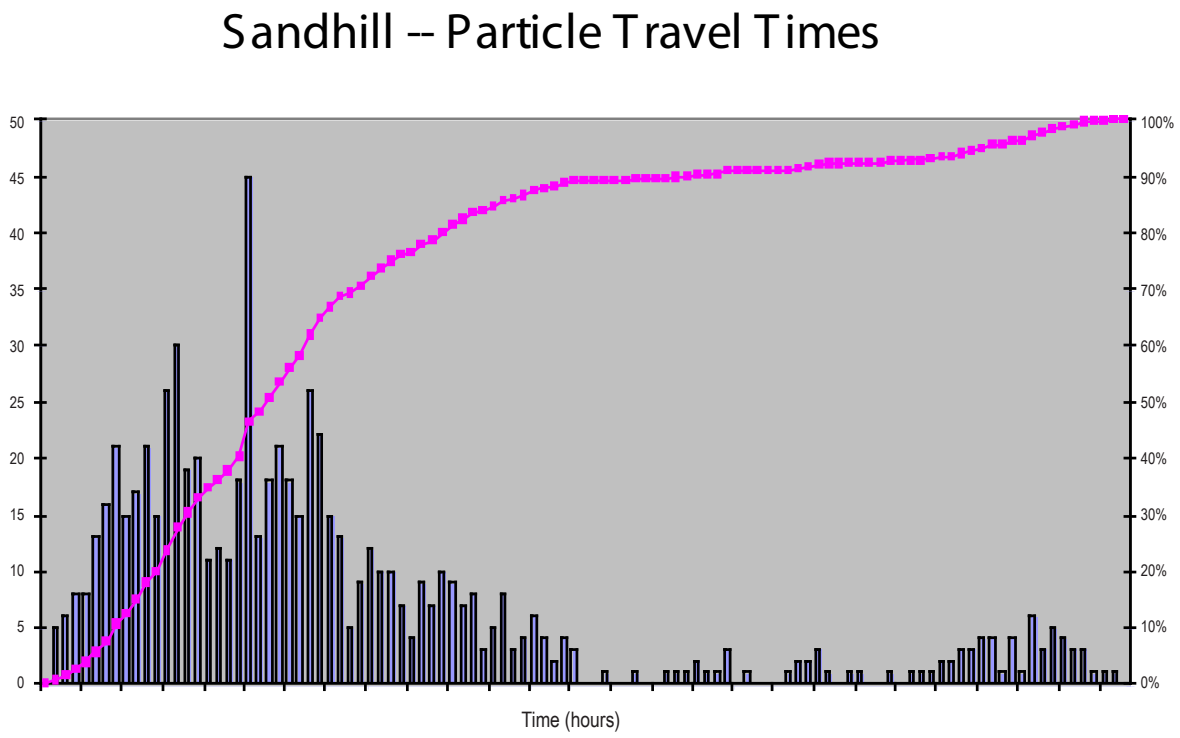



Figure 5: Breakthrough distribution of particles at downgradient end of the model. This shows a strong non-Fickian character.

We expect to continue evaluating these results over the next several years.

Continued work on this proposal will be conducted over the next two years under a DOE-BES grant (in collaboration with Sandia and Colorado School of Mines). Additionally, we are using this approach in collaboration with colleagues at Pacific Northwest National Laboratory and the University of Buffalo to evaluate the influence of small-scale heterogeneity on reactive transport of contaminants.

Further evaluation of these results will help us develop new proposals to further investigate the implications of small-scale heterogeneity on contaminant transport and remediation.

*Presentations*

The work from the first year of research is being presented at both the Geological Society of America annual meeting in October (Denver) and the American Geophysical Union meeting in December (San Francisco). Additionally, we plan to submit the results from this work for publication in Water Resources Research during this project year.

Weissmann, G.S., "HydroGEOLOGY: A Geologic Approach to Groundwater Studies", University of Colorado, Department of Civil, Environmental, and Architectural Engineering, October 31, 2007.

*GSA Abstracts*

J.D. Frechette, G.S. Weissmann, and T.F. Wawrzyniec, "Classification and Segmentation of Terrestrial Lidar Data for Lithofacies Analysis," Paper 55-28, poster session, October 28, 2007.

K.A. Klise, S.A. McKenna, V.C. Tidwell, and G.S. Weissmann, "Numerical Investigation on the Ability to Predict non-Fickian Dispersion from Aquifer Properties," Paper 128-2, October 30, 2007.

G.S. Weissmann, J. Frechette, T. Wawrzyniec, and K. Klise, "Investigation of non-Fickian Dispersion using Lidar Imagery on Outcrops," Paper #178-2, poster session, October 30, 2007.

*AGU Abstracts*

K.A. Klise, G.S. Weissmann, S.A. McKenna, V.C. Tidwell, J.D. Frechette, JD, and T.F. Wawrzyniec, "Dispersion Analysis Using Particle Tracking Simulations through Heterogeneity Based on Outcrop Lidar Imagery," Session H23G, poster session, December 11, 2007.

G.S. Weissmann, J.D. Frechette, W.Woodruff, E. Nichols, T.F Wawrzyniec, and K.A. Klise, "Outcrop-Based Lidar Imagery to Develop Millimeter-Scale Models of Heterogeneity," Session H11I, December 10, 2007.

## UNIVERSITY OF TEXAS SYSTEM

The University Research Programs Office supports interactions with some universities that do not have "campus executive" status. Such interactions are meant to explore niche technical areas of interest and forge new strategic relationships in critical skills areas. These programs are evaluated regularly to determine their value toward achievement of Sandia's mission objectives.

In FY 2006, Sandia and the University of Texas System (UTS) renewed their commitment to the joint Memorandum of Understanding established in 2005, charging their institutions with strengthening Research Program Interfaces and Collaborations, Peer Review and Scientific Accountability, and Education and Transformation. Their overarching goal is to achieve a greater mutual impact on national security issues. Its strategic purpose is to participate with Sandia scientists on collaborative research projects, to provide peer review for Sandia's research programs, and to provide specialized courses taught by UT professors to increase educational opportunities for Sandians.

Research program interfaces and collaborations in the areas of bioscience and biodefense, healthcare modeling, the National Institute for Nanoengineering (NINE), the National Initiative for Modeling and Simulation (NIMS), and in High Energy Density Physics have been identified. Work began in late 2007.

One outcome of the commitment by SNL and UTS is a joint postdoctoral fellowship program across Sandia's Bioscience Research Foundation and UTS Medical Branch in Galveston, which began in February 2007. Areas of research being explored include host/pathogen interactions, new bioresearch techniques in microfluidics and other microengineered platforms, advanced imaging, and computational biology. This program is rapidly growing the Research Program Interfaces across the two institutions and will serve as the springboard for building future programs.

UTS is providing independent oversight to assess and enhance Sandia's Science, Technology and Engineering excellence through the Peer Review process. In 2007, at the request of the Science and Technology Subcommittee of the Missions Committee of the Sandia Board of Directors, the UTS Vice Chancellor for Research and Technology Transfer assumed responsibility for decisions associated with the membership of the six Research Foundation External Review Panels (ERPs). Chairs of each ERP also serve as members of the Sandia Science Advisory Board (SSAB). Working in concert with the Sandia Chief Technology Officer, formal, independent UTS oversight of the panel vetting process is now considered critical to the integrity of the external advisory and review process.

The partnership in Education has directly benefited Sandians. The Texas State legislature, in 2005, granted the UT System permission to charge in-state tuition and fees to employees and dependents of organizations working with UTS in science and technology development. Sandians and their dependents can pay in-state rates when enrolled at a University of Texas System institution. This benefit also extends to those taking distance-learning classes.

Sandia has had memoranda of understanding with UT Austin for approximately six years and with UT El Paso for eight years. Various research projects have been ongoing. As a result of the emphasis on new collaborations, at least 30 research projects exist, up from 23 research projects last year. This number includes 3 new projects at UT Medical Branch, Galveston.

In FY07, Sandia had research contracts totaling $3.9 million with UT Austin, UT El Paso, and UT Medical Branch, up from $3.5 million in 2006. There were no contracts placed with UT Arlington, Dallas, or Southwestern Medical Center. Approximately 156 UT System graduates are currently employed at Sandia. In addition, 7 students in the UT System currently work for Sandia.