SURF 2008

summer undergraduate research fellowship

Program and Activities

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

NSF

- INTENTIONALLY BLANK -

Table of Contents

2008 SURF Summer Seminars and Tours 1

2008 SURF Summer Activities 8

2008 SURF Program Student Abstracts at NIST Gaithersburg, MD 17

American University .....
Nathan Behm .....
Brian Kelleher .....

Appalachian State University
Benjamin Madison .....

California Institute of Technology
Andrew Durnford .....

California State University, Fresno
Kennedy-Kiet Tuan Vu 18

Carnegie Mellon University
David Bunker 18
Benjamin Greer .....
Jennifer Shih .....

Centre College
Brittany Devine 19

Clemson University
Lauren Miller 19

Colorado School of Mines
Justin Anderson 20

Colorado State University, Pueblo
George Fosu 21

Cornell University
Brian Bolz 21
Eric Huang 22
Jonathan Ligda .....
Yanan (Henry) Wen .....

Florida Gulf Coast University
Joshua Johnson 22

Franciscan University, Steubenville
Stephen Nowak 23

George Mason University
Meghan Kern 23

George Washington University
Philip Naudus 24

Gettysburg College
Anne Marie Forney 24

Harvey Mudd College
Akash Rakholia 27

Haverford College
Alex Cahill 28
David Winogradoff .....

Hood College
Hilary Stauffer .....
Eric Walton .....

Indiana University of Pennsylvania
Lauren Abbott .....

Iowa State University
Bethany Juhnke .....

James Madison University
Lydia Barker 28
David Berry 29

Johns Hopkins University
Tiffany Ng 30

Juniata College
Justin T. Schultz 31

Lehigh University
Joseph Sabol 33

Loyola College in Maryland
Lisa Schneider 34

Massachusetts Institute of Technology
Tammy Ngai 36
Beatrice Parker .....

Miami Dade College
Tyler Bonnen 36
Sebastian Palacios .....
Jonathan Vega .....

Miami University Ohio
Jesse Manders .....

Millersville University of Pennsylvania
Kevin Workman 37

Montgomery College
Semme Yilma 38

Mount Saint Mary's University
Christine Wroge 40

North Carolina State University
Courtney Taylor 41

Oberlin College
Jacob Schalch 41

Pennsylvania State University
Adam Brockett 42
Matthew Chang 43
Matthew Ebert 43
Adam Neal .....

Purdue University
Craig Bouis 44

Rensselear Polytechnic Institute
Joseph Gibney .....
Johannes Craig Kutten 44

Rice University
Laura Timmerman .....

Saint Joseph's University
Nicholas Minutillo .....

Saint Mary's College of Maryland
Patrick Bowers 45
Sara DeSavage 45
Martin Mooney 46
Amelia Tebbe 46

Southern University and A&M College
Wade Reimonenq 47

State University of New York, Binghamton
Theodore White 47

Swarthmore College
James MacArthur 50

Tulane University
Tessa Johnson 51

University of California, Irvine
Nhieli Ly 52

University of California, Santa Barbara
Griffin Rowell 53

University of the District of Columbia
Amine Lambarqui .....

University of Florida
Kevin Tierney 54
Carlos Manuel Torres, Jr. .....

University of Illinois, Urbana-Champaign
Sibu Kuruvilla 54

University of Iowa
Grady Payson .....

University of Maryland, Baltimore County
Izath Aguilar 55
Derek Fertig .....
Brandi Jackson .....
Jeong-O Jeong .....
Andrew Schuldenfrei .....

Nadezhda Serova .....
Kimberly Shurupoff .....
Christopher Sims .....
Julian Spiegler .....
Malcolm Taylor .....

University of Maryland, College Park
Jeffrey Birenbaum 59
Dustin Biser .....
Olivia Buzek .....
Suehyun Cho .....
Shauna Dorsey .....
Marina Feric .....
Nicholas Franson .....
Aleksandr Gorbashev .....
Christine He .....
Marc Howell .....
Amy Hudson .....
Shifra Katz .....
Hilary Lane .....
Christine Lau .....
Donna Le .....
Timothy Lee .....
Song Li .....
Keddy Liu .....
George Luo .....
Devon MacNeill .....
Stephanie Martin .....
Alexander Mont .....
Peter Niarhos .....
Kelly Opert .....
Sindhushree Raghunandan .....
Scott Robertson .....
Cameron Rose .....
Mark Sailey .....
Thomas Sarvey .....
Roshan Shah .....
Kathy Tang .....
Nicholas Wagman .....
Andrew Ward .....
Minghui Yang .....

University of Puerto Rico
Raiza Cortes
Paul Fuentes-Martinez
Angelica Muniz-Mercado
Stephanie Montalvo-Delgado
Axel Rivera Rodriguez 70

University of Rochester
Daniel Green 73

University of San Diego
Emmett Perl 74

University of Texas, Austin
Chong Jiang 77

University of Texas, Pan American
Ike Muniez, Jr. 78

University of Wisconsin, Stout
Jarrod Feight 80

Virginia Polytechnic Institute and State University
Matthew Glazer 81
Brian Mayer

Washington University in St. Louis
Nathan Shemonski 81

Wellesley College
Willa Freedman 82

Western New England College
Alexander Boutin 83
Kathryn Purdum

Whitman College
Jackson Cahn 83

Worcester Polytechnic Institute
Timothy Lontz 85
Long Tong

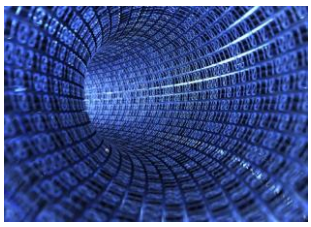
Appendix A: Quick Cross-Reference (Student, University, OU) 87

2008 SURF Summer Seminars and Tours

May 27 First official work day and orientation for SURF Session I students

June 5 James Filliben
NIST Information Technology Laboratory, Statistical Engineering Division

Catapults, Funnels, Science and Statistically Designed Experiments



In years past as part of one of its stat courses, the Air Force Academy had its students examine and optimize the distance accuracy of a simple catapult system. In a week-long NIST stat course, one of the props used was an elementary funnel apparatus with the goal of characterizing, understanding, and maximizing the "roll-time" of such a system. In 2001 Congress mandated that NIST study the collapse causes of the World Trade Center disaster; to that end, the amount of core damage that was done to the South Tower based on video evidence and FEA (finite element analysis) computational code became of interest—such damage needed to be estimated, characterized and understood. In last year's SURF program, one of the students conducted a scientific investigation of carbon nanotube contamination in water; in her study it became necessary to identify primary factors and interactions that affected the degree of such contamination.

In all of the above four examples—plus a large number of other NIST and non-NIST scientific studies—the systematic, structured, rigorous approach known as statistically designed experiments (DEX) played a critical role 1) to produce a dataset that had the capacity to answer the scientific question at hand, and 2) to do so with the minimal expenditure of money and time (as is especially relevant in your SURF environment with its 10 week window of data-generation and analysis). This seminar provided an introduction to the DEX approach, described selected important principles and techniques, and applied the approach to the above-described four problem areas.

June 12 Tom Juliano
American Society for Engineering Education, Washington, DC

Free Money: Secrets of Effective Grants for Graduate School

The American Society for Engineering Education (ASEE) manages over 1,400 research fellowships and scholarships totaling over 60 million dollars for both undergraduate and

graduate students for most federal agencies including NSF, DOD, NASA, etc. As the administrator for these fellowships, we are in a unique position to offer advice about these opportunities, how to apply and be awarded these fellowships. Receiving a graduate fellowship significantly increases your potential opportunities in graduate school and beyond.

June 19 David J. Gundlach
NIST Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division

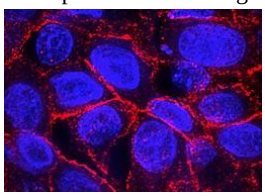
Plastic Electronics

Human-scale electronics like flat panel displays and sensor arrays are pervasive in today's society. Cost, size and performance requiements make single crystal silicon ill-suited for these applications, thus amorphous silicon thin films deposited on thin glass substrates have become the dominant technology for any human-scale electronic applications. Plastic electronics (electronics based on thin films of organic semiconductors) is an attractive alternative to thin fim electronics based on inorganic materials like amorphous silicon. Organic semiconductors have several potential advantages notably their compatibility with low-cost, high-volume solution processing, the ability to chemically-tune their electronic and optical properties, and their ability to be processed at relatively low temperatures. Taken together these properties will enable the fabrication of low-cost, large-area electronics with increased electronic functionality on flexible substrates. In this presentation, Dr. Gundlach discussed the tremendous potential for plastic electronics to impact all aspects of life through revolutions in lighting, sensing, displays and energy harvesting.

June 26 Michael Amos
NIST Chemical Science and Technology Laboratory

Disease Signatures

The future of biology and medicine depends on the development of technologies and research approaches that embrace the high degree of complexity in biological systems. Therapeutic or preventative interventions will be based on "disease signatures" – unique descriptors that can be definitive markers of health status – which will be derived from the integration of quantitative and qualitative measurements (biochemical, biophysical and bioelectronic) of hundreds or thousands of biomolecules and/or intermolecular and cellular interactions.

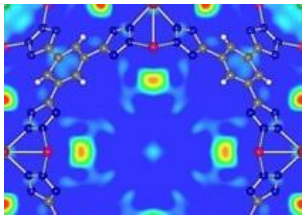


Likewise the next generation of health assessment diagnostic tests will be based on multiplex determinations constituting a unique complex signature rather than single markers of biological activities. The shift to signature analysis in diagnostics will help to enable routine health status monitoring that uses each person's own signatures of wellness and disease as the controls against which to detect pathological changes. This new focus will enable a new comprehensive and integrated approach to wellness that includes prevention of disease, early detection of disease risk and individualized treatment plans for individual patients. The new approach to wellness, in turn, may help control the rising cost of health care, for which spending now consumes nearly one fifth of the U.S. gross national product. This lecture will highlight current needs and future opportunities of this important sector of biosciences.

July 2 Craig Brown
NIST Center for Neutron Research

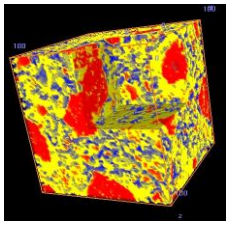
Probing Hydrogen Storage Materials Using Neutrons

Storing hydrogen molecules in porous media based on a physisorption mechanism is one possible approach to reach the U.S. Department of Energy targets for on-board hydrogen storage. Although the storage capacities of coordination polymers have progressed significantly over recent years, some technological obstacles pose challenges for their future improvement. These include the generally low hydrogen adsorption enthalpy limiting room temperature applications and the lack of understanding of surface packing density hindering the efficient improvement of hydrogen adsorption uptake. Results of various neutron scattering experiments help to shed light on both of these topics and recent results were presented.



July 10 Dale Benz
NIST Building and Fire Research Laboratory, Materials and Construction Research Division

When Water Meets Cement

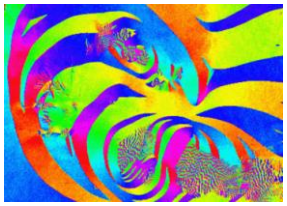


Concrete is the second most consumed material on a worldwide basis, after water. The key components of concrete are water and cement (along with sand and stone) and their interactions are responsible for the amazing transition that concrete undergoes, from a viscous suspension into a rigid load-bearing solid. The talk provided overviews of concrete and cement production and then proceeded into a presentation of what happens when water

meets cement. Hydration reactions, chemical shrinkage, and autogenous expansions and shrinkages were introduced. The importance of proper curing of concrete was emphasized and the talk finished by considering the long term interactions between water and cement that influence durability and service life.

July 17 Mark Stiles
NIST Center for Nanoscale Science and Technology

Magnetic Materials: More Than What You See Everyday

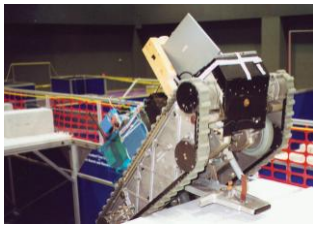


Electricity, sound, motors, information storage, sensors… Magnetic materials play an important role in these applications and are crucial for many aspects of modern life. Traditional applications of magnetic materials are based on the interaction between the magnetic materials and the electric fields generated by currents. Newer applications are based on the direct interaction between these materials and current. The 2007 Physics Nobel Prize for Giant Magnetoresistance is an example of this newer interaction. In this talk, Dr. Stiles described the interactions between currents and magnetic fields and discussed some of the ways in which this interaction is exploited.

July 23 Elena Messina
NIST Manufacturing Engineering Laboratory, Intelligent Systems Division

Robots – Ready or Not?

Robots hold much promise as tools that will aid humans in a wide variety of missions and applications. They are being developed for military missions, transportation systems, factory automation, health care, and homeland security, to mention a few examples. Yet there are very few means – if any—of objectively and quantifiably determining whether robots are ready to be fielded or how effective they will be in accomplishing a particular job. To address this shortcoming, NIST is working with end-users and developers to define application-specific requirements for robot performance, devise test methods and metrics for evaluating the performance, and in generation of consensus standards. This talk presented the challenges in developing a measurement science for robotics and provided examples of the process used that abstracts application-specific real world challenges into quantifiable and reproducible tests.



August 5 Final presentations by SURF students moderated by invited guests.

August 5	Lunch: SURF Directors and special invited guests.
August 6	Final presentations by SURF students moderated by invited guests.
August 7	Final presentations by SURF students moderated by invited guests.
August 8	Last day for SURF students and farewell pizza party.

2008 SURF Summer Activities

Gaithersburg, MD may not be around the world like the the 2008 Beijing Summer Olympics, but it's still difficult when you're in a new city. NIST Gaithersburg SURF students all find themselves in the same boat and thus forge bonds that may last a lifetime. They work together AND play together. In fact, to make life easier they can get it all scheduled using their own forum for social and work-related chatting.

NIST SURF Forum
(For NIST SURF-reated chat & info (this is not a U.S. Government website)

Before you Arrive
Travel, Living Arrangements & Money (how to get here, info on roommates, and the all important money)
Meet your Roommates (chat with your new suite mates)

NIST Research and Other Opportunities
Important Meetings & Dates (NIST seminars, tours, special meetings, off-campus visits, socials & more)
Working at NIST (guidelines to the NIST workplace)
Please help… (Solve a problem / find something I need for my project)
Complaints (Post a complaint about NIST or Summerfield – solutions welcomed!)
After the NIST SURF Program (Graduate school options and other career opportunities)

SURF Student Activities
Chat Central (off topic chat, forum games and everything else)
Outdoor Activities (organize hiking, biking, camping trips)
Apartment Life (organize parties, BBQ's and other Summerfield Suite gatherings)
Sports (Organize sports activities at our outside of NIST)
Take a Trip (organize trips to DC, Baltimore, New York, amusement parks & more)
Religion (Find friends of faith)

General Category
General Board (This is the board for general discussions)
Test Zone (Test the forum out here. Posts made in this board will not add to your post count.)

SURF BBQ – NIST Picnic Grove

July 4th in the Nation's Capitol

On the Fourth of July, we pause to remember and celebrate the values of liberty and justice that make our country great, and to be thankful for the remarkable freedoms that we enjoy in the United States of America. The significance of this day has inspired speeches, literary works, and musical compositions. It is also an opportunity for each of us to ponder the meaning of our nation's heritage and to celebrate in our own unique way. Check out how this year's SURFers celebrated the holiday…

2008 SURF T-Shirt Design

What better way to remember your summer at NIST than to design your very own souvenir T-shirt. It may not be the Olympic rings, the world's most recognized symbol, but this year's SURF T-shirt will provide the students with lots of memories. The T-shirt has a symbol for each of the nine organizational units at NIST, the bear that wandered onto the NIST grounds, a tornado that shook up the area during their stay, and the water main break that left many SURFers without the ability to wash their clothes or do other tasks we take for granted, to name a few.

NIST Summer Institute for Middle School Science Teachers

This summer NIST sponsored a workshop for ~17 middle school science teachers from schools in the Montgomery County area. One of the goals of the two-week workshop was to help the teachers learn more about how to encourage their student's interest in science in the crucial middle school years. Since SURFers were closer to the middle school years than most of the other staff at NIST, they asked for the SURF students to provide insights into the issue. Also the SURFers were involved in interesting projects and learning how to explain what they were doing to others. This made them great examples for the teachers of how scientists work. Who knows, the SURFers may have even got to meet their science teacher from years ago if they went to school in the area – wouldn't that have been cool – in addition to making that teacher proud!!

White House and Capitol Hill Tour

The White House - For two hundred years, the White House has stood as a symbol of the Presidency, the United States government, and the American people. The 2008 SURFers got to see the White House up close and personal on a special tour arranged just for them. Hmm, I wonder if they saw Barney and Miss Beazley running around during their visit.

The White House has a unique and fascinating history. It survived a fire at the hands of the British in 1814 (during the war of 1812) and another fire in the West Wing in 1929, while Herbert Hoover was President. Nonetheless, the exterior stone walls are those first put in place when the White House was constructed two centuries ago.

Presidents can express their individual style in how they decorate some parts of the house and in how they receive the public during their stay. In 1829, a horde of 20,000 Inaugural callers forced President Andrew Jackson to flee to the safety of a hotel while, on the lawn, aides filled washtubs with orange juice and whiskey to lure the mob out of the mud-tracked White House.

There are 132 rooms, 35 bathrooms, and 6 levels in the Residence. There are also 412 doors, 147 windows, 28 fireplaces, 8 staircases, and 3 elevators.

Capitol Hill, aside from being a metonym for the United States Congress, is the largest historic residential neighborhood in Washington D.C., stretching easterly in front of the U.S. Capitol along wide avenues. It is one of the oldest residential communities in Washington, and with roughly 35,000 people in just under two square miles, it is also one of the most densely populated. Capitol Hill's landmarks include not only the United States Capitol, but also the Senate and House office buildings, the Supreme Court, the Library of Congress, the U.S. Marine Barracks, the Washington Navy Yard, and Congressional Cemetery.

Neighbor Helping Neighbor

The honor, spirit and resources of the American people comes forth with neighbors helping neighbors in need — during earthquakes, floods, fires, storms — and also for the deeply personal and often quiet disasters that require a gift of blood. Quietly, without fanfare, SURFers gave the gift of blood during the NIST blood drive.

Pentagon Tour

The Pentagon is virtually a city in itself. Approximately 23,000 employees, both military and civilian, contribute to the planning and execution of the defense of our country.

The Pentagon tours program was established on May 17, 1976 to support the nation's Bicentennial Celebration. Initially, the program was to last through the 4th of July and then be disbanded; however, internal support and public demand were so great that the program has been continued ever since – with a few SURFers adding to those numbers.

SURFer Girl Night at the Cold Stone Creamery

The SURFer "girls" needed someplace to wind down from a hot Washington area summer week and hard work, so they headed to the Cold Stone Creamery for their favorite ice cream indulgence and some "girl" talk.

Artscape 2008 was a free public arts festival in nearby Baltimore, MD. The festival had multiple music stages going non-stop with such greats as Roberta Flack, Joan Jett and the Blackhearts, the Wailers, Ne-Yo, and the Baltimore Symphony Orchestra, along with visual and performance art.

A pretty good deal, even considering the price of gas to Baltimore, but ever conscience of their funds and the environment, the group carpooled.

Where you can you get your start to win the Fox Network contest "So You Think You Can Dance"? Several SURF students took up two NIST staff (not professional dance instructors) on their offer of free dance lessons to learn the East Coast Swing and Cha Cha. Who knows we just might see a former SURFer on the new season's show.

Volunteers Wanted – Linear Algebra & Synthetic Worlds

Contrary to popular belief, students do not just *play* video games all day; sometimes that *play* is really a serious scientific experiment. A SURF student and advisor were looking for a few students to help evaluate a software prototype designed to be used for linear algebra. The only requirements were that you needed to be pretty familiar with linear algebra (think high school precalculus), be free during the time slots to participate, and, of course have your advisor's permission.

SURF Students Hard at Work

MSEL/NCNR SURF students Tiffany Ng and Sindhushree Raghunandan describe their summer research projects to Senator Ben Cardin (left) and Dr. James Turner, NIST Deputy Director

Jacob Schalch tending to the helium cryostat while performing neutron experiments at the NCNR

A group of SURFers touring the CNST Nanofabrication Cleanroom.

SURF Farewell Pizza Party

Every year the SURF Directors treat the students to a farewell pizza party. This year the SURF T-shirt committee made a few dollars profit selling NIST's hottest fashion item – the SURF 2008 T-shirt. Luckily for their fellow SURFers, the T-shirt committee decided to treat everyone to Rita's Ice in three yummy flavors – mint chocolate chip, blueberry, and mango – pizza and dessert, what's not to love.

Student Abstracts
2008 SURF Program

American University

Using Magneto-Optical Trapped Lithium Atoms to Create a Versatile FIB
Nathan Behm

Focused ion beams, (FIB) are useful for applications in nanoscale fabrication and observation, as a FIB can be used for ion milling and deposition as well as microscopy. However, as things stand today there are few options available when it comes to creating a focused ion beam. The FIB makes use of a liquid metal ion source which in practice can only be used with the element gallium. Gallium is good for processes such as ion milling, but microscopy is hindered by its large mass, with both processes resulting in implantation of Ga in the sample, contaminating the sample.

In order to improve FIB's this study has focused on the creation of a magneto-optical trap (MOT) that will trap lithium to use as an ion source. Once completed the Lithium MOT will provide a source that is better suited for microscopy since its small mass will prevent implantation. It will also be possible to modify the system to use other elements depending on the need of the individual experiment. This system provides a prototype to create a system capable of microscopy, deposition, ion milling, and doping all with relatively minor changes to the basic design of the system.

In order for the MOT to function correctly, it is important to create a laser-lock system, consisting of a lithium heat pipe, laser optics, and laser-locking electronics. The laser-lock keeps the lasers functioning at the resonant frequency of lithium, corresponding to a wavelength of 671 nm. Further work included creating a lithium oven capable of heating the lithium to the temperature necessary for vaporization. Finally fiber-optically coupling was performed to make the entire system more compact and user-friendly.

Rate Dependent Magnetization Reversal in Thin Co/Pt Multilayer Film
Brian Kelleher

Magnetic films with perpendicular anisotropy, such as Co/Pt(Pd) multilayers have helped to dramatically expand the storage density in magnetic media such as hard-drives over the past two years. Further application of such films requires a thorough understanding of the magnetization reversal behavior. By using Kerr microscopy, I have observed the reversal behavior of three perpendicularly oriented films, (Co/Pt)x=2, (Co/Pt)x=3, and [Pt/(Co/Pt)x=2]/Ta . The samples were grown via DC magnetron sputtering in a low pressure Ar environment. In these films, large circular domains nucleate and expand when enough magnetic field is applied. A variety of effects occur during the domain growth process which are dependent on several parameters, including the amplitude of the applied field, the slew rate of the field, and the frequency of the field in AC measurements. Applying both DC and AC fields, I have expanded and contracted isolated domains leading to exotic behavior. As a

domain undergoes expansion and contraction the domain wall (edge) becomes less uniform. I have devised a method to quantify this asymmetrical domain wall 'roughness' by calculating the average magnitude of the slope of the domain wall. Interestingly, cusping domain walls are sometimes observed as a function of field slew rate, which adds to the roughness. These cusps can be attributed to oppositely magnetized domains, which I call *ghost* domains. Ghost domains have nucleation sites near the domain wall which can dramatically influence the shape of a growing or shrinking domain. Using AC fields I was able to nucleate and observe the hidden locations of the ghost domains as well as define other interesting reversal modes.

Appalachian State University

Characterization of Femtosecond Laser Frequency Comb and a Micro-Channel Plate (MCP) Detector for High Resolution Atomic Spectroscopy
Benjamin Madison

We are developing tools useful for high resolution atomic spectroscopy. In the Atomic Spectroscopy Group, a femtosecond laser frequency comb has been installed recently, and is being characterized for use in experiments with simple atomic systems. As a test of this 250 MHz fiber-laser comb, optical frequency measurements of an iodine-stabilized helium-neon laser will be presented. Applications include planned experiments with stored ions extracted from the NIST electron beam ion trap (EBIT), for which a position-sensitive, micro-channel plate (MCP) detector is being developed. The capabilities of this imaging detector will also be discussed.

California Institute of Technology

Simulating Diffusion from Laser-Excited Gold-Coated Silica Nanoparticles
Andrew Durnford

A persistent problem with most cancer treatments has been the difficulty in avoiding damage to healthy tissue while killing the cancerous cells. Recently, more selective treatments have been devised that exploit the porosity of blood vessels produced by tumor angiogenesis by using intravenous injections of nanoparticles large enough that they are only capable of passing out of the bloodstream into surrounding tissues through the "leaky" walls of the tumor-generated vasculature. These nanoparticles are thus able to congregate only in the aberrant tissue, where they are agitated by an outside field, inducing apoptosis through hyperthermia. Our research uses a Python-based, finite volume method to simulate one such treatment method: gold-coated, silica-core nanoparticles are illuminated by near infrared laser light to generate the heat necessary to induce hyperthermia. By exploring influences of nanoparticle dimensions, distribution, and concentration, and of the laser illumination intensity on the resulting thermal diffusion process in a flesh-like medium, we intend to determine effective mesoscale thermal transport properties for macro-scale tumor ablation models and to derive an empirical model of the phenomenon.

California State University, Fresno

Fate and Behavior of TiO_2 Nanoparticles in the Natural Environment
Kennnedy-Kiet Tuan Vu

The stability and behavior of titanium dioxide (TiO_2) nanoparticles in aquatic environments will likely govern their toxicity and photocatalytic properties. This research investigates the early stage aggregation kinetics of a commercially available TiO2 powder using time-resolve dynamic light scattering (DLS). A stable solution of primary TiO_2 particles could not be generated through any investigated means (extended sonication, UV-ozone cleaning, pH adjustment, and polymer addition). Consequently, this work focuses on the behavior of stable, primary particle aggregates (nanoaggregates) that are either bare or have been coated with either natural organic matter (NOM) or alginate, a biopolymer produced by algae, under basic conditions (pH range = 8.8 - 9.3). The ionic strength was adjusted with different concentrations of several electrolytes, namely NaCl, $CaCl_2$ and $MgCl_2$. The stability of the TiO_2 nanoaggregates coated with NOM or alginate varied according to the electrolyte type and concentration. However, aggregation of the bare TiO_2 nanoaggregates was not observed for any electrolyte. This suggests that, depending on the environmental conditions, NOM and alginate can act as both a stabilizing or destabilizing agent for TiO_2 nanoaggregates. Subsequently, solution chemistry will be critical for understanding the behavior of TiO_2 powder in the natural environment.

Carnegie Mellon University

Materials Informatics Tools and Crystallographic Databases
David Bunker

From the aluminum alloy in airplane fuselage to the steel in bridge girders, to the Li-ion battery in cell phones the properties of alloys are becoming increasingly important in modern life. Designing the next generation of materials will involve alloys of steadily more complex chemical compositions and so will require more information about the structural, mechanical, electrical, and magnetic properties. One field emerging to face this challenge is combinatorial materials research. In the past, material scientists would extensively study a single chemical composition, such as $Fe_{.5}Ga_{.25}Pd_{.25}$, before moving onto another composition. However, with procedures such as co-sputter deposition it is feasible to get spectral data from every possible composition of Fe, Ga, and Pd in a single experiment. After this data is acquired, materials informatics can be used in conjunction with the available materials property databases to analyze the massive amounts of data obtained from the combinatorial experiments.

It is vital that the data entries in the databases are of high quality to ensure that the conclusions drawn from the databases are valid. In addition to the evaluation of database information, materials informatics tools are also important in data extraction. Using NIST's crystallographic databases it is possible to resolve a large number of experimental spectral data into a ternary phase diagram complete with chemical and structural information. The informatics tools developed provide group-theoretic and matrix-based algorithms for both

crystallographic theory, and the clustering analysis of X-ray spectral data. The informatics tools can be used to evaluate the databases as well as perform experimental data processing. This summer, the creation of these tools has included writing graph theoretic and spectra clustering libraries in Matlab and C++ as well as porting NIST's crystallographic databases such that it is available on multiple platforms. The efficiency and quality of data processing was also evaluated.

Terahertz Spectroscopy and Modeling of Biological Molecules in Reverse Micelles
Benjamin Greer

Terahertz spectroscopy has become a useful tool in studying molecules and how they interact with their environment. While mid-infrared spectroscopy can give information on specific bonds within a molecule, spectroscopy in the terahertz region (1-20 THz or 35-700 cm-1) reveals information about the molecule on a larger scale. Normal modes of the molecules as well as molecule-to-molecule interactions show up as absorption features in this region, allowing analysis of crystal structures and other molecular environments. One area of interest has been looking at biological molecules (sugars, peptides..) in aqueous environments, as that is where they are naturally found and many of them may change conformation when surrounded by water. However, water strongly absorbs in this region, so the biochemical in question is saturated in water and placed in inverse micelles, where a surfactant creates tiny pockets of solution surrounded by a non-polar solvent that does not absorb the terahertz light. A modified Fourier Transform Infrared Spectroscopy (FTIR) machine is used at room temperature to produce an absorption spectrum. Spectra for L-Proline, ß-D-fructose, and sucrose will be shown.

To understand the measured spectra and how various peaks relate to molecular movement, density functional theory (DFT) calculations were done using both GAUSSIAN 03W and CASTEP software packages. GAUSSIAN was first used to determine the vibrational spectra of molecules in gas phase at 0 K. Molecular structures from various crystallography papers were used as input, but many of the structures had to be optimized using DFT calculations before the vibrational spectra gave realistic answers. Comparisons between THz crystalline sample spectra and GAUSSIAN calculations will be discussed. Due to computational and theoretical restrictions in the GAUSSIAN calculations, we switched to using the CASTEP software package designed for calculating the vibrational spectra of molecules in crystal lattices.

SANS-USANS Investigation of Magnetic Nanoparticles Chaining in Polymer Epoxy Nanocomposites
Jennifer Shih

Incorporation of magnetic nanoparticles (MNPs) into aqueous ferrofluids can be used with DC magnetic fields to shape and cure MNP loaded polymer epoxies. Specifically, the MNPs form rigid chains that depend upon the magnetic field configuration. These systems can be used in applications such as tissue engineering and magnetoelastic polymer epoxy nanocomposites.

The FeCo MNPs used in this study were synthesized in a radio-frequency induction plasma torch (PT) with the option of cryo-milling (CM) afterwards. During cryo-milling, the as-synthesized nanopowders are ground in a cryogen slurry to improve the monodispersity of the particles. The PT or CM MNPs were then ultrasonicated in bisphenyl F to form a viscous ferrofluid. An NdFeB permanent magnet was used to induce chain growth in the ferrofluids. The macroscopic chains are formed radially, circumferentially or laterally depending on the field geometry or randomly with no applied field. MNPs were also dispersed on pieces of tape for characterization of the nanoparticles themselves.

We examined CM and PT nanoparticles with varying weight concentrations and chain geometries using small angle neutron scattering (SANS) and ultra small angle neutron scattering (USANS) to learn about the nanoparticle and chain structure. The SANS and USANS instruments at the NCNR are ideally suited for probing the structural features of materials with length scales between 10 to 500 nm and 100 to 10000 nm respectively. Fits to these data provide information about the average nanoparticle size, dispersity and length of chaining. A SQUID magnetometer was also used in order to measure the average magnetic response of the epoxy samples in an applied field.

In both the SANS and USANS scattering regimes, all of the CM and PT samples showed strong scattering with distinguishing features such as slope changes and weak peaks. In the data for the tape samples, distinct differences between CM and PT samples were evident at intermediate values of the wavevector Q. In particular, the PT samples had more disparate particle sizes, while the CM samples had better monodispersity with an average particle size of about 30-50 nm. As a result of these differences, the CM epoxy samples were chosen as the focus of our in-depth analysis. Both the random and chained CM epoxy samples exhibited low Q scattering indicative of collective clustering of the MNPs. For the chained samples, this clustering is evident both parallel and perpendicular to the macroscopic chains. The 2-D SANS scattering was asymmetric, and the sector-averaged data were split due to the asymmetry of the MNP chains. In the direction parallel to the chain, the scattering is greater at a smaller Q signifying that the length scales associated with these clusters are longer, as expected. The lengthscales extracted from fits to the SANS and USANS data will be interpreted in light of the SQUID magnetometry results which revealed a difference in the crystallographic anisotropy for a CM chained sample.

Centre College

Measuring User Experience in Large Simulated Networks
Brittany Devine

Current models to compare congestion-control algorithms proposed for the future Internet show effects of such algorithms in small-scale networks. To compare macroscopic network behavior and user experience for proposed congestion-control algorithms in large-scale networks, NIST has created a simulation model (MesoNet), which mimics real-life networks, like those comprising the Internet. As first constructed, MesoNet could compare only average throughputs for flow groups, classified based on characteristics of routes (very advantaged, advantaged or typical) transited in a simulated network topology. MesoNet did not consider a range of other,

key, flow characteristics, such as maximum flow capacity (e.g., 100 Mbps or 1 Gbps), flow size (e.g., web objects, documents, service packs, and movies) and congestion-control algorithm, which can also affect user experience.

The research project discussed in this colloquium added the capability for MesoNet to classify simulated flows along four dimensions and to capture and report 14 statistics for flows within each 4D class. This additional classification and statistical information allows researchers to obtain a nuanced picture of user experience. After upgrading MesoNet, the research project conducted experiments to demonstrate the value of the improved measurement capability. This colloquium introduces MesoNet, along with the concept of congestion control, and describes the 4D classification technique and 14 statistics added to the model over the summer. The colloquium also presents some results comparing two, proposed congestion-control algorithms (Scalable TCP and H-TCP) under 32 simulated conditions. A series of future experiments will use the new measurement capability of MesoNet to compare macroscopic network behavior and user experience in a large network with a heterogeneous mix of congestion-control algorithms, network-interface speeds, file sizes and flow routes.

Clemson University

Influence of Temperature on the Molecular Conformation in Gold-Monolayer-Semiconductor Structure

Lauren Miller

The use of organic molecules in replacing existing electrical functionality, such as switching or wires is an emerging technology which holds great potential to meet the demands of the electronics world for "More than Moore" devices. One of the main challenges to this technology is the application of the top metal electrode on molecule-semiconductor hybrid devices because metal filaments diffuse through the organic monolayer and alter the electrical response instead of forming the idealized metal-molecule-substrate sandwich structure. To approach this issue, it is necessary to consider metallization methods beyond traditional evaporation such as Nanotransfer printing (nTP). The principle of this method consists in transferring material from one substrate to another by mechanical contact and sometimes it requires applying temperature and pressure. Since the molecular conformation is an integral aspect of the functionality of the components, understanding the influence of temperature on monolayers, in conjunction with related studies in the influence of pressure, is a needed step toward their future application that will help explain changes in molecular conformation during the placement of the electrode on the monolayer. Then, this structural knowledge will be correlated with electrical properties to begin to engineer devices with desired properties.

We have investigated molecules of varying hydrocarbon length and terminal functional groups to ensure chemical bonds between the molecules and the substrate. In addition, the effect of UV-Ozone treatments on monofunctional monolayers was studied in hopes of converting the methyl-terminated molecules to bifunctional molecules. Then, we have utilized these molecules to explore the influence of temperature (70-120ºC) on self assembled monolayers on three different substrates: evaporated gold on silicon, nanolaminated gold on

plastic substrate (PET), which presents an atomically flat surface and enhances the conformal contact with the molecules, and Silicon substrate. The monolayers are characterized by means of FT-Infrared spectroscopy and contact angle measurements. In general, the monolayers became more disordered and trends based on molecule and substrate was observed. Long chain molecules exhibited different behavior depending on the substrate: molecules on Au/PET are more ordered than Au/Si and desorb at a higher temperature. Short chain molecules lead to less well packed chains and show no dependence on the substrate. The temperature tests were performed on a silicon substrate with similarly structured molecules to draw comparisons.

Colorado School of Mines

Theory of Quantum Corrals on Graphene
Justin Anderson

Graphene, a one-atom-thick crystal of graphite, is a material that can exist as either a typical metal or as a semiconductor under ambient conditions. In addition to this inherent versatility, graphene's unusually long mean free path for charge carriers yields a resistivity lower than that of silver; this low resistivity casts graphene as a major candidate to replace current nanowire and silicon transistor technologies. In the four years since graphene was first isolated and characterized experimentally, a large effort has been made to develop the material from a theoretical sandbox into next generation devices. Matching this push to manufacture and commercialize has been a revival of theoretical interest in graphene, with a particular focus on its unique band structure which causes the nonrelativistic electrons to behave like relativistic particles.

Scanning tunneling microscopy (STM) permits arbitrary arrangements of atoms to be placed on metal surfaces, and also permits imaging of electron waves scattering from these atoms. When the electron waves are confined in a closed arrangement of atoms the resulting structure is called a "quantum corral." Experimental work is currently ongoing at NIST to use STM to build quantum corrals on graphene. The ultimate goal is to construct devices using STM that will exploit graphene's unique electronic attributes for use in such fields as spintronics and microelectronics.

With the goals of interpreting the results of NIST STM experiments and proposing useful device applications, we develop a multiple scattering theory for an electron wave scattering from atoms deposited on a graphene substrate. Our method is an extension of previous theoretical work on quantum corrals on metallic surfaces, which has successfully matched the interference patterns produced in experiment. Mathematically, the method modifies the wave function incident on a scatterer to include the contributions of waves scattered from every other impurity. The results are combined to produce a total wave function that includes the interference resulting from the electron scattering from multiple atoms.

Using a partial wave expansion, we generate an expression for the wave function of an electron in graphene scattering from a single hard-disk impurity. The model is numerically

evaluated in a low energy regime (*s*-wave approximation). Generated results will be compared to NIST STM experiments when they are available.

Colorado State University, Pueblo

Validation of the SysML Tools and Specifications
George Fosu

Systems engineering (SE) is any methodical approach to the synthesis of a system that (1) defines views of that system to help elicit and elaborate requirements, and; (2) manages the relationship of requirements to performance measures, constraints, risk, components, and discipline-specific system views. Systems engineering is part of the development of complex systems, such as aircraft and automobiles. SysML is a modeling language based on the Unified Modeling Language (UML). It enables the expression of systems engineering viewpoints. NIST's Systems Engineering Tool Interoperability project is an ongoing effort to allow engineers, who use SysML tools, to reliably communicate SysML content. In order to collaborate effectively, the various tools must conform to the system of expression defined in the SysML spec. In our work, various systems engineering models were created using SysML-capable tools. These models are being used to define formal expressions of requirements that are currently only informally described in the SysML spec. The formal expressions we develop, when validated, will become part of the next version of the SysML spec. Validation of these constraints, and of SysML tools, can be confirmed by the use of NIST's SE Tool Interoperability facilities.

Cornell University

Controlled Electrostatic Deposition of Graphene
Brian Bolz

Since the discovery of graphene and its startling electronic properties two different methods for producing graphene have developed, mechanical exfoliation and chemical exfoliation. These techniques have created a working foundation for graphene devices, but there exist several obstacles hindering standardized fabrication. The size and location of exfoliated graphene are particularly important characteristics for constructing graphene devices. Thus far every device is uniquely fabricated depending on these two key features. A recent study has shown that graphene can be deposited electrostatically, but control over size and location is not applied.

This research is based on controlling the electrostatic deposition of graphene through a localized electric field. Tests have produced unsystematic deposition caused by an electric field across the entire substrate. It is believed that by fabricating a substrate with patterned electrodes beneath the surface a local field can be produced causing a field effect between the graphene and the restricted substrate surface above the electrode. The type of graphite used in these experiments may also have a considerable impact on its deposition ability.

Microwave and Radio-Frequency Addressing of Bose-Einstein Condensate
Eric Huang

A Bose-Einstein condensate (BEC) forms when atoms are cooled to nearly absolute zero. At these temperatures the kinetic energy of the ensemble is virtually zero and a large percentage of the atoms can be characterized as occupying the ground state of their confining potential. This leads to a dramatic phase transition that defines BEC as a unique state of matter.

However, working with BEC is rather difficult; even slight interactions can heat the atoms past the point of condensation. Nevertheless, their unique properties make them an appealing subject for a variety of experimental and practical research, including the formation of coherent atom lasers, the examination of quantum behavior, and, more relevant to this project, quantum computing, in which the quantum nature of atoms can lead to exponentially more information processing than conventional computers.

In order for a BEC quantum computer to work, there would need to be a method to communicate with atoms at an individual level. This is achieved by trapping the atoms in a double-well-lattice optical potential, and loading them into precise quantum states through the use of microwave and radio-frequency radiation. The creation and manipulation of sub-millisecond radiation pulses of varying frequency, phase, and amplitude will be discussed.

Mechanically Exfoliated Graphene
Jonathan Ligda

Production of graphene has no doubt been on going ever since the invention of the pencil lead, however, identifying the single layer of carbon known as graphene only occurred a few years ago by Giem and Novosolov. There are different avenues for the creation of graphene; chemical exfoliation, mechanical cleavage, and thermal processing of SiC. The method I investigated this summer at NIST to produce graphene is mechanical exfoliation. Although very simplistic in nature, with specific process conditions it can yield high numbers of large graphene flakes. Producing these large flakes allows investigation of some of the interesting material and electrical qualities of graphene.

Mechanical Exfoliation is accomplished by using Nitto tape and a bulk piece of Highly-Oriented Pyrolytic Graphite (HOPG). Using the tape to peel off a graphite layer from the HOPG and placing the tape onto a silicon sample with a specific thickness of SiO_2 allows a transfer of graphene from tape to the substrate surface. Graphene flakes are located using optical microscopy and confirmed as single layer using Raman spectroscopy. Once located, these flakes can have devices fabricated on them. Using electron-beam lithography, Focused-Ion-Beam milling, and metal evaporation, devices are made to test electron transport properties and to obtain Scanning Tunneling Microscope (STM) images.

Single Molecule Studies on Membrane Protein Using Hydrosomes and Optical Trapping
Yanan (Henry) Wen

We combine IR-optical trapping, femtoliter water droplets (hydrosomes) and single molecule fluorescence techniques to manipulate and study membrane proteins in their native environment. We investigate and report on the feasibility of single molecule fluorescence detection on lipophilic dye molecules (DiIC16) embedded in a liposome encapsulated inside a hydrosome all of which is trapped by optical tweezers. We aim to use the well understood membrane protein Gramicidin-A dimer system to investigate the feasibility of FRET detection in such a confinement and to study the dimerization process and its relation to ion flux. We hope to demonstrate a single molecule manipulation and detection technique that enables studies on membrane protein in an environment more similar to *in vivo* conditions than have been previously possible, and at the same time allowing unprecedented confinement, access and control for single molecule biochemical studies using hydrosomes as femtoliter reaction chambers. To date we have achieved liposome-in-hydrosome encapsulation as well as single molecule level characterization of residual fluorescence and other competing signals that arise from the lipid.

Florida Gulf Coast University

Development of Static and Dynamic Stability Test Standards for a Load Carrying Device
Joshua Johnson

The HLPR is a semi-autonomous load carrying device that was originally developed as a patient lift and wheelchair. It has recently undergone a transformation into a material handling apparatus. The HLPR is designed to be load-assisted by human counterparts, and then autonomously deliver the load to a known location. Using International (ISO) and American standards (ANSI) for similar devices, a series of tests were developed and implemented to determine the static and dynamic stability of the HLPR. These standards are used for apparatus optimization and quantifying environmental limitations.

In addition to creating stability standards, an economical indoor tracking system was installed that enables operators to know where the HLPR is located within a facility. The system, called Sky-Trax, uses an onboard-vehicle camera with ceiling mounted, 2D barcodes. Together, the tracking system along with the HLPR will be integrated into a semi-autonomous controller to allow loads to be safely distributed throughout facilities while workers continue their load/unload tasks.

Franciscan University, Steubenville

Simulating CO Pollution Across the Indoor/Outdoor Interface
Stephen Nowak

The long-term health and well-being of a building's occupants is determined largely by the number of pollutants present in a building's atmosphere. One particularly worrisome pollutant is CO, carbon monoxide, which is odorless, colorless, quite toxic, and obviously very dangerous. CO can reach lethal concentrations inside a living space through humerous potential combustion sources including improper use of a gasoline-powered generator.

Two primary simulation methods are used to model airflow for indoor and outdoor environments. Computational fluid dynamics (CFD) has the potential for great resolution at great computational expense, often on the scale of hours or days. Multizone analysis gives much less resolution but for less operator time and only a few seconds' processing time. NIST is working on combining the two approaches into one seamless method to study problems such as the entry of airborne contaminants into living spaces from outdoor air.

My work centers on two distinct tasks: to generate suitable test model data for the simulation to process, and to perform upgrading and debugging on the CFD simulation program. This talk will cover the elementary aspects of the airflow simulation programs and what we hope to achieve, the difficulties encountered, and some sample simulation results.

George Mason University

Gamma-Gamma Coincidence Detection
Philip Naudus

Gamma-gamma coincidence detection was first used by Eldridge for the purpose of measuring the activity of ^{125}I. Involving two detectors and a radioactive source which emits two or more gamma rays simultaneously, one can infer the activity of the source by examining both coincident and non-coincident counts of gamma rays on the detectors. Although this method has previously been used for sources which emit low-energy gamma rays, where the effect of Compton scattering is negligible, the purpose of this project was to demonstrate that it can be implemented for sources with high-energy gamma rays. While ^{60}Co was the primary focus of this project, we also considered ^{22}Na and ^{108m}Ag.

A significant advantage of gamma-gamma coincidence detection is that it does not depend on the geometric configuration of the experiment. In order to verify this, we applied this method to data collected for radioactive sources placed at equal distances from the two detectors, or closer to one detector than another. In both cases, the same value for the activity was produced with small differences (less than 0.5%), while our results coincided with measurements made using beta-gamma coincidence detection.

Gettysburg College

Examination of the B3 Dosimeter Temperature-Dose Response Dependence
Anne Marie Forney

High energy radiation (gamma rays, electrons and x-rays) is used for a broad range of applications that include cancer therapy, food processing, and medical device sterilization. In order to apply this type of processing safely and accurately, dosimetry is used as a tool to measure the dosage of the radiation. The two types of dosimeters are chemical and physical. The chemical dosimeters used in this experiment were solid B3 radiochromic devices made by GEX, which change color with exposure to radiation. The optical density at a certain wavelength (554nm) is measured using a spectrophotometer, because it is reliant on the radiation response of the dosimeter.

The radiation response for most chemical dosimeters varies with temperature during irradiation. Many industrial irradiation processes can have temperatures up to 60 degrees Celsius, thus in order for a dosimetry system to be accurate and applicable the interdependence between temperature and absorbed dose must be resolved. Using a high-dose rate Cobalt-60 gamma source, the temperature dependence of the dosimeters in the range of 10kGy to 70kGy is examined. Previously collected data has suggested there is a change in the optical density as a function of the absorbed dose. The clarification of dosimeter response and temperature dependence will lead to an accurate dose reading of the irradiated product.

Harvey Mudd College

Reverse Monte Carlo Refinements of Local Structure Using Atomic Pair-Distribution Functions and EXAFS
Akash Rakholia

Reverse Monte Carlo simulations (RMC) are widely used for studies of structural and chemical atomic disorder in crystals and amorphous materials. Total x-ray/neutron scattering is used to generate pair distribution functions (PDF), which provide information on instantaneous interatomic distances. Radial and angular information can also be acquired through Extended X-Ray Absorption Fine Structure (EXAFS), which analyzes oscillations in x-ray absorption as a function of photon energy, caused by scattering of photoelectrons on neighboring atoms.

The RMC algorithm involves a simulated box containing thousands of atoms distributed in a certain configuration. Atoms are moved sequentially and the corresponding PDF and EXAFS are simulated. If the change decreases the discrepancy between theoretical and experimental PDF/EXAFS, it is accepted unconditionally; otherwise, the change is accepted with a certain probability. Work was performed to optimize the input/output of structural refinements utilizing combined PDF/EXAFS data, and to analyze the three-body distribution function in the structures studied. Test systems included Ni and $SrAl_{0.5}Nb_{0.5}O_3$ perovskites.

Haverford College

Refining the Fine Structure Constant: Theoretical Calculations of Fine Structure Splittings in Highly Ionized Atoms
Alex Cahill

The fine structure constant is important for physics, this fundamental constant is a measure of the strength of the electromagnetic interaction, and used in many calculations of atomic structure and quantum electro-dynamics. In addition, the fine structure constant is useful because it appears in varying fields of physics, such as condensed matter, particle, and atomic physics. This creates the possibility of testing the theories of these different fields against each other; which could help make sure physics has continuous properties across the different fields. Therefore, obtaining an accurate value of the fine structure constant is important. Usually the fine structure constant is determined through measurements of the quantum hall effect or the electron anomalous magnetic moment. These experiments have produced values of the fine structure constant with accuracies to 5 parts per billion. In this talk I will describe a possible new method to calculate the fine structure constant using fine structure splittings in potassium, sodium, or aluminum ions. To acquire a more precise value for the fine structure constant, calculations of the fine structure splitting will be compared to experimental values of the same splitting. Many different programs were examined. These programs, though good for approximate numbers, were not accurate enough for the purposes of this research. Many body perturbation theory is another option. In many body perturbation theory the atomic system is assumed, at first, to be a single electron orbiting a nucleus with a screening potential between the two, and then the fine structure splitting is solved for. Subsequently, effects that stem from other electrons are added as perturbations. Many body perturbation theory may provide a more accurate method for calculating the fine structure splitting; this approach will be pursued in the coming months.

Neutron Optics and the Beam-Stop Problem
David Winogradoff

Thermal and cold neutrons can be treated similarly to rays of light. There are materials that allow neutrons to pass through, such as Aluminum, materials that stop neutrons, such as Cadmium, and materials that serve as neutron mirrors, such as Nickel. When looking at my problem, one of the important types of materials that affect neutrons is the neutron mirrors. One of the defining characteristics for a ray of neutrons in a specific situation is theta critical – the maximum angle at which the neutron will reflect off the surface of the neutron mirror.

Theta critical depends on several variables relating both to the reflecting surface and the neutron beam: the neutron wavelength, the atomic number density of the scattering surface, and the coherent scattering amplitude. For most materials, the coherent scattering amplitude is positive, but for some materials, such as Hydrogen, this value is negative, making theta critical imaginary, meaning all the neutrons that come in contact with the surface are scattered (i.e. no reflections occur). Similar to how light is directed through light fibers, tubes of neutron reflective materials,

known as neutron guides, are used to efficiently transport, through long distances, neutrons from a neutron source to a medium scattering instrument such as a collimator, a monochromator, or a detector.

In order to optimize the performance of such an instrument, it is important to understand how each part interacts with the incoming neutrons. In many cases, these multi-dimensional interactions can be simplified to the product of several lower dimensional interactions. In the case of reflecting rectangular guides, their performance may be characterized by defining a plane normal to the mean neutron direction and a set of cross-wise spatial and angular coordinates of the neutrons crossing the plane. Together, these coordinates define polygons in a 2-dimensional phase space. Each polygon can be associated with a specific group of neutrons. If their distributions are uniform, the area of each polygon gives the number of neutrons crossing a given plane per unit time. The total number of these polygons for a given system defines the acceptance diagram for the system.

I am working on a program that, given a system with several parameters, creates an acceptance diagram. I am working with John Copley, who has written a similar and more general IDL procedure, and Jeremy Cook, who has developed a Monte Carlo program. The system involves a beam exit, a sample, a beam-stop, and a set of detectors. We know the ideal placement of the beam-stop, but the current experimental results do not match the expected ones, and we would like to know why. Even though many of the parameters are fixed for the specific situation for which the three programs (Copley's, Cook's and mine) are geared, they would allow for greater generalization and use in future projects. As for more specific information concerning the system, the beam-stop has the same width as the guide, the detectors are 4 m away from the sample, and the neutrons being used have wavelengths between 4 and 8 Å. In my presentation, I will provide equations and sample diagrams and explain the results produced by my procedure.

Hood College

Combinatorial Pulsed Laser Deposition of Functional Oxides
Hilary Stauffer

This talk will highlight research in combinatorial methodology on oxide thin film systems grown via pulsed laser deposition (PLD). The growth and characterization of functional oxides, the ferroelectric material $BaTiO_3$, and the conductive material $SrRuO_3$, were studied to optimize their use as thin films in electronic device applications.

Combinatorial library film preparation by means of PLD allows for an easy and efficient way to study processing space. The use of an aperture makes possible the deposition of multiple films on a single substrate with differing growth conditions, such as temperature and oxygen pressure. Characterization of crystallinity and electrical properties of the $BaTiO_3$ library films were done using x-ray diffraction and electrical measurements done using a probe station. A high-throughput screening tool was used to measure the resistivity of $SrRuO_3$ films and the degradation of these films after room temperature annealing over time. Other work studying

the effects of annealing on capacitor devices, including annealing in forming gas and oxygen annealing, will be discussed.

High-Fidelity Simulation Environment for Testing Virtual Robots
Eric Walton

Eliminating unnecessary risks for humans is a concern of many companies whose jobs are often unavoidably dangerous. Replacing these hazardous positions with autonomous robits is the ideal solution since there is no loss of life when a robot is damaged. Unfortunately, it is very expensive to build these robots and equally impractical to test programs on actual robots. An alternative to testing the robots in reality is to test them through a computerized simulation.

The Urban Search and Rescue Simulation (USARsim) Department has focused its attention primarily on all aspects required to reach and identify humans who have been involved in a disaster so that a rescue team can m inimize the risk of injury upon rescue. USARsim has been using a computerized simulation based on the Unreal Tournament 2004 game engine and physics to test algorithms. Fortunately, better software exists that allows USARsim to be more complex in its sensors and physics.

Three game engines have been chosen as potential candidates to replace Unreal Tournament 2004: Unreal Tournament 3, Panda 3D, and Ogre 3D. The best suited candidate will be chosen based on graphics and realism of physics, a visual world editor, compatibility with old code and graphics models, and the ability to maintain a fast and accurate simulation since the complexity increases with the addition of robots and sensors.

To test the abilities of the three game engines, each software has a goal of producing a simple robot that could navigate the world with applied physics. Using code from Unreal Tournament 2004 would be ideal as it would eliminate the time spent recoding.

Ultimately, even though Unreal Tournament 3 required some modification of code it is the best candidate that was able to effectively use the old Unreal Tournament 2004 code.

Indiana University of Pennsylvania

Quantum Mechanics and the Mystery of Life: Quantifying DNA's Interactions
Lauren Abbott

A distinct gap exists between theoretical and experimental science. Computational science has started to bridge that gap. By explaining experimental data theoretically, scientists can advance science through predictions based on these theories. Computational scientists are able to obtain results for systems that complement those found experimentally, using modeling and simulation methods based on varying levels on theory. Simulations run at the atomic scale are more time consuming due to the quantum theory required. Even though computing power has increased significantly, scientists are able to run high level calculations on only the smallest of molecular

structures. Thus, the dilemma with computational science is finding a balance between speed and accuracy.

Within computational chemistry and biology, there is a big interest in modeling DNA, the backbone of life. Even small strands of DNA structures have hundreds of atoms, systems far too complex to model using quantum theory. However, by running varying levels of calculations on the stacking and bond interactions of different pairs of nucleotides, we can compare how the lower level methods perform with respect to the more accurate, higher level ones. From our results, we will be able to determine which low level calculations represent the molecular interactions in DNA most accurately and are best to use on more complex systems. With an accurate computational model of DNA, not only will we be able to improve our understanding of the structure of DNA, but also how it functions.

Iowa State University

Assessing Cell Morphology and Adhesion of a Small Library of Tyrosine-Derived Polycarbonates
Bethany Juhnke

Advances in material synthesis have yielded new polymers possessing a wide variety of functional groups and architectures and corresponding physical properties. Identifying materials exhibiting favorable interactions with cells is challenging especially within libraries of closely related materials. This presentation will focus on the assessment of cell morphology on a small library of tyrosine derived polycarbonates synthesized by the New Jersey Center for Biomaterials. The materials, some of which are in the FDA approval process, are being applied as active and passive devices in orthopedic, cardiovascular and wound healing applications. The cells were MC3T3-E1 preosteoblast cells. First, the cells were seeded, cultured, fixed and stained on polymer spin-coated slides. Second, a LEICA DM RXA2 automated microscope was used to image the cells. A cell analysis software, created within the Polymers Division, enabled an automated analysis of the cells and defined the morphological characteristics of the cells. This study allowed us to better understand the cells interaction with different polymeric surfaces.

James Madison University

Optimizing Standard Addition Design for Minimal Uncertainty
Lydia Barker

The calibration curve is the most frequently used experimental method for chemical determinations. The uncertainty of measurement based on this approach is often assumed to be fixed, but is actually heavily dependent on the details of the design, including homoskedasticity of the data, location of calibrant points along the curve, and number of repetitions. A design with evenly spaced points is the most common, but it may not be the best. Optimal design suggests an evenly clustered one, wherein all points are located at the two extrema.

Based on our previous experiments analyzing sulfur in biodiesel using the standard addition method (SAM) for calibration, it was hypothesized that a different design might yield better uncertainty for this particular technique. Subsequent modeling demonstrated a significant improvement in uncertainty with use of asymmetric clustering: n-1 points at the minimum and 1 point at the maximum. This design greatly simplifies SAM because only one calibrant need be prepared. This design was tested by laboratory experiments using monochromatic X-ray fluorescence spectrometry to measure low-level sulfur in diesel SRMs.

Determination of Toxic Metals at Trace Levels in SRM 955c Caprine Blood by Isotope Dilution Inductively Coupled Mass Spectrometry

David Berry

NIST Standard Reference Materials (SRMs) are relied upon to provide quality assurance and comparability of analytical measurements. Measurement results without these two components are not very useful. SRM 966 L1 and L2 is a bovine blood-based standard containing trace levels of toxic metals such as cadmium (Cd) and mercury (Hg). SRM 966 L1 contains natural levels of toxic elements which are present in the pg/mL range. SRM 966 L2 contains elevated levels of toxic metals in the ng/mL range, representative of someone who has been exposed to unsafe levels of these elements. Since Cd, Hg and their compounds are highly toxic, accurate measurements in blood are needed to correctly evaluate exposure to these toxic metals. Clinical laboratories perform millions of blood measurements each year and they rely on SRM 966 to provide quality assurance for their results. However, the supply of SRM 966 is running out and NIST has plans to replace it with an existing material, SRM 955c. SRM 955c contains Cd, Hg and additional toxic species at concentration levels similar to SRM 966, but the Cd and Hg are not certified.

In this project we used isotope dilution inductively coupled plasma mass spectrometry (ID ICP-MS) to measure Cd and Hg. ID-ICP-MS is a method that can produce very accurate and precise results, but the determination of such low concentrations presents challenges with regard to procedure blank and interference from the blood matrix. For the previous determination of Cd in SRM 966, Cd was not separated from the matrix because blank from the more complicated analytical procedure could cause additional uncertainty in the measurement. We investigated ways to separate Cd from the blood matrix without increasing the procedure blank. A procedure using anion exchange chromatography was developed and successfully applied to the determination of Cd in the elevated level of SRM 955c. The expanded uncertainty for the Cd concentration of SRM 955c L2 was improved by a factor of 5 relative to that for SRM 966 L2. However, additional research is required to effect improvement in the uncertainty of the L1 Cd concentration. Mercury was determined by cold vapor ID ICP-MS. In this procedure Hg is separated from the matrix as Hg vapor and introduced directly into the ICP-MS, which gives high selectivity and sensitivity.

Johns Hopkins University

Preparation and Characterization of a New Tethered Bilayer Lipid Membrane (TBLM) Model Membrane System

Tiffany Ng

The structure of biological lipid bilayers is facilitated by the creation of biomimetic membranes at or near electrically conductive solid supports. However, when placed directly on a solid support, the space between the inner leaflet of the membrane and the support surface is too small to allow the significant presence of an aqueous space necessary for the full incorporation of integral membrane proteins (IMPs). This perturbs the natural conformation of the IMP and the bilayer, preventing the study of structure and function of accurate biological models.

To remedy this, tethered lipid membranes have been developed, such that the bilayer can be suspended above the support surface, maintaining its fluidity and increasing the space between the membrane and the support. In the past, an anchor molecule (synthetic lipid) developed at NIST, WC14, has been used to tether the bilayers above the solid support. More recently, a new anchor molecule has been prepared, FC16, which may allow more water to fill the space between the inner leaflet of the bilayer and substrate (solid surface).

In order to allow for the presence of water, however, the FC16 molecules cannot be packed too closely. Therefore, spacer molecules are used to decrease the surface concentration of FC16. The ideal ratio of FC16 to the spacer, β-mercaptoethanol, would be one in which there are as few anchors as possible, while at the same time allowing the formation of the bilayer with few or no defects. To prepare these bilayers, rapid solvent exchange was used with various types of phospholipids needed to complete the inner and outer leaflet of the biomimetic bilayer.

We are using various techniques to characterize this new system and determine the ideal molar proportion of tether to spacer, including spectroscopic ellipsometry, contact angle measurements, infrared spectroscopy, electrochemical impedance spectroscopy (EIS), and neutron reflectometry. From the ellipsometry, it was determined that the self-assembled monolayer (SAM) that forms from the tether molecules has a maximum thickness of 43 Å, approximately 10 Å longer than WC14. EIS revealed that one can create a tethered, fully insulated bilayer on lower concentrations of FC16 than on WC14.

In addition, investigations on tethered bilayer formation on WC14 with various concentrations of charged and uncharged lipids were performed using fluorescence microscopy. As time permitted, certain aspects of the synthesis of FC16 were carried out and the products were analyzed.

Juniata College

Development of an Axicon MOT for Rubidium Atoms
Justin Schultz

The development of the magneto-optical trap (MOT) has been pivotal in the control and manipulation of neutral atoms, and is an enabling technology in ultracold atomic physics. In a MOT, laser light and a magnetic field combine to trap atoms spatially and dampen their thermal motion, in essence, cooling them. Atoms captured and pre-cooled by a MOT can be transferred into conservative traps such as an optical dipole traps or magnetic traps can be evaporative cooled to form a Bose Einstein condensate (BEC) — which forms when the atoms de Broglie wavelength becomes comparable to the inter-particle spacing. Starting with a BEC, various experiments can be preformed, many of which include loading the BEC into an "optical lattice" — a standing wave of light forming a corrugated lattice potential.

Light can transfer momentum to and from atoms through the absorption and spontaneous emission of photons. In a conventional MOT, six laser beams (two counter-propagating beams along each principle direction) intersect in the center of a pair of magnetic coils in an anti-Helmholtz configuration. The circularly polarized beams are detuned below atomic resonance such that atoms moving more rapidly are Doppler shifted into resonance and slowed down; likewise, atoms which are displaced from the center of the system field are Zeeman shifted into resonance and are pushed back into the trap-center. Together, the light and magnetic fields combine, cooling the atoms and also creating a force that pushes the atoms to the center of the MOT (the magnetic field zero).

Unlike conventional MOTs, our arrangement uses a single slightly-focused laser beam with a 6 cm beam width incident on an axicon mirror. The laser has 6.835 GHz sidebands which is equal to the ground state hyperfine splitting in ^{87}Rb. The light reflects off the mirror twice before being directed back parallel to the direction from which it came. Rays from opposite sides of the axicon intersect in the center and have will have the correspondingly opposite circular polarizations necessary to form a MOT. Since the beam is focused, a portion passes through the axicon and is retro-reflected, counter-propagating with itself to provide confinement in the z-direction. Without the retro-reflected beam, this system essentially acts as a Zeeman slower creating a slow-moving, cool atomic beam. This system serves as a transition between a cool atomic beam source and a MOT.

Lehigh University

Microwave Methods Generating CdSe/ZnS Nanostructures
Joseph Sabol

CdSe/ZnS (core/shell) nanoparticles possess fluorescent optical properties in the visible range making them useful for biological imaging applications. The size of the nanocrystal controls the bandgap which intur controls the wavelength of the fluorescence properties. Recently, NIST researchers developed a method with which to synthesize CdSe/ZnS nanoparticles using

a microwave synthesis. Earlier procedures required synthesis in air-free environments and operating temperatures as high as 360˚C, but the microwave synthesis can be performed in short times, at relatively low temperatures (50˚C - 150˚C) and in normal atmospheric conditions. The new method requires a microwave irradiation unit and commercially available materials make synthesis in atmospheric conditions possible. Using experimentally determined synthesis times and temperatures quantum dots with size-dependent luminescent properties were produced. These wavelengths are in the 500 nm to 600 nm range, where smaller nanoparticles fluoresce closer to 500 nm and larger ones closer to 600 nm. However, the microwave synthesis procedure has thusfar been limited to producing spherical-shaped quantum dots.

Rod-shaped nanoparticles have some advantages over spherical nanoparticles. Not only do they fluoresce like spherical nanoparticles, but their fluorescence is also constant. Both the spherical and rod-shaped nanoparticles can be used as bioluminescent markers for cancer cells. The nanorods, with their constant fluorescence, will be better suited for imaging while still possessing the luminescent properties found in the spherical nanoparticles.

In order to produce rod-shaped nanoparticles using the microwave synthesis procedure, other conditions that are capable of synthesizing different shaped nanoparticles needed to be considered. A procedure published by Alivisatos et al. uses hexylphosphonic acid (HPA) to control the growth of CdSe nanoparticles. This procedure, like the microwave synthesis procedure, uses trioctlyphosphine oxide (TOPO) as a solvent, which shows potential for adaptation to the microwave synthesis. This presentation will highlight our efforts toward this goal.

Loyola College of Maryland

External Calibration of a Camera and Laser Range Finder
Lisa Schneider

The goal of this project is to examine existing methods for external sensor calibration, to evaluate them, and to appropriately estimate their relative and absolute accuracy. External calibration refers to the determination of the relative orientation and position of two sensors, and it provides the ability to analyze and fuse data from multiple sensors. This project is motivated by a number of robotic applications, including an increased focus on robotic navigation and manufacturing automation.

This evaluation observed the external calibration between a camera and a SICK 1-dimensional range sensor. For the different methods, points in the image and data points from the laser scan are used to determine the relative orientation and position between the camera and SICK. Also, these methods utilized closed-form solutions followed by optimization steps to obtain external calibration results. Furthermore, these methods which we implemented included different targets and techniques of optimization. Through testing and evaluating the error for each method, we can assess the robustness of the methods. Additionally, it helps to

determine what method should be recommended for robotics and to better establish the validity of visual data from cameras and sensors.

Massachusetts Institute of Technology

Standardizing Base Metric Scoring for the National Vulnerabilities Database Operations Team and Other Users of the Common Vulnerabilities Scoring System

Tammy Ngai

In this day and age, software and hardware vulnerabilities are almost unavoidable. More and more vulnerabilities are discovered daily and this makes keeping track of all these vulnerabilities a difficult challenge. For some vendors, not only do multiple vulnerabilities need to be fixed, some vulnerabilities are more dangerous than others and thus need to be addressed first. Unfortunately, the existence of various scoring systems complicates the analysis of a vulnerability's true risk and makes prioritizing fixes for vulnerabilities difficult. As a solution, the National Institute of Standards and Technology developed a public, online database of security vulnerabilities called the National Vulnerabilities Database (NVD). Not only does the NVD keep an ongoing list of security vulnerabilities, it also assigns a base impact score, computed using the Common Vulnerabilities Scoring System (CVSS) standard, to each vulnerability.

The authors of the Common Vulnerabilities Scoring System intended for the standard to provide standardization, consistency, accuracy, and transparency in scoring. Unfortunately, insufficient clarification and guidelines in the Common Vulnerabilities Scoring System documentation concerning particular types of vulnerabilities has led to scoring inconsistencies in all four areas as well as vendor complaints. The overall CVSS score is composed of three parts: a base score, a temporal score, and an environmental score. While individuals can assign temporal and environmental scores to a vulnerability to accurately represent their specific machines, the base score should be consistent across time and user environments. Ideally, anyone using the Common Vulnerabilities Scoring System should be able to arrive to the same base score regardless of prior security experience. Unfortunately, this has not been the case and it is clear that either the CVSS documentation needs to be revised or an addendum needs to be added to the documentation to provide both the NVD Operations Team and outside parties with further clarification of how current base scoring practices should be executed.

This presentation will give an overview of general scoring issues, scoring issues related to specific base metrics, and how the National Vulnerabilities Database Operations Team hopes to address some of these inconsistencies. Coming in as a vulnerability analyst with no prior experience in computer security, my project was to help format a CVSS guidance document by researching the origins of these scoring inconsistencies by doing daily vulnerability analysis and looking at my base metric impact scores compared those of seasoned analysts.

Contributions to the Electronic Kilogram Experiment: Measuring the Acceleration of Gravity and Configuring a Motion Control System
Beatrice Parker

The kilogram is the only base unit in the SI (International System/ Metric System) whose definition is based on a physical artifact instead of quantum references and the fundamental properties of nature. The scatter of the primary prototype artifacts is about 50 parts per billion after a century, affecting the uncertainty of other physical constants based on the mass standard. The goal of the Electronic Kilogram Experiment is to improve the measurement of Planck's constant *h* (by measuring the ratio of mechanical and electrical power in a watt balance) and provide an alternate definition to the mass standard.

Many measured values and quantum constants go into the mathematics of the watt balance, and the acceleration of gravity still holds a substantial uncertainty. Vertical gravity gradients at a standard location (U.S. Geological Survey marker) on the laboratory floor and 4 m up to the reference mass on the watt balance, as well as a comparison between the two locations, was necessary to "transfer" the absolute value from the standard location to the watt balance. Measurements with a portable relative gravity meter reduced the uncertainty from 12 parts in 10^9 (2007) to 6 parts in 10^9. These gravity and uncertainty values have proved to be reproducible within the better uncertainty.

There are two measurement modes needed to obtain the power comparison, one of which measures the force on a kilogram mass. This implies that a mass must be placed on and off the balance. A system of two stepper motors controls the vertical translation of the two separate masses. The second goal of this project was to configure a new motion control system for the two motors and encoder position sensor. New hardware was installed and re-wired, and the LabVIEW control program was updated and debugged for the new system requirements. Finally, the new system was tested, with further adjustments made to increase efficiency and smoothness of operation.

Miami Dade College

The Morphology of C_{60}/Pentacene Heterojunctions
Tyler Bonnen

The use of organic semiconductors in electronic devices is a developing industry driven by the promise of inexpensive materials, low temperature processing, and compatibility with flexible substrates. These unique properties have encouraged industrial pioneers to envision novel applications for these technologies. But while innovations may one day reshape the electronic industry, experimental applications have demonstrated that the transport properties and operating lifetimes of organics are far from suitable for most commercial applications.

The growth of organic thin films is not well understood, in part due to the complexity of the molecular building blocks and their interactions. Nonetheless, the use of organics in high performance devices depends on developing a greater understanding of interface morphology as it relates to electron transport. With an understanding of the growth of these interfaces, traits

such as grain size and crystallinity, which in part determine device performance, can be controlled.

As a donor and acceptor interface, Pentacene/ C60 heterojunctions serve as a prototypical model to understand device performance in organic light emitting diodes and photovoltaic cells. But while the growth of Pentacene thin films on many substrates has been categorized, outlining the utility and limitations of its morphology, far less is understood of C60 growth on Pentacene.

We have grown C60 on top of Pentacene under high vacuum conditions and studied the resulting interface morphology with Atomic Force Microscopy (AFM). The density of C60 grains and the surface roughness was measured as a function of film thickness, C60 deposition flux, and annealing. We have observed that C60 films tend to be granular in nature from their earliest stages even after moderate heating in vacuum. While some grain coalescence was observed as C60 film thickness was increased, the surface roughness was always considerable. These observations will be discussed using phenomenological growth models and previous molecular dynamics calculations of C60 transport on Pentacene.

Interoperability of Building-Related CAD Applications
Sebastian Palacios

Interoperability is a key component to the successful use of Building Information Modeling (BIM) across the building industry. An important aspect of interoperability is the exchange of files among different building-related CAD applications. Some of the file formats are IFC (Industry Foundation Classes) and CIS/2 (CIMsteel Integration Standards) product models. Over the past 10 years, IFC has been developed and published by the International Alliance of Interoperability (IAI), and is a commonly used format for exchanging Building Information Models (BIM). The IAI is an alliance of organizations, builders, software companies, information publishers, owners, designers, building product manufacturers, students, architects, and engineers whose goal is to develop a universal standard for information sharing and interoperability.

There are numerous issues affecting the exchange of information using IFC: (1) problems mapping from the CAD software's internal representation of objects to the standard file formats; (2) multiple methods of representing the same object in IFC; (3) lack of data structures in these standard formats to support certain building information and (4) imported information from the files being inaccessible in the CAD software.

This research involved analyzing and characterizing problems with the IFC exchange process with the following tasks: (1) modeling simple structures in different CAD applications and exporting them as IFC files to analyze, characterize differences, and track the flow of data transfer; (2) exchanging IFC files among different CAD applications, analyzing their import and export user interfaces, and characterizing the behavior of the data transfer; (3) analyzing past IFC exchange experiments, and building knowledge to find options to enhance their results and (4) building knowledge on the research results to continue developing the IFC to Excel translator which is used to asses, test, and improve interoperability via IFC files.

Time-of-Flight Laser Scanners and 3D Modeling
Jonathan Vega

At the National Institute of Standards and Technology (NIST) the Construction Metrology and Automation Group (CMAG) is developing a testbed. A testbed is an area in which an object can be tested in a controlled scenario. The testbed developed by the CMAG is formally known as the Intelligent and Automated Construction Job Site (IACJS) Testbed. The testbed is designed in partnership with the U.S. construction industry and academia and will provide the measurement tools necessary for testing the performance of and demonstrating new construction technologies (such as robots, positioning systems, information exchange protocols, construction methods, and etc.). Initial efforts are focused on developing a conceptual model of the testbed, which will serve as a tool for describing this research to industry and academia, and as a starting point for the final design. Currently the IACJS testbed is still a concept; no 3D model had been created to represent how the testbed will look or function. The IACJS testbed is projected to replace the tri-directional test facility (a current highbay lab at NIST in building 226). Using a 3D imaging device the highbay was scanned in its existing conditions. The 3D imaging device used in this case was a pulsed time-of-flight laser scanner. When using this type of instrument the output data is a 3D point cloud that can be manipulated within a computer program. Typically, after a scan the data is used as a reference for measurement purposes. The data can be used to query for exact coordinates of points in 3D space and, these scans are an ideal foundation for creating 3D models. In the IACJS Testbed model the 3D point clouds were used to create the 3D model, photo realistic renders and fly-through animations via a Non-uniform Rational B-Spline (NURBS) software (Rhinoceros). Rhinoceros functioned as the primary model software, Flamingo a separate plug in was used for rendering images and materials on surfaces and Bongo another plug in was used to create the animations.

Miami University, Ohio

An Atom-by-Atom Approach to Alzheimer's: Coordination in Metal-Peptide Complexes
Jesse Manders

Although metal ions play a critical role in biological processes ranging from nutrition, growth, and development to toxicity and neurodegeneration, the fundamental interactions between metals and biomolecules are often not fully understood. In recent years, numerous studies have investigated the role of metal ions in neurodegenerative diseases such as Alzheimer's and Parkinson's. These studies have identified active coordination sites on the amyloid-β protein, but the fundamental inorganic chemistry that drives processes, such as protein misfolding associated with the diseases, require further study. Using electrospray ionization mass spectrometry (ESI-MS), we achieve an atom-by-atom picture of the chemical interactions prevalent in metal-peptide complexes.

It is known that peptides with active basic coordination sites interact strongly with metals due to their Lewis Acid properties. We examine complexes with the monopeptides, histidine (His) and arginine (Arg), as well as the dipeptides, His-His and Arg-His, whose basic side chains bind

strongly with metal ions. The selected dipeptides are related to specific active sites identified on the amyloid-β protein.

ESI gently delivers ions from solution to the gas phase, giving us the ability to investigate the complexes as they are found *in vivo*. We further analyze the gas phase complexes *via* collision-induced dissociation (CID), revealing more detailed structural and energetic information.

We find, when comparing Zn^{2+} and Cu^{2+}, that the coordination energies are competitive. However, once one metal complexes to a site, the dissociation barriers are too great to allow a direct displacement by the other. CID indicates that metal coordination can occur at either residue on the Arg-His dipeptide, and both isomers are present in room temperature solutions with no strong suggestion as to the rank in coordination preference.

Millersville University of Pennsylvania

Using Video Games to Improve Visual Analytical Software for Digital Natives
Kevin Workman

Members of the generation currently entering the professional field have grown up surrounded by electronics. They are completely comfortable using text messages, social networking sites, and video game interfaces. Thanks to their immersion in technology, these "digital natives" have more highly developed eyesight along with the cognitive ability to handle larger amounts of information than their older coworkers. They have also developed new styles of communicating their ideas and forming collaborative knowledge.

To take advantage of these skills, the visual analytic field must develop software to accommodate the abilities of the incoming workforce. As older visual analysts retire, new employees will rely less on mentors and more on software for guidance in the field. Software that makes the most of the digital natives' skills will help them collaborate, form connections between data, and generally accomplish the goals of the field.

The software will include visually intensive graphical user interfaces conveying heavy loads of different kinds of information, much like a video game interface. This summer I designed, organized, and performed an experiment to examine behavior in a synthetic world with a focus on the effect of roles and communication on collaboration. The synthetic world served as a metaphor for the visual analytic field, sharing qualities such as personal interaction over the internet, collaborative knowledge, and both synchronous and asynchronous communication.

Results of the experiment will directly impact the development of visual analytical software. The next generation of graphical user interfaces must match the users' skills and expectations, and this study will help developers understand the needs of digital natives.

Montgomery College

Modeling of a Reinforced Concrete Portal Frame Under Fire
Semme Yilma

Concrete is among the most commonly used construction materials in the world. It is an intricate material that has complex properties which are difficult to model. Even though it has a high compressive strength, it is very weak in tension and can fail easily by cracking. This is why using reinforcement materials such as steel are required. It also shows a nonlinear compressive stress-strain behavior. In addition, it has the property of good thermal insulation. An experiment was done here at NIST to investigate its behavior under fire for a certain period of time. In order to simulate this experiment, it was necessary to build a representative computer model of the portal frame and make an analysis using finite element method. Finite element method is a method of piecewise approximation in which the approximating function is formed by connecting simple functions derived over elements. 3D solid elements were chosen instead of beam elements to represent the thermal flow more accurately. The presentation will cover a brief introduction to reinforced concrete behavior and finite-element analysis and it will also discuss the steps taken in building the model using the program ANSYS and the preliminary results of the modeling efforts.

Mount Saint Mary's University

ρ-Aminophenyl Phosphoryl Choline Purification of C-Reactive Protein for Development of a Mass Spectral Internal Standard
Christine Wroge

C-reactive protein (CRP) is an ancient evolutionarily preserved serum protein that is released by hepatocytes as part of the immune response. It has become one of the primary biomarkers for inflammation and organ rejection, and has also been linked to heart problems. Various assays are used by the medical community to quantify CRP in serum. NIST is working on a Standard Reference Material (SRM) and standard reference method in an effort to standardize them.

Comment [j1]: It would probably be helpful to mention why we want to make our own CRP (labeled) since you make it clear that pure CRP is commercially available

As a part of this overall project, there are efforts to develop isotopically labeled CRP for use as an internal standard in mass spectrometry applications. Current internal standards in mass spectral proteomics are labeled peptides, spiked into a mixture after protein digestion. These approximate but do not completely mimic the whole protein analyte. A part of this project involved performing a tryptic digest of pure commercially-made recombinant CRP in solution. Analysis of the digest by MALDI-TOF-TOF mass spectrometry revealed mis-cleavages in at least two locations. These results indicate that whole CRP is susceptible to mis-cleavage by trypsin and further support the need for a whole protein internal standard.

Efforts to develop these internal standards hinge upon producing pure recombinant CRP. Traditional purification methods involve Immobilized Metal Affinity Chromatography (IMAC), in which Ni columns are used to purify histidine-tagged protein (CRP) from cell extract. However, this technique is not very specific. A number of other cellular proteins have been

shown to have a high affinity to this column, preventing CRP purification. The goal of this project was to reduce these contaminants and impurities.

This project investigated a different approach in which immobilized ρ-aminophenyl phosphorylcholine was used to purify CRP directly from *Escherichia coli* (*E. coli*) cell extract. The specificity of CRP to phosphorylcholine has been well-established.

The phosphorylcholine affinity column was tested using commercially available recombinant CRP to assess the recovery. It was then tested using *E. coli* cell extract containing ^{15}N labeled, his-tagged CRP. The procedure demonstrated a high recovery in the elutions when pure CRP was used. Preliminary results from cell extracts showed a specific affinity but rather low recovery of CRP. Further complications were revealed by the presence of an unknown protein in the elutions of later trials and an inability to reproduce the level of recovery of the initial trial.

In all, the phosphorylcholine resin did not yield reliably reproducible results for the cell extract. Future work will investigate the preparation of the cell extract, to determine problems with ^{15}N labeled CRP structure and affinity to the column. These results will be used in future projects to optimize this CRP purification procedure, and to develop a SRM and a mass spectrometry-based standard method for C-reactive protein in human serum.

North Carolina State University

Design of a Detection Calibration System for Use in the Neutron Lifetime Project
Courtney Taylor

The Ultra-Cold Neutron (UCN) Lifetime Project is an ongoing experiment with the objective of improving the average measurement of the neutron beta-decay lifetime. A more accurate measurement may increase understanding of the electroweak interaction and improve cosmological theories on big bang nucleosynthesis. The current apparatus uses .89nm cold neutron beams to produce UCN through inelastic collisions with superfluid ^4He in what is known as the superthermal process. The experimental cell is located within a magnetic trap which serves to contain the UCN. The lifetime is then measured by detection of scintillation light from the superfluid ^4He created by electrons produced in the neutron decay.

Calibration of the detection system is needed to estimate the neutron beta decay detection efficiency within the experimental cell as a function of position along the length of cell. A calibration curve of light detected versus length along the cell from a light guide simulation program, GuideIt, has been made but comparison with experimental results is needed for accurate efficiency estimates. A radioactive source with beta decay energy similar to neutron beta decay will be inserted into the cell and moved along the length. Then a calibration curve will be taken. This is achieved using an earlier design from the previous generation of the Lifetime Project and improving it. This apparatus will be able to move the source the entire length of the cell under liquid helium temperatures. Design and construction will be discussed.

Oberlin College

Understanding Hydrogen Adsorption in Carbon-Templated Zeolites
Jacob Schalch

As a result of rising demand, dwindling supply, and pollution associated with traditional fuels, as well as global warming associated with excess emissions of CO_2, hydrogen fuel cells have become an attractive alternative as a clean, high capacity energy source. However, many obstacles must be overcome before a hydrogen energy infrastructure is possible. One impediment to use of hydrogen as a fuel is the lack of an efficient and recyclable means of hydrogen storage. My research here at the Center for Neutron Research has focused on understanding the structure and dynamics of hydrogen adsorbed in carbonaceous materials. In particular, I have been examining a NaY zeolites-templated carbon.

We began experimentation using a suite of analytical techniques to confirm the basic properties and characteristics of the materials. X-ray diffraction allowed us to confirm the short-range order in the carbon and successful removal of the zeolite. Use of Prompt Gamma Activation Analysis allowed us to find the approximate molar and mass ratios of elements that are present in the sample, confirming chemical composition and impurity levels. Both low-pressure and high-pressure gas adsorption isotherms, at various temperatures, helped us understand adsorption capacities as well as important characteristics such as surface area and enthalpy of adsorption.

Unlike x-rays, neutrons have a very strong interaction with hydrogen and can be used to probe the local adsorption environment and provide a measure of how strongly the hydrogen is attracted to that site. Filter Analyzer Neutron Spectrometer offered detailed insight into the quantum mechanical rotation of hydrogen at the local level in this carbonaceous material as a function of loading. Other neutron spectroscopic measurements using the time-of-flight Disk Chopper Spectrometer allowed us to observe the diffusion (or dynamics) of the hydrogen within the material at different temperatures. Having obtained a timescale for the hydrogen diffusing within the narrow pores of the carbon, we attempted to obtain higher resolution quasi-elastic data using the High Flux Backscattering Spectrometer.

Ultimately, this information may help us, and all hydrogen storage scientists, to understand and optimize the hydrogen-substrate interactions with various storage materials in order to create the most viable fuel storage solution for hydrogen fuel cell vehicles as well as other applications.

Pennsylvania State University

Ontological and User Interface Development for the Urban Search and Rescue Robotics Program
Adam Brockett

In the past few years, many advancements have been made in the field of robotics. Specifically, interest in using robots to assist search and rescue first responders has grown recently. Robots have the ability to fit in spaces not previously possible and use thermal imaging and other

advanced sensors to locate victims. However, this advancement is meaningless if first responders do not know how to best use these new resources and how well this technology works in different scenarios. Thus the advancement in robotic capabilities has to be matched with training and new tools for first responders.

In 2005, the Knowledge Systems Group of MEL at NIST started the Urban Search and Rescue Robot Performance Standards project in conjunction with the Department of Homeland Security's Technology Directorate. This project aims to assess which characteristics of US&R robots are of the most interest to first responders and subsequently develop tests for quantifying the performance of these characteristics. Once this data is gathered, it needs to be stored in a robust form and presented to a user who needs timely and simple access. Additionally, as first responders may not be familiar with the capabilities of given robots, a function to find a suitable robot given a set of requirements is needed.

To store the information about robot capabilities, an ontology implemented in OWL (Web Ontology Language) was developed. This format allows a more flexible representation of information than that provided by traditional relational databases. Additionally, OWL is a W3C standard and one of the backing technologies of the next generation Semantic Web. Thus, the knowledge stored in this ontology will be available to a wide range of applications in the future. To present this information to the user, a GUI application was written in Java. Characteristics that would affect a robot's suitability for a situation were identified. The application allows users to search over these terms and provides an intuitive, graphical representation of the results. For example, a first responder may require a robot with wireless communication that is able to operate for over 30 minutes on battery. The user can input these requirements using convenient drop down menus and the application will display a list of robots from the ontology that fulfill these requirements. As the ontology is still developing, these characteristics are easily expanded without requiring the entire application to be rebuilt.

An Atom Thick: Graphene Based Quantum Hall Resistance Standard

Matthew Chang

Once claimed to be a scientific myth, graphene, an *atom-thick* sheet of carbon, has demonstrated a multitude of fascinating electrical transport properties since its shocking discovery in 2004. These properties, along with graphene's two-dimensional nature, allow the Quantum Hall Effect (QHE), the quantum mechanical version of the classical Hall Effect, to be observed on graphene's surface even at room temperature. In the QHE, the Hall resistance depends solely on the invariant fundamental constant h/e^2. Moreover, the accuracy of the quantized Hall resistance is two orders of magnitude better than the current SI standard of the ohm and it is highly reproducible, making the QHE a new and valuable standard for electrical resistance.

The QHE is primarily measured in gallium arsenide (GaAs) heterostructures at liquid-helium temperatures and high magnetic fields. Only a handful of GaAs devices are of high enough metrological quality; consequently, most labs do not have direct access to the accuracy of the QHE resistance standard. Graphene's 2-D structure is ideal for observing the QHE. In addition, graphene's ability to display the QHE at room temperature makes graphene based QHE devices much more feasible than 3-D GaAs devices for many labs. This research focuses on the isolation

of graphene from graphite through mechanical exfoliation followed by the fabrication of a graphene based quantum Hall bar. If the resulting measurements are as accurate as those of GaAs devices, this will be the first step in a long-term goal in which QHE graphene devices, and thus a highly accurate standard of the ohm, will be disseminated to labs across the United States.

Two Photon Microscopy
Matthew Ebert

There are different microscope techniques to obtain images of samples. They include traditional optical, florescence, scanning tunneling, and atomic force microscopes. Each type of microscopy has its own advantages and disadvantages. In our group we look at how proteins diffuse in and on the surface of cells, so we label these proteins with luminescent probes so that we can easily see their behavior. In this case florescence microscopy is extremely useful.

We use fluorescent quantum dots (QD) as labels, which mark specific proteins so that we can easily record the motion of target proteins. Since the emission spectrum of a QD depends on its composition and size, we can even attach different kind of QDs to different proteins and track multiple protein interactions/movements. In order for these QDs to fluoresce they must be excited, usually by a laser, and each photon from the excitation beam is capable of easily exciting a QD. High resolution imaging of small numbers of proteins is challenging because scattered light can excite other QDs which are not at the focal plane of the excitation light. One solution to this problem is to use a total internal reflection florescence (TIRF) microscope which uses evanescent waves (from total internal reflection) to excite the targets only on or near (within about 100 nm or less) the surface of a substrate. However even with a TIRF, the confinement of the florescence isn't always good enough since the evanescence can extend up to several hundreds of nanometers depending on the excitation condition.

In the search for more refined ways to measure florescence in the focal plane of the excitation beam, I spent this summer constructing a two-photon confocal florescence microscope. It is the same principle as standard (one-photon) florescence but instead of using a beam that will be absorbed by the sample; we use a beam that is twice the wavelength of the one photon excitation. In order to facilitate two photon excitation, which is a rare transition process in photoexication, a powerful femtosecond-pulse laser was used. Even then is it unlikely that the quantum dots will be excited. For confocal imaging, we have the sample raster scanned over a focused laser spot, and the florescence emission from each point in the scan line is collected with a photomultiplier tube (PMT). A two dimensional intensity map was produced from these raster scanned pixels. This method has a high degree of accuracy but takes a relatively long time to produce an image making it useful for static samples. As a complementary approach to this slow technique, I also constructed a full-field fluorescence imaging technique to look at relatively larger areas of the sample at a high acquisition rate. Several samples including microarray spots on a glass substrate or on the surface in a single well of a 96 well plate as well as fluorescent beads on a glass substrate were imaged.

Process for In-House Soldering of Printed Circuit Boards
Adam Neal

In the CMOS Device and Reliability project, our goal is to advance measurement capabilities to enable a better understanding of transistor reliability.

With transistors operating at Gigahertz frequencies, the understanding of their transient response after stress is increasingly important in predicting their long-term reliability. To measure the transient response requires us to build high bandwidth, high gain, and low noise circuits not available commercially. Realizing circuits which fit all of these criteria requires that we use surface mount components to minimize parasitic circuit elements. Surface mount components must also be used to achieve a small enough printed circuit board (PCB) so that it can be placed very close to the actual source of signal.

Surface mount technology is well-established in the electronics industry; however, it is viable only to customers who need large quantities of a PCB. In research, we use one-of-a-kind circuits and will have to pay a high premium to get our PCBs custom-built. To make surface mount technology available to our research, my project is to devise and test a process to solder PCBs using readily available equipment - a toaster oven.

The important criteria for the surface mount soldering process are that the process be easy to use, be reliable, and have high yield. The importance of the first two criteria is obvious. The last one is important because there are many components on a PCB, so the yield must be high to ensure that the resulting PCB will work every time. I will describe how I planed and executed my experiments to achieve all of these goals.

To verify that I have a successful process, I will use it to design and build a high-speed (DC to 1.8 GHz), high gain (60 db), and low noise amplifier that will fit into the small housing of our probe station's electrical probe. If all works well, I will use this new measurement capability to demonstrate that we can take an existing experiment to new territory.

Purdue University

Characterization of the UV Degradation of Photocatalytic Nanoparticle-Filled Polymers
Craig Bouis

Inorganic pigments, such as titanium dioxide (TiO_2), are added to polymeric materials to enhance both the appearance properties and the mechanical durability. A common misconception is that these fillers are considered to be inert, despite their semiconductor properties. Research has revealed films dispersed with TiO_2 films exhibit measurable photocatalytic activity when exposed to ultraviolet (UV) radiation. A clear understanding of the degradation mechanism is needed in order to engineer nanocomposite coatings that take advantage of the particle photoreactivity by maximizing beneficial photocatalytic activity, minimizing negative effects of the photoactivity, and enhancing mechanical strength and fire resistance.

The focus of this work is to determine the role that TiO_2 pigments play in the degradation of polymer films and to develop a metrology for the photodegradation of polymeric nanocomposites. Previous studies within the research group have examined the degradation of filled polymer films in dry conditions at ambient temperature (25^oC and 0 % RH) and found that the the degradation of the films depended significantly on the polymer matrix.

That is, the photodegradable epoxy amine degraded to the approximately the same extent for all pigments making it difficult to determine the effect of particle reactivity on the degradation of the polymer film. The experiments conducted in this study were conducted at high temperature and high relative humidity (55^{o}C and 75% RH), a condition that is considered more realistic to an outdoor weathering atmosphere. Under these conditions it was observed that the extent of degradation between pigments was greatly enhanced. Laser Scanning Confocal Microscopy (LSCM) was used to follow the changes in morphology of the pigmented polymer films and to determine the changes in particle agglomerate size, polymer matrix pits/holes, and surface roughness of the film as function of UV exposure time. Attenuated Total Reflectance – Fourier Transform Infrared Spectroscopy (ATR-FTIR) was used to monitor the chemical changes within the model polymer as a function of exposure time.

Rensselaer Polytechnic Institute

Modeling Holey Fibers
Joseph Gibney

Photonic crystals fibers (PCFs) are a relatively new development in optics that is finding applications in a wide area of science and technology. Sophisticated fabrication techniques allow the manufacture of PCFs with remarkable accuracy which gives precise control over optical properties of the fiber such as dispersion, birefringence, and nonlinearity by varying structural parameters of the fiber. Fibers can be designed and manufactured for specific purposes with highly tuned optical properties without being limited by material properties. The type of PCF primarily studied is a periodic hexagonal lattice of air holes in fused silica with a central defect where light is confined. These fibers offer low loss, high nonlinearity, and potentially high birefringence with control of the zero dispersion wavelengths over a wide range.

Photonics modeling software was used to model PCFs and solve for the fundamental guiding modes, effective refractive index, and confinement loss of various fibers over a range of wavelengths. The finite element method (FEM) was employed for these calculations, and all calculations were made for both the principle and secondary axis. From these calculations it was possible to obtain dispersion curves up to a high order. By varying parameters of the microstructure such as air hole diameter and pitch, the dependence of dispersion on these factors was determined. The effects of compressing one axis of the array to induce birefringence were also explored. The calculated values of the effective refractive index were fit to polynomials, and used to study four-wave mixing in the fibers. Inclusion of high order dispersion should allow for a more accurate description of the parametric processes occurring in these photonic crystal fibers.

Measuring the Effect of Cytotoxic Compounds Using an Engineeered Reporter Cell Line

Johannes Kutten

Cell-based cytotoxicity assays are commonly used for initial identification of potential toxic compounds that are produced by pharmaceutical and other chemical manufacturing companies. For our experiment, *vero* (monkey kidney) cells engineered to produce green florescent protein (GFP) were used tested for use in a cell-based cytotoxicity assay. The assay is based on the knowledge that a healthy cell constantly produces and degrades proteins whereas unhealthy cells will downregulate protein production while continuing to degrade proteins at a normal rate. We hypothesize that this will be true even when the toxin does not directly affect protein synthesis. We can quantify the effect of the toxins on the cell culture by measuring the fluorescent intensity of each cell after they have been exposed to the cytotoxin. The eventual goal of this experiment is to demonstrate the effectiveness of this cellular assay in determining the toxicity of a given compound.

The "Multicenter Evaluation of *In Vitro* Cytotoxicity" study (MEIC, September 2000) had a similar objective. MEIC chose fifty compounds that were known to be lethal to humans and animals. These substances were chosen because toxicity data was readily available. We selected forty-four of these chemicals for our experiment, eliminating those which require a special permit to transport. For our initial toxicity screening assay, this list was further narrowed to sixteen substances. The final substances were selected to represent a compounds with varying commercial applications, lethal doses, and toxicity mechanisms.

For the experiment, *vero* cells were deposited into 120 wells of two 96-well cell culture plates. After 24 hours, the sixteen compounds, each with six concentrations, were deposited into cells. Each plate also contained four blank control wells, two "negative" control wells, and six "positive" control wells. The four blank wells were used to determine background florescent intensity. The two "negative" wells contained cells and a low concentration of DMSO, with no other drug present, to show how the cells would behave in absence of a toxin. Finally, the "positive" control wells contained cells exposed to a cycloheximide-DMSO solution at four different concentrations. Cycloheximide is known to inhibit protein expression.

After drug treatment, an automated microscope was used to take four fluorescent photographs of the cells in each well. Each photo was analyzed to determine cell count, nuclear area, nuclear stain intensity (a measure of DNA replication) and GFP intensity. With this method we were able to rapidly perform 60 experiments on each plate and obtain valuable data for comparing this new cell-based cytotoxicity assay to existing assays.

Rice University

Toward Monodispersity of Single-Walled Carbon Nanotubes via Ultracentrifugation
Laura Timmerman

Single-walled carbon nanotubes (SWNTs), which may be visualized as sheets of graphene rolled into a cylinder, possess extraordinary optical, thermal, electronic, and mechanical properties. These attributes make SWNTs a popular area of research for materials, nanoelectronic, and biomedical applications. However, as-produced SWNTs come in a wide range of lengths, diameters, and chiralities. Each combination of these dimensions possesses its own unique characteristics. Many applications would greatly benefit from the availability of monodisperse SWNTs; that is, nanotubes of the same geometric proportions.

Recent efforts toward monodispersity include the use of ultracentrifugation, a highly scalable technique in which liquid SWNT dispersions are spun at very high accelerations. In a centrifugal field, the minute differences in hydrodynamic properties of the nanotubes are magnified, allowing for separation by both length and diameter. Additionally, separation by chirality or electronic type may be achieved by exploiting selective affinity and packing structure of dispersants. In this work, ultracentrifugation process parameters were explored in an effort to optimize the sorting of nanotubes by diameter, chirality, and electronic type.

Saint Joseph's University

The Silk Purse from the Pig's Ear – Optimization of a Prototype Detector for Large Area Radionuclide Contaminated Urban Material Characterization
Nicholas Minutillo

One important aspect of dealing with cleanup of nuclear contamination should there be an RDD or IND incident in a heavily populated urban area is finding effective cleanup technology for the task. Reference Materials characterized for radionuclide content would be useful to evaluate the efficacy of the various cleanup technologies for effective remediation of the contaminated areas. The instrument I have been working with this summer is an alpha detector with a unique ability to accept samples that are tens of cm in x,y dimensions and a few cm thick. These samples could be a piece of concrete, metal, or other debris one might find within the blast radius of a dirty bomb. We are interested in knowing how this detector can be used to develop reference materials for the cleanup leg of a nuclear disaster response.

This ion chamber detector is a prototype built by XIA LLC (formerly X-Ray Instrumentation Associates) designed to detect extremely low activity alpha radiation in solid-state computer components. It was thought that as these products became smaller, the "soft-errors" that alpha particles can cause by flipping bits would become a serious concern. In our case, it is advantageous to have the ability to count large samples for the development of nuclear radiation cleanup materials like concrete and asphalt. Our efforts this summer were first focused on understanding how the detector can be best operated to sense emitted radiation and processes the information. Using a statistical experimental design, our goal for this part of the research is to understand how large a sample the detector can accurately count, how to best prepare a sample

for counting, and the range of radioactivity within which the detector best operates. As would be expected based on its original design intentions, the detector is efficient in very low ranges of activity and it appears to be able to accurately count samples up to 10 cm from the center of the detector anode, however, it needs a considerable purge time to operate reliably. Further work should include redesigning the counting chamber to be more gas tight, debugging the software of overflow errors at extremely low counting rates, improving the algorithm the software uses to classify signals as either alpha particles or noise, and an in-depth look at the many parameters built into the processing software for added flexibility in operating the instrument.

Saint Mary's College of Maryland

2D vs. 3D Measurement of HER2 FISH Bioimaging in a Cell
Patrick Bowers

Bioimaging may be used to visualize and quantitate the number and intensity of molecules within the natural architecture of an individual cell. Thirty percent of breast cancer patients exhibit an abnormal increase above the expected HER2 gene copy number of two. Clinical quantitation of HER2 gene copy number demands accurate measurement for the prescription of expensive medical treatment. Individual HER2 Gene spots in 2D, 3D, and deconvolved 3D images were numbered and the optical density of individual spots was measured using an image analysis application in IPLabs software. A flat 2D image of a breast cancer cell with HER2 genes was dependent on the focal plane and produced an opaque image. Undesirable light scatter observed in 2D and 3D images was greatly reduced with deconvolution performed with Huygens software. Deconvolution allowed for an increased quantitation of HER2 gene copy spots and produced a lower standard deviation for average optical density among individual HER2 spots. Optimal imaging and quantification of the multiple gene copies of HER2 in cancerous cells may be achieved using 3D images produced with a stack of deconvolved photographs.

Characterization of a Medical Imaging Camera for Improved Color Contrast of Human Tissues
Sara DeSavage

Cameras can be used to view still images as well as video images. In clinical medicine, cameras are often used to capture images to aid a practitioner during examination or surgery (example, surgical camera). The information from this type of camera is red, green and blue color corresponding to the human eye's receptors. However, the appearance of objects is greatly influenced by the color of the incident light.

Through the study of spectrophotometry, it is hoped to be able to use different spectral distributions of light to "stretch" the "red" colors (wavelengths approximately 600-750 nanometers) for applications in the medical field. As a result, colors like pink and red could possibly be more noticeably different. An application of this outcome would be to make the difference between various tissues, veins or arteries more distinct. A separate project is using a monochrome camera but having only light at distinct wavelengths incident on the object. One application is the measurement of oxy and deoxyhemoglobin through the skin using light in the near infrared region.

The focus of my project was to prepare the reference camera (CoolSNAP HQ2) to test images with the different spectral distributions. Various tests were run on the camera (Qimaging) for measuring hemoglobins. The absolute responsivity of the camera was characterized at the wavelengths of 640, 700, 760, 820 and 850 nm. Several lenses were tested for relative transmission at the longest wavelength to determine the optimal lens for our study. To write the program for future use with the CoolSNAP HQ2, the dynamic link library of the camera was explored. This library is the form of communication used between the computer and the camera.

The Effect of the Floor on Thermoplastic Melt Spread Rate in a Fire
Martin Mooney

In a fire, thermoplastic materials such as upholstered furniture, mattresses, and solid plastic assemblies often melt and drip onto the floor, forming a liquid pool that, if ignited, interacts with the fire on the object itself. This has a large effect on flame spread and fire growth. The thermal properties of the floor influence whether the polymeric material melt cools and solidifies or remains fluid and carries fuel (and the fire) far from the burning object.

The goal of this project is to model the effects of flooring on two-dimensional melt spread from burning thermoplastics. A computational model is used to investigate the effect of different parameters, such as floor material, floor angle, and boundary heat flux, on the spread rate of the thermoplastic melt. To model the movement of the melting thermoplastic, a mesh is simulated and properties of individual vertices are calculated at each time step. Comparison between experiments using different mesh sizes leads to a linear regression that estimates the spread rate of an actual thermoplastic with an infinitesimal mesh size.

Estimating Volumes of Simulated Lung Cancers by B-Spline Modeling
Amelia Tebbe

The change of volumes of lung cancer lesions is a potential diagnosis tool to evaluate the effectiveness of various therapies. Lung cancer lesions are usually detected through Computed Tomography (CT) scans. There scans provide 2-d slice images of the lungs and are evaluated by Radiologists. This project aims at developing a means of estimating the volume of a lesion detected by a Radiologist by combining the scan slices into a 3-D image and computing a volume estimate. The Federal Drug Administration (FDA) has developed simulated lung cancer lesions, called phantoms, which are used to measure the accuracy of CT scans. The FDA has given NIST two such simulated lung cancer phantoms. The outer surfaces of these phantoms have been probed by a Coordinate Measuring Machine (CMM) in MEL. A program has been written to convert these scattered (x, y, z) points into spherical coordinates. These can be interpreted as coordinate of a surface in rectangular coordinates. Work is under way to model this surface using B-splines (Basis Splines). Once an adequate model has been developed, Green's Theorem can be invoked to estimate the phantom volumes.

Southern University and A&M College

Efficiency of 35S Promoter PCR Assays for Quantitation of Biotech Maize
Wade Reimonenq

"A biotech crop is a crop plant that has been genetically engineered using recombinant DNA technology either to promote or to prevent the production of a particular protein, with the objective of introducing or enhancing a desirable characteristic in the plant or seed" (Deynze et al 1). Seven lines of biotech maize that were genetically engineered with genes for pesticides and/or herbicides, were examined using Real Time Polymerase Chain Reaction. RT-PCR is used to amplify, isolate or identify known sequence from cellular or tissue RNA or DNA. Each of the biotech corn lines has a transgenic construct in its genome. The genomic DNA sequences of the transgenes were known. All of the transgene constructs shared a small promoter sequence, 35S, in common. The RT-PCR process was run using five different primer sets on seven DNA isolated from biotech maize. The isolated corn DNA's were diluted in a series of most concentrated to least concentrated. These dilutions varied with each different maize DNA isolations. The primer sets were to amplify the modified corn DNA in the region of the 35S promoter. The crossing threshold (Ct) values were plotted against the log of maize DNA concentration to form the standard curve. The goal was to determine which set of primers was more robust and gave the best efficiency of amplification.

State University of New York, Binghamton

First Order Reversal Curve Measurements of Magnetic Tunnel Junctions
Theodore White

Tunneling magneto-resistance (TMR) based first order reversal curves (FORCs) were measured for several magnetic tunnel junctions (MTJ) and analyzed to determine the magnetic "soft" layer's distribution of switching fields. FORC measurements characterize the reversible and irreversible switching of magnetization (M) using a series of magnetic field sweeps. MTJ's consist of an insulating layer, in this case oxidized aluminum, between two ferromagnetic layers. A voltage applied perpendicular to the MTJ's layers produces a current due to electron tunneling through the insulating layer. Both the insulating barrier and the dot product of the M's of the ferromagnets contribute to the MTJ's resistance. In the magnetic field range of interest the change in resistance depends only on the M of the soft layer. Typical FORC measurements characterize the changes in a material's M by using B-H loops. In our case FORC measurements are taken using R-H loops because resistance is dependent on the soft layer's M. Traditional analysis of these R-H FORCs should allow calculation of the switching field distribution in the MTJ's soft layer. To our knowledge this is the first application of FORCs to MTJ's.

Swarthmore College

Using Interference Lithography to Create Magnetic Nano-stripes
James MacArthur

As feature size advances into the nano-scale in today's magnetic devices, the need for property measurements at the edges of patterned films is clear – for small enough structures everything becomes an edge. However, the edge properties of magnetic thin films are as yet an unexplored area in the study of magnetic nanostructures. Regular stripe patterns are ideal for edge measurement because they provide a large edge-to-surface area ratio. In this talk I will present the design and construction of an interference lithography setup coupled with a bi-layer resist stack lift-off technique as a method for creating arrays of parallel stripes to be analyzed using ferromagnetic resonance (FMR).

A regular stripe pattern is created using interference lithography. This technique relies on the superposition of two coherent plane waves of light to create a sinusoidal interference pattern over a large area. A spatially filtered 405 nm diode laser was used as the source. A Lloyd's Mirror configuration was employed to allow the top half of the incident beam to be superposed onto the bottom half, creating an interference pattern. A silicon wafer coated with photoresist was placed in this pattern, allowing for an exposure. To limit the intensity of the undesirable reflections off of the substrate, an anti-reflective coating was placed between the photoresist and wafer. After photoresist development, a layer of $Ni_{20}Fe_{80}$ will be evaporated on top of the patterned resist stack. The remaining photoresist and anti reflective will dissolve away during lift-off, leaving only the stripes of $Ni_{20}Fe_{80}$. These stripes will range from 120 nm to 300 nm in width, suitable for FMR analysis.

Because of the variable spatial period of the interference pattern, grating patterns of specific period can be manufactured. And although the Lloyd's mirror interference lithography setup is implemented to create regular stripes of magnetic material, it has potential for additional use. Regular arrays of dots or antidots can be created using perpendicular exposures.

Tulane University

Probing the UnderlyingPhysics of Graphene with Raman Spectroscopy
Tessa Johnson

Graphene, a monolayer of tightly-bound carbon atoms, has long enjoyed theoretical study as the starting point for a range of interesting carbon allotropes including graphite, Bucky balls, and single-walled carbon nanotubes. Prior to the physical discovery of graphene in 2004, an isolated atomic monolayer was considered an unstable, unobtainable structure. Currently there exists a great demand in graphene for experimental research and potential applications utilizing its in-plane strength and novel electronic properties. Barriers to applications include the difficulty producing large (>10 micron) free-standing sheets of graphene and distinguishing a monolayer from multiple layers or bulk graphite.

A NIST wide effort is underway to produce and characterize graphene and to fabricate and test graphene-based devices. A group of SURF students joined the team and participated in many levels of the project.

Raman spectroscopy provides a rapid and non-destructive tool to probe the underlying physics of graphene. The unique and rich Raman signature of graphene affords studying the layer number, the quality/defects of those layers, and electron-phonon coupling, just to name a few. The position and shape of the Raman peaks of graphene enables a definitive determination of the presence of the desired single layer. Raman spatial imaging of graphene is a key part of the NIST arsenal to enable the realization of applications.

University of California, Irvine

Influence of Nanoparticles on Short-term and Long-term Performances of Polymeric Materials
Nhieli Ly

This experiment is designed to test the influence of ZnO-nanoparticles (NANOBYK-3820) on the short-term and long-term performance of a-one component water-borne polyurethane system (BAYHYDROL 110). Thin and thick polyurethane films with various concentrations of ZnO-nanoparticles are prepared via spin coating and drawdown methods. Samples are then exposed to UV light in the SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) accelerated laboratory exposure device and outdoor conditions (on the roof top of NIST building 226 at Gaithersburg, MD). FTIR (Fourier Transform Infer-Red) spectroscopy and UV-Vis (ultraviolet - visible) spectroscopy are employed to monitor chemical changes of spin-coated thin polyurethane films with thickness about 6 μm. Films of approximately 100 μm thick are monitored for changes of mechanical properties for instance, elastic modulus, tensile strength, and elongation. Confocal microscopy and atomic force microscopy are applied to the polyurethane thin films to evaluate the surface morphological changes such as surface roughness from micrometer scale to nanometer scale. To investigate the effect of nanoparticles on the short-term performance of polyurethane, chemical, physical, and mechanical properties will be measured on fresh, unexposed samples. For long-term influence of nano-ZnO on polyurethane, all data from chemical, physical, and mechanical properties will be analyzed as a function of UV exposure time or UV dose.

University of California, Santa Barbara

The Normalization of Alanine Dosimeter Films
Griffin Rowell

Irradiated products are ever present in modern society. The uses of irradiation range from food sterilization to the strengthening of polymers. Even medical instruments are irradiated in order to ensure the safety of use on patients with even the most compromised immune systems. As the safety of the population can rely on properly irradiated items, this process must be accurate. In

addition to safety concerns, an inefficient industrial process can cost industry millions of dollars. Radiation dosimetry plays an important role in the feasibility of irradiation in industrial processes.

If an industrial processing facility uses irradiation in its process, radiation dosimetry enables the facility to track the dose of radiation the item is exposed to. While there are many types of dosimeters, one notable material is alanine. When exposed to radiation, alanine ionizes and becomes a free radical. Unlike most substances in this state, alanine remains stable. Due to this stability alanine is extremely useful in the radiation dosimetry field.

Many irradiation processes call for alanine pellets. In these pellets alanine penetrates through the pellet and known values for the number of alanine free radicals reveal the dose delivered to the material. In processes using less penetrating radiation thin films are necessary. However, the system of the film and the device used to measure the dose absorbed by the dosimeter have an inherent error of approximately 1.5%. Calculating a normalization factor and applying this to the calibration of the system improves efficiency and, thus, the usefulness of the dosimeter film.

University of the District of Columbia

Microfluidic Chips and Microwve-PCR for DNA Amplification
Amine Lambarqui

Specific fragments of DNA can be amplified for analysis using a technique called Polymerase Chain Reaction (PCR). This technique can generate millions of copies of a target DNA sequence *in vitro* to conduct DNA analysis for various purposes, such as paternity testing, hereditary studies, and forensic DNA profiling. During the process of PCR, the original DNA template is exponentially amplified in cycles of three steps occurring at different temperatures. Although PCR is widely used for its sensitivity and accuracy, it requires large sample volumes and it is labor-intensive, time-consuming and prone to contamination. Efforts at NIST aim to develop an on-chip system that uses microwave dielectric heating to carry out PCR. This would add automation to the PCR process, enabling faster reaction time and minimizing risks of contamination.

Our experimental set up includes a sophisticated microwave oven with a waveguide used to deliver microwave energy to the plastic chip inserted into an opening on the waveguide. The chip is a microfluidic device that has a well where the PCR sample can be deposited. PCR samples are made by mixing optimized volumes of deoxyribonucleotide triphosphates (dNTPs), enzyme, primers, buffer, and DNA template. A thermocouple of type T (copper/Constantine) is used to provide temperature feed-back from the sample in the Chip to a computer programmed to control the power of the microwave generator. However, it has been reported that copper in the thermocouple inhibits PCR (possibly by changing the molecular configuration of the enzyme).

The goal of this study is to avoid the inhibition of PCR samples by using a dual-well chip designed to use a thermocouple only in one well to provide temperature feedback for control, leaving the second well free for PCR sample. A temperature correlation between the two well

needed to be established first. A thermoclycling protocol is then determined by testing the dual-well chips using (water/oil) samples to mimic the nature of the actual PCR sample. The dual-well chips are designed and fabricated here at NIST. The plastic materials used for fabrication are called Zeonor 1020 R and Zeonex 690 R.. In testing the dual-well chip, we used 15 µL of water and 10 µL of oil (to prevent evaporation) in each of the two wells. Additionally, we applied the use of two thermocouples. The first is used for control feed-back in one well and the second thermocouple is used to record temperature in the other well. This allowed us to adjust the temperature profile in each of the two wells, to see which would be most fit for microwave-heated PCR.

The control themocycling protocol suited best for microwave-heated PCR is as follows: 15 seconds at 85°C in the denaturation step, 50 seconds at 50°C in the annealing steps, and 40 seconds at 60°C for the extension steps. The three steps are one cycle repeated 40 times during each PCR process run. We apply this particular thermocycling to run microwave-heated PCR, by placing the PCR sample in one of the well without using a thermocouple. Analysis of the results is done using gel electrophoresis to quantify the yield for on-chip microwave-based PCR.

As a consequence of this study, PCR inhibition was avoided. Successful on-chip experiments should stem from these results, paving the way for a more comprehensive DNA analysis chip that will comprise exciting capabilities such as cell lysis and DNA extraction.

University of Florida

Diagramming the Phase Relations of the CeO_2-$Nd_2O_3Sm_2O_3$ System
Kevin Tierney

In these days of high priced oil, there is pressure to find an alternate method of energy production. Fuel cell technology represents a possible substitute to fossil fuel. Solid oxide fuel cells (SOFCs) are highly efficient, stable, cost effective electrochemical conversion devices that produce electricity by oxidizing a fuel. While fossil fuels can be used to run SOFCs, the most common fuel is hydrogen gas, which can be produced by using natural renewable energy sources to electrolyze water.

A solid oxide fuel cell is made of three basic parts: a cathode, an anode, and a solid oxide electrolyte which connects them. Oxygen gas is ionized at the cathode. These ions diffuse through the electrolyte to the anode, where they react with hydrogen gas to create water, heat and two electrons per oxygen ion. These electrons are sent through a load, creating electricity, and return to the cathode where they again ionize oxygen.

One of the barriers to widespread SOFC use is operating temperature; it is not uncommon for SOFCs to operate at up to 1000 ˚C. Yttria stabilized zirconia is the current electrolyte material of choice, but it is only usable at high temperatures. $Ce_{1-2x}Nd_xSm_xO_{2-\delta}$ is a possible material that could be used as an SOFC electrolyte at lower temperatures of approximately 600 ˚C.

A phase equilibria study of the CeO_2-Nd_2O_3-Sm_2O_3 system has been performed. From the phase relationships of the CeO_2-Nd_2O_3-Sm_2O_3 system, researchers will be better prepared to choose what molar concentrations to test. Disordered ceria is the only phase that works as an electrolyte material, and this phase diagram pinpoints its boundary. This will allow deeper investigation into the ionic conductivity and other properties of Sm_2O_3-Nd_2O_3 doped ceria.

Powders of various compositions were ground and heated repeatedly until equilibrated, then analyzed using X-ray diffraction. Attention was paid to concentrations near phase boundaries and more samples were created until the boundary was determined to within a few mole percent. Areas of interest for fuel cell applications are compounds within the disordered ceria phase and particularly those which are close in molar ratio to $Ce_{.85}Nd_{.075}Sm_{.075}O_{1.925}$.

Green's Functions, Scattering Effects, Impurities…Oh My!
Predicting the Behavior of Electrons Confined to Quantum Structures
Carlos Manuel Torres, Jr.

The study of nanostructures, such as quantum corrals and quantum dots, allows us to detect, observe, and exploit quantum phenomena that are quite different from the macroscopic world we are accustomed to. One motivation for studying these quantum structures is to observe their electronic properties, which may be used to develop novel concepts and benchmarks for post-CMOS (Complementary Metal Oxide Semiconductor) devices. A powerful tool to probe these structures is Scanning Tunneling Microscopy (STM), which is a measurement technique that detects the tunneling of electrons between an STM tip and the sample substrate. The tunneling current is related to the density of states, giving a topographical image of the substrate surface and allowing us to peer into the nanoscale.

In this talk, I investigate the electron interference patterns which result from embedding impurities into various arrangements on a substrate surface. On this surface, electrons form a two-dimensional electron gas (2DEG). We describe the propagation of electrons in this 2DEG, accounting for the multiple-scattering effects an electron experiences from the impurities (or scatterers) using Green's functions. I implement these Green's functions in MATLAB to calculate and display the change in density of states due to these impurities. Our goal is to develop a software tool which can predict the electron interference patterns resulting from diverse impurity arrangements (ie. circles, lines, ellipses, etc.) with specified parameters (ie. energy, scatterer phase shifts, scanning lengths, etc.). Comparisons are made with existing experimental results taken via STM in Joseph Stroscio's group.

<u>University of Illinois, Urbana-Champaign</u>

Modeling of Nanotube Separation in Field Flow Fractionation
Sibu Kuruvilla

The growing industry of nanotubes, a discipline of nanotechnology, has a very promising future. Carbon nanotubes, particularly single wall carbon nanotubes (SWNTs), have extraordinary properties. They are light, flexible, thermally stable, and can be up to 100 times stronger than

steel. SWNTs have the ability to be either metallic or semi-conducting depending on the "twist" (chirality) of the tube, and can be produced in different lengths and diameters. These traits provide the potential for their application in nanotechnology, electronics, optics, energy-efficiency, space travel and more. Although this range of properties is potentially very valuable, current nanotube synthesis techniques result in mixtures that are polydisperse with respect to both size and type. This presents an obstacle, because many applications require SWNTs with well-controlled electronic properties and of specific sizes. Thus, techniques to physically separate tubes by size and chirality are an active area of research.

One method being studied to separate nanotubes is a technique called field-flow fractionation (FFF). The basic technique, called flow-FFF, is able to size separate nanotubes with respect to length. In the present work, we used flow simulation to study a modification of the basic technique called Electric Field, Field Flow Fractionation (EF-FFF), as a means to separate tubes with respect to type. In EF-FFF, in addition to the usual FFF cross-flow, an AC electric field acts in the gradient direction. The AC field acts to align the nanotubes normal to the flow direction, working to overcome the shear field and Brownian motion – effects conventional to the particles while in flow. The simulation results show that as the rods become increasingly aligned, they undergo a transition from normal mode to steric mode separation, and thus provides a mechanism for type separation based on preferential alignment of metallics. In addition, the electric field strength needed to confine the tubes in near perpendicular orientation as a function of the anisotropy of the polarizability is estimated.

University of Iowa

Metric Evaluation and Report Generation for the NIST 2008 Metrics for Machine Translation Challenge (Metrics MATR)
Grady Payson

Machine Translation (MT) is a translation done by computers from one natural language to another. The desire for Machine Translation systems which could produce translations on par with those done by humans has been around nearly as long as there have been computers. One of the significant hurdles faced by the MT community has been the difficulty of developing standardized automated metrics. To date, the accepted measure for evaluating MT has been human assessment. This method, however, is often prohibitively expensive and time consuming to the point that it serves to bottleneck development.

In 2002, the development of BLEU [2002, Papineni et al.], a new metric for MT, sparked increased interest in the field. Despite today's widespread use of BLEU, it is not without its shortcomings [2006 Callison-Burch et al.] and a considerable amount of research continues in the field of MT metrology. However, individual metrics continue to be implemented and used in isolation of each other, giving rise to difficulties assessing the relative progress of any given new metric with respect to the rest of the field. To address this situation, the ITL's Speech Group has announced the NIST 2008 Metrics for MAchine TRanslation Challenge (Metrics MATR), in which research groups have been invited to have their metrics run on NIST's set of machine translations. All metrics are then evaluated on the basis of the correlation between the generated

scores and the human assessments of the same data's quality, as well as their ability to differentiate between MT systems of differing quality. In addition, several other factors including speed, repeatability, automaticity, and intuitiveness of interpretation are taken into account.

Given the enormous amount of data generated by any one metric, the decision was made to automate the evaluation of metric scores. This has been the primary focus of my involvement with Metrics MATR. In particular, I have had three main tasks. The first was to write Perl scripts which collect metric scores and run various correlation tests, and statistical tests, with results being stored in XML files. The second task was to produce graphs displaying human assessment scores versus metric scores. The final task was to automate the creation of web pages for each of the various metrics. In this manner we are able to create a complete workflow to quickly and efficiently automate the task of evaluating the metrics, creating graphs, and displaying the results on the web.

The 2008 Metrics MATR challenge is the first in what will be an ongoing series of evaluations. We anticipate making additions and modifications to subsequent year's challenges. With this in mind, my goal in this project has been to produce code that, in addition to performing the tasks it is designed for, may be easily extended for future use. We hope that this challenge will serve to raise interest and stimulate research in the evaluation of MT metrology.

University of Maryland, Baltimore County

Molecular Electronic Devices
Izath Aguilar

Molecular electronic devices are being studied as a possible alternative to traditional electronic devices, complementary metal-oxide-semiconductor (CMOS). In this work, I fabricated molecular electronic devices using organic molecules with different molecular dipoles to study the effect of the dipoles on the electrical characteristics of the junctions. After the native oxide was etched from wells in pre-fabricated device structures using a hydrofluoric acid solution, I self-assembled organic molecules in the devices. The two types of molecules used were: 1-Decanethiol (non-fluorinated) and Heptadecafluoro-1-decanethiol (fluorinated). I then evaporated silver on samples to produce top contacts and electrically characterized the devices with a probe station. Because the fluorinated and non-fluorinated molecules have different molecular dipoles, we expected to see electrical characteristics of the devices that were dependent on not only the resistivity of the silicon used in the device, but also on the molecular dipole of the molecules used. By studying how the molecules with each of the two dipoles affect the electrical characteristics of silicon with different resistivities, we will gain an improved understanding of electron transport through these molecular electronic devices.

Water Calorimetry and Heat Transport
Derek Fertig

The primary reference standard used to determine the calibration of field instruments used in medical radiation clinics in the US is based on water calorimetry, in which radiation dose is assessed by measuring temperature changes in ultrahigh purity water. Water is used because it is present in human tissue, and thus constitutes a sort of tissue-equivalent substance for dose measurements. However, it also presents certain experimental difficulties to the measurement of dose because it conducts heat and is susceptible to convection. The latter, being a nonlinear phenomenon, is particularly problematic if it occurs in the calorimeter; thus, nearly all water calorimeters employed as primary standards throughout the world are operated at 4^{o}C to eliminate the effects of convection. While such refrigeration is eventually envisaged for the NIST device, finding appropriate correction factors that would allow one to operate at room temperature would save both money and time when determining the absorbed dose to water. We have developed an experimental technique for studying incipient convection and conduction effects in water calorimeter vessels that may lead to precise estimates of heat-transport correction factors for such devices. Initial experimental results show very good agreement with the output of finite-element simulations.

Characterization of Local Mechanical Properties in Epoxy Nancomposites
Brandi Jackson

Nanoparticles are defined as particles that have a diameter less than 100 nm. They have been shown to provide significant enhancement of composite properties such as modulus, hardness, and oxygen transport at lower particle concentrations compared to micrometer size particles. These improvements are attributed to the large surface area to volume ratio of the particles. Mechanical properties of nanocomposites are often measured using bulk techniques. These techniques assume the mechanical properties are uniform throughout the material; however, this may not be the case. One question in nanocomposite research is whether mechanical properties are homogenous throughout the material.

In this research project, we investigated the impact of the silica nanoparticle concentration, matrix glass transition temperature, and matrix chemistry on the bulk material and local properties of the nanocomposite. Model Diglycidylether of Bisphenol A (DGEBA) epoxy materials were combined with silica nanoparticles at levels of 1 wt % and 5 wt %. Bulk properties such as T_g, dynamic mechanical properties (E' and E"), and decomposition temperature were characterized using differential scanning calorimetry, dynamic mechanical analysis, and thermogravimetric analysis. Local chemical and mechanical properties were characterized by ATR-FTIR and depth sensing indentation. Indentation measurements were conducted at the surface and along the cross section of the composite.

Development of Software Tools for Extracting Model Parameters of SiC Power Diodes
Jeong-O Jeong

The emergence of High-Voltage, High-Frequency Silicon-Carbide power devices is expected to revolutionize industrial and military power generation, transmission, and distribution systems.

Progress has been made in developing 10 kV SiC Junction Barrier Schottky (JBS), PiN, and Merge PiN Schottky (MPS) power diodes. The goal of the Defense Advanced Research Projects Agency (DARPA) Wide Bandgap Semiconductor Technology- High Power Electronics (WBST-HPE) Phase II program is to develop 100 A, 10 kV SiC power modules required to demonstrate a 13.8 kV, 2.75 MVA Solid State Power Substation (SSPS) in DARPA WBST-HPE Phase III. NIST is playing a critical role in enabling the development of SiC devices by providing electrical and thermal measurements, as well as developing and delivering electro-thermal models for circuit simulations to industry and other government agencies.

The goal of the SURF project is to develop and demonstrate a new software package called DIode Model Parameter extrACtion Tools (DIMACT) that is necessary to extract parameters for both Si and SiC power diode models. The software package is developed using LabWindows/CVI and consists of three programs: 1) JBS MeaSuRement (JBSMSR) program, 2) MPS MeaSuRement (MPSMSR) program, and 3) PiN MeaSuRement (PiNMSR) program. Each program incorporates graphical user interfaces (GUIs) for monitoring and acquiring data for diode forward characteristics, reverse recovery switching, and junction capacitance characteristics. The DIMACT software tools then uses an extraction sequence consisting of linear curve fitting and Gauss-Newton algorithm optimization procedures to determine the diode model parameters.

The model parameters extracted from the new DIMPACT tools are incorporated into diode models for simulation in the Saber circuit simulator. The simulated results obtained using these models is compared with measured data to validate the extracted parameters. The results demonstrate that the model parameters extracted from the JBSMSR program are accurate for both low voltage (e.g. 45 V) Si JBS diodes and high voltage (e.g. 10 kV) SiC JBS diodes. These models are being used as part of a 100 A, 10 kV half-bridge SiC MOSFET/JBS power module model that will be used to perform the simulations necessary to design the SSPS in WBST-HPE Phase III.

Observations of the Oxidation of Pentacene Thin Films in Air by Photoluminescence Spectroscopy

Andrew Schuldenfrei

In recent years, there has been significant interest in developing electronic devices using organic semiconductors. Such devices may eventually be inexpensive to make compared to present day silicon-based devices. In addition to their mechanical flexibility and ease of large area processing, they can be used in niche applications such as large area lighting, RFID, and solar cells.

One of the biggest problems encountered with organic electronics is that in contrast to silicon, they have a tendency to degrade rather rapidly under ambient conditions. This will limit their ultimate technological impact since the benefits in processing cost compared to silicon may be offset by the short lifespan of organic devices. It is therefore necessary to explore the phenomena and mechanisms of the gradual degradation of organic devices.

To this end, we have used photoluminescence (PL) spectroscopy to track the oxidation of thin films of pentacene ($C_{22}H_{14}$) in air. Pentacene transistors typically have among the highest carrier mobilities of any thin film organic semiconductor. However, this mobility has been observed to decrease over long periods of operation in air. This degradation process has been attributed to the formation of 6,13-pentacenequinone ($C_{22}H_{12}O_2$).

We measured PL spectra of pentacene thing films grown on SiO_2 under high vacuum conditions as a function of time for several days. The gradual oxidation of pentacene was tracked using the increase in intensity of the PL peak at about 570 nm associated with pentacenequinone. The rate of oxidation was measured as a function of initial pentacene film thickness and also measured for films stored in ambient fluorescent light compared to films stored in the dark. These observations show a gradual but nonetheless dramatic chemical degradation of pentacene thin films due to exposure to air.

Non-Linear Polymer Film Thickness Gradients Through Flow Coating

Nadezhda Serova

In sub-micron thick polymer film production, higher control and precision can be achieved with flow coating than the more popular spin coating method. This can be done through manipulation of factors such as the flow coater geometry and motion as well as the solution properties. In addition, flow coating can generate gradients of thicknesses in films as opposed to constant thicknesses created through spin coating. These gradients are vital in combinatorial research of polymers.

The flow coater in our lab was controlled by a simple Python program written a few years ago. The program allowed for only linear accelerations of the flow coater stage. Since film thickness is proportional to the flow coater stage velocity, it was only possible to make constant thickness films or linear gradients. My project included recreating the Python written programs in the more practical LabView code. More importantly, I was to implement the ability to program non-linear accelerations into the flow coater in a user-friendly program to be used for combinatorial research. I have created a program which can generate customizable linear, exponential, sinusoidal, step, and sawtooth film thickness gradients. In addition, the program supports a custom, user-entered function for the velocity profile. Finally, it is possible to combine multiple individually configured regions into one profile.

In addition to the flow coater control, I was to fix and improve another program responsible for automating the measurement of polymer films using the flow coater stage and an interferometer. I combined this functionality into the flow coater control program. The resulting program has several different limitations, but they can be minimized through optimization of a few factors. The program is easy to use and includes various error checking. The program I created as part of my project widens the range of possibilities of the flow coater and subsequent polymer research.

Large Building Evacuation
Kimberly Shurupoff

Currently, egress systems for buildings are designed around a concept of providing stair capacity (e.g. stair width) based on the largest number of people on any one floor in the building with little or no consideration for the number of people using the entire stairway, the presence of emergency responders, and occupant behavior on the stairs. In order to better understand what needs to be done to improve building design and evacuation procedures, a group in the fire research division at NIST is collecting video and RFID data from mid- and high-rise building evacuations from cities across the United States. The goal of this work is to provide building evacuation data to improve the overall level of occupant safety in buildings and to provide sound technical basis for improving current egress requirements in building codes/standards.

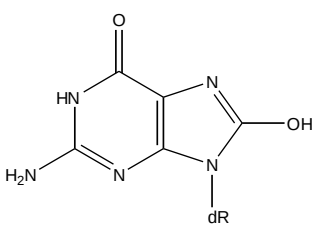
For my project, I participated in the video data collection of an 18-story building evacuation drill in Montgomery County. Cameras were set up in four stairwells and an exit corridor. The following day, I participated in the full building evacuation, exiting from the eighteenth floor. During this drill, 17 firefighters in full turnout gear ascended one of the stairwells while occupants were exiting. After all video data was collected, I digitized all footage from the evacuation and analyzed the footage from two stairwells, one of which included the firefighters ascending against the exiting occupants.

Analysis includes descriptions of all occupants (including their appearance, and whether they were helping someone exit, exiting in a group, and/or carrying objects), the floor exited from, entrance and exit times on each floor recorded, and time the alarm sounded. Using this information and dimensions of the stairwells, each occupant's speed was calculated over different distances traveled in the stairwells. Density, or number of people in a frame at a given time, was calculated over equal intervals as well for each stair. Using this specific data, we hope to gain a better understanding of how firefighters impact building evacuation in order to design and implement better procedures and building designs in the future.

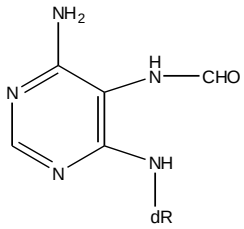
Fundamental Interaction Mechanisms of Engineered Nanomaterials with DNA
Christopher Sims

Reactive oxygen species (ROS) are generally small molecules such as free radicals, oxygen ions and peroxides that are naturally present in the body. However, an overabundance of ROS can overwhelm the body's natural antioxidant defense system and lead to a condition termed oxidative stress. Oxidative damage to the body's genomic DNA is one of the consequences of oxidative stress and is a direct result of the interaction of ROS with our DNA. It is not known at a fundamental molecular level if biomedically-relevant nanomaterials promote or hinder the formation of ROS in the body. If excess ROS are formed by nanomaterials, oxidative damage to our DNA could occur, leading to genotoxicity and/or cytotoxicity. This short-term research project is focused on determining if specific oxidatively modified DNA lesions can be formed in simple bicomponent solutions containing calf-thymus DNA (ct-DNA) and selected engineered nanomaterials. Gas chromatography/mass spectrometry (GC/MS) and liquid chromatography/mass spectrometry (LC/MS) will be utilized as tools to determine the presence

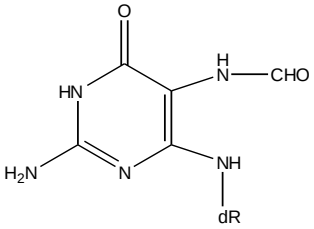
of oxidatively modified DNA lesions (See below, dR = 2'-deoxyribose) after test solutions have been incubated at 37 °C for 1 hour.



8-hydroxyguanine



4,6-diamino-
5-formamidopyrimidine



2,6-diamino-4-hydroxy-
5-formamidopyrimidine

An Energy Model on the IAQVG Test House
Julian Spiegler

Energy conservation in buildings has been an issue for many decades, but recent concerns over rising energy costs have fueled a bigger push for the standardization of energy conservation techniques in commercial and residential buildings. The Indoor Air Quality and Ventilation Group maintains a test house wherein data is collected that relates to indoor air quality, airflow, and energy usage. There are current models of the house that seek to study airflow and contaminant transport within the house, but until now, no energy model had been created.

The in-house airflow program, CONTAM, was coupled with the popular energy analysis software TRNSYS in order to create a model of the test house. The coupled method of energy modeling was first assessed by applying several industry-standard test cases for validating energy analysis software to the TRNSYS/CONTAM couple. After successful validation, building data with regards to heating, ventilation and air conditioning (HVAC), dimensions, weather and airflow was gathered. A basic model was created in TRNSYS/CONTAM that relied on a multizone approach. Rooms within the house were simplified to zones that function as control volumes in a thermal airflow system. Results for zone temperatures, air flows and heating/cooling loads were gathered from simulations and compared to experimental data. This is a continuing process; further modifications should be made to bring the model to a higher standard of conformity with actual data.

Results show that effective leakage area (ELA) of the building envelope plays a critical role in energy transport. The leakiest rooms experience the highest heating and cooling loads due to infiltration. Temperature differences between indoors and outdoors create pressure differences due to the stack effect which can increase infiltration. Higher air change rates in leaky rooms allow for good ventilation, but maintaining proper temperatures and comfort levels is a challenge. The goal is to minimize energy consumption while maintaining good indoor air quality and occupant comfort.

Parallel Covering Array Generation: The Future of Combinatorial Testing
Malcolm Taylor

Pairwise testing has become a popular way to validate software, check for bugs and uncover security vulnerabilities due to its ability to ensure that every variable value is tested interacting with every other variable value by covering all pairs. For this type of testing to be applied, sets of data must be generated that cover all of the possible variable interactions for a given variable group size. These sets of data are called covering arrays. When testing 2-way or pair wise interactions the covering array is not very time consuming to generate but as the variable count, values per variable or interaction size increase the amount of time begins to increase due to the NP-hard time bound on covering array generation. Prior research at NIST shows that software failures appear to be caused by a maximum of 4-way to 6-way interactions. Generating covering arrays for combinations this large with prior algorithms can take several days to weeks because the algorithms are highly sequential and therefore cannot be fragmented for parallel processing. However, a new method named Paintball has been developed here at NIST that allows for parallelization by generating large random numbers on multiple machines then aggregating them together and analyzing which of the numbers tests the most individual combinations. This type of algorithm allows for scalability and architecture independence while lowering run times. This research evaluates the parameters, constraints and metrics that apply to this type of parallel covering array generation as well as the ability to lower complexity of the test generation by automation and integration with model checking software.

University of Maryland, College Park

Optimizing the Nano-Manufacturing of Crystalline Single Electron Transistors
Jeffrey Birenbaum

Single electron tunneling transistors (SETs), transistors that rely on quantum tunneling for current flow, produce current one electron at a time. This behavior can be controlled to produce a single electron pump. SETs are also the world's most sensitive charge detectors and can therefore be used to develop current and capacitance standards. In addition, modified SETs can be used in quantum information, an exciting field that offers a radically different approach to computing based on the wavelike behavior of particles. The problem with current metal-based SET devices, however, is the charge offset drift, a phenomenon that prevents the devices from being used for more than a few hours.

In an SET electrons must tunnel from a source lead through a tunnel barrier onto a metal island. Once on the island the electrons tunnel out another tunnel barrier onto a drain lead. Standard SETs consist of layered Al-AlO_x-Al deposited via double-angle deposition. This process produces SETs with amorphous aluminum oxide as the tunnel barrier and aluminum as the metallic island. These SETs, however, experience a phenomenon known as charge offset drift, which randomly shifts the control curves of these devices over a period of a few hours. This prevents Al-AlO_x-Al SETs from being used over periods longer than a few hours without recalibration, preventing their integration into more complicated circuits. Most researchers

believe the charge offset drift is caused by motion of charges in the amorphous insulator changing the polarization of the island. Our goal was to produce an SET with crystalline aluminum oxide (Al_2O_3) and thereby greatly reduce the charge offset drift. We developed a new technique using a focused ion beam in combination with standard photolithography and ion milling to create the devices. We characterized and analyzed each step of the process to produce a robust method for producing the SETs.

Development of an Optical Waveform Generator Using Digital Micromirror Devices

Dustin Biser

The optical waveform generator (OWG) under development is a software based controller that converts time varying voltage signals into time varying optical signals by means of a digital micromirror device, or DMD. A DMD is a small electronic chip with a rectangular array of about a million programmable mirrors. Each mirror is close to 16 micrometers in width and has the ability to pivot ±10-12° along a fixed axis for reflecting light in different directions. The direction in which light is reflected corresponds to a particular mirror being on or off. A user defined voltage waveform is sent to the OWG which then issues commands to the DMD in order to create an optical signal that mimics the form of the voltage wave. A collimated light source is projected onto the surface of the DMD as its mirrors pivot in various directions. When all the mirrors are pivoted to the "on" position the DMD projects the maximum amount of light, and projects the minimum amount of light when the mirrors are pivoted to the "off" position. Each mirror can be independently pivoted so that a wide arrange of light intensities can be obtained within a given time frame. One important use of the OWG is the validation of remote sensing equipment, such as radiometers and hyperspectral imagers. During the validation of such equipment static images are often used, which consist of a large array of pixels. Each pixel has the ability to project different spectral wavelengths over a given bandwidth. In order to create scenes that simulate reality much more accurately it is desirable to have the ability to vary the intensity of any section of the image up to the maximum resolution of a single pixel. Therefore, with the combination of the OWG and other standard calibration equipment, an optical instrument can be validated with conditions that not only vary spatially and spectrally, but now also temporally.

Inclusion of Parallel Vectors in FiPy

Olivia Buzek

FiPy is a partial differential equation solver which uses the finite volume discretization method to obtain numerical solutions. Numerical solutions to these equations are often useful in materials science. FiPy obtains its solutions by creating a system of linear equations to represent the problem and solving them with a matrix representation of the system. The software then takes advantage of Python's interactive functionality to provide a straightforward interface to obtain solutions. This project focused on improving FiPy by including the mechanisms to solve equations in parallel using MPI.

The parallel functionality extends on an earlier SURF project to include packages from the Trilinos solvers software suite. To show an improvement in FiPy's efficiency, it is necessary for

matrices and vectors to be solvable across multiple processors. Previously, a Trilinos matrix wrapper was developed. To extend upon this work, the matrix wrapper was parallelized and a wrapper for Trilinos's parallel vector classes was developed for smoother integration with the rest of the FiPy software suite, effectively creating a parallel replacement for FiPy's previous use of NumPy arrays. This allows for faster evaluation of numerical solutions using FiPy.

I will present the results of our tests, which determined the calculable improvement using parallel matrices and vectors over previous serial operations.

Cheerios Gone Micro!
Suehyun Cho

In *The "Cheerios Effect,"* (Am. J. Phys., Vol. 73, No. 9, September 2005) Dominic Vella and L. Mahadevan discuss the driving forces behind self assembly of objects pinned at a liquid interface, Vella and Mahadevan challenge the common misconception that wetting properties solely determine the movement of self assembled objects through a simple experiment using two drawing pins. They explain that buoyancy plays a significant role in the assembly process. This claim is confirmed by an observation of two drawing pins pinned at the air and water interface, one complete and the other with the pin removed, repelling one another. The authors state that for smaller particles, the buoyancy effect should dominate the interaction.

One of the important challenges with measuring the Cheerios effect at the micoscale or nanoscale involves preparing suitable containters, "cereal bowls," for confining the particles laterally above a microscope. In other words, one would like to prepare bowls that will support and stabilize microscopic liquid menisci, and which can be filled with the appropriate fluids such that menisci are formed at the focal plane of the microscope.

In this talk, I will discuss methods that we have devised for creating various sizes of microwells through photolithography in order to image the Cheerios effect at the microscale.

Using X-Rayed Microcomputed Tomography to Assess Cell Adhesion and Proliferation in Polymer Scaffolds
Shauna Dorsey

Tissue scaffold research is a multidisciplinary field that involves designing, fabricating, and implanting artificial tissue scaffolds to repair damaged or diseased tissues and organs. A common example is bone tissue engineering. When trauma or diseases cause extensive bone tissue damage, polymer scaffolds can be used as templates to facilitate bone regeneration. Scaffolds provide the initial support necessary for bone formation as new bone cells adhere to their surface and proliferate. The scaffolds are biodegradable, leaving behind new bone tissue to heal the damaged area.

This project examines a new technique for assessing bone cell adhesion and proliferation in polymer scaffolds using X-ray microcomputed tomography (μCT). μCT is an imaging technique that uses scattered X-rays to create 3D images of test specimens for quantitative analysis. 3D imaging is important because cells behave more physiologically in a 3D

environment and biomaterials are typically used in a 3D format for tissue engineering applications. Traditional methods for assessing cell adhesion and proliferation are fluorescence microscopy and soluble colorimetric assays for DNA, protein or enzyme activity. Fluorescence microscopy is generally qualitative and cannot be used to examine cell adhesion and proliferation on the scaffold *interior*. Soluble colorimetric cell assays are quantitative but do not yield images for qualitative evaluation. The benefits of μCT over traditional methods are that it enables 3D imaging *throughout* the scaffold and quantitative analysis.

In order to test the ability of μCT to assess cell adhesion and proliferation in polymer scaffolds, MC3T3-E1 preosteoblast cells were seeded on scaffolds at six different concentrations and incubated for 1d, 7d, or 14d. Cells were cultured on the scaffolds, fixed and stained with osmium tetraoxide. Osmium is a heavy metal that stains cells, scatters X-rays and makes cells visible by μCT. The results show that μCT can be used to image osmium-stained cells on scaffolds for quantitative evaluation of cell adhesion and proliferation and examine cell penetration depth into scaffolds using 3D imaging.

This new μCT approach was validated against the traditional methods of fluorescence microscopy and a picogreen DNA assay. For microscopy analysis, cells were seeded on polymer scaffolds, cultured, fixed and stained with a florescent dye for cell nuclei. Cells were imaged by fluorescence microscopy to assess cell adhesion and proliferation. The picogreen DNA assay was also used to verify the μCT approach. Picogreen is a fluorescent stain for nucleic acids that is used to quantitate double-stranded DNA (dsDNA). The intensity of picogreen fluorescence is directly proportional to the concentration of dsDNA in a solution. The results from microscopy and picogreen agreed well the μCT approach. In summary, a new μCT approach was successfully established to quantitatively examine 3D cell adhesion and proliferation in polymer scaffolds.

Manipulating Microstructure to Achieve High Performance Organic Thin Film Transistors

Marina Feric

Organic semiconductors are expected to play a critical role in next generation electronics: notably, low-cost large area applications for which single crystal silicon is ill-suited such as, smart cards, sensor arrays, photovoltaics, displays, and RFID tags. This new generation of semiconductor materials is appealing due to their ability to be processed at reduced temperatures (near room temperature) using low cost manufacturing techniques and flexible plastic substrate materials. The organic thin film transistor (OTFT) is a key component in many of the anticipated applications.

High performance field-effect transistors are fabricated by inducing preferred crystallization of the organic semiconductor material at the contact interfaces via chemical modification of the metal surface. The thin film formation of different molecular structures was investigated on pentafluorobenzenethiol (PFBT) treated gold contacts to explore the role of different chemical interactions on the film microstructure. In particular, two similar organic molecules, tri-isopropylsilylethynyl perifluoropentacene (TIPS PFP) and tri-isopropylsilylethynyl

catafluoropentacene (TIPS CFP), were studied extensively and compared to better understand how the crystal structure and thin film properties influence their electrical behavior. These two molecules vary solely in the position of the fluorine substitution along the conjugated backbone, but exhibit significantly different interactions with both the chemically treated and untreated substrates. Overall, the field-effect mobility of these devices is directly related to their thin film microstructure.

Flow Table Reference Material
Nicholas Franson

The flow table at NIST is used as a reference in order to calibrate the rest of the flow tables in the USA. The material used to obtain the reference values is composed of silica powder and mineral oil, and the properties of the material needed to obtain reproducible data from batch to batch are yield stress and plastic viscosity. The purpose of the project is to study the influence of particle size distribution and viscosity of oil on the yield stress and plastic viscosity of the reference material in order to determine what the values of the constituents should be to ensure a proper value for the flow table.

The flow table test is an empirical standardized test that does not use fundamental properties of the material. Therefore, it is important for the flow table to be properly calibrated in order to ensure the correct consistency of the cement paste. If the paste does not have the proper workability, improper consolidation may result inside the hard concrete which lowers the stress the concrete is able to support. This project studied the influence of temperature on the reference material flow properties, and on the oil viscosity. Additionally, silica powder was ground and the change in particle size distribution was monitored. This will allow to determine the optimum grinding time for the reference material. The results obtained will be presented.

Robot Sensor Evaluation and Calibration
Aleksandr Gorbashev

In today's world, many robots and other intelligent systems rely on various sensors to evaluate the environment. Some of such sensors may include color cameras, infrared cameras and laser range sensors (Lidars). In recent years, the use of laser range sensors (Lidars) in intelligent systems such as robotics and automation has grown rapidly. In most cases, Lidar sensors are combined with other lidars or cameras to allow recognition, tracking and other applications including robot navigation and manufacturing automation. In order for such multi sensors systems to be useful, they must produce measurements in a common coordinate system.

In the Intelligent Systems Division, the Knowledge Systems Group is interested in calibrating SICK Lidar with a 3D Color Camera that would be used for robot navigation and manufacturing automation. In order for this multi sensor system to be calibrated to use common coordinate system, a special Pyramid type target was constructed. Such target must have a unique geometry in order for the SICK Lidar to provide a distinctive data sample for the external color camera calibration.

When the SICK Lidar images the target, it produces an array of points which are extrapolated to produce virtual intersection points. Such intersection points allow us to determine the orientation and position of the slicing Lidar plane, or the full 6 degree of freedom pose. Knowledge of the Lidar pose, allows the group to create the calibration.

Because of this target imaging process, the consistency in geometry and precision in target manufacturing is highly desirable. Before such precision can be achieved through NIST shops, two generations of targets were built for experimentation and experiment design. In this presentation, I plan to address technical issues involved in construction of the targets that affect the calibration process. These factors include the significance of the pyramid type geometry, surface characteristics, manufacturing challenges and other key considerations.

Facilitating Structure-Based Drug Design: Updating the HIV Structural Database
Christine He

NIST's HIV Structural Database (HIVSDB) is an online repository that organizes structural data related to HIV/AIDS research into an easily retrievable form with the aim of facilitating structure-based drug design. In structure-based drug design, drug discovery is guided by the three-dimensional structure of a drug's viral target, such as HIV protease. Drugs developed using this method are based on inhibition of viral proteins, and so the target's active site is treated as a space to be filled by a drug molecule that complements the site's size, shape, charge, and other bonding properties. For a single active site, many chemical structures may exist that effectively complement it. Thus in structural chemistry, the need exists for an efficient way to collect and compare these structures, called "fragments," which are pieced together to create an overall drug.

The HIVSDB fulfills this need by organizing HIV/AIDS related structural data into a chemical taxonomy that users query not with the name of an individual fragment, as is the case with existing databases, but with the structural category that the desired fragment(s) falls in. Structures are organized into a hierarchical tree so that a user may, for example, browse the category "six-member rings" and the subcategory "benzene" to retrieve a list of all benzene-containing fragments. Alternatively, users may query an individual fragment and retrieve a list of all inhibitors containing that fragment. In this way, structural chemists looking for compounds that exhibit a certain chemical property can efficiently find the entire range of potential structures without inputting any alphanumeric information, making the HIVSDB unique among all structural databases.

This project involves updating the current HIVSDB in two main ways. First, the existing database contains only structures relevant to HIV/AIDS research. This project aims to expand the database to incorporate all 50,000+ proteins documented in the Protein Data Bank, the world's largest public online repository of 3D structural data for proteins and nucleic acids. When this goal is achieved, the database will no longer be specific to HIV/AIDS but will be pertinent to research of all human diseases. The second major change that the database will undergo is the addition of 3D images to the existing 2D representations, adding a valuable dimension to the database.

Using Microfluidic Devices to Amplify Small mRNA Samples

Marc Howell

Studies in gene expression have many applications in biological research, including the understanding and detection of major health problems such as genetic disease and cancer. Microarray platforms are often used in these studies because they allow simultaneous detection of more than 2400 genes and can help identify changes in gene expression. With an understanding of these differences, it is possible to find the genetic basis for the phenotypic differences between cells (e.g. the genetic difference between a healthy and a diseased cell) and then to test for these genes of interest (markers) to detect disease.

There is a minimum mRNA sample size required for detection on current microarray platforms. In situations where only a few cells are available in a sample (such as biopsies or rare cell types), an amplification of 10^6-10^7 fold is needed to get usable results. A reliable method of amplifying such small mRNA sample sizes for use on microarrays would enable greater gene detection which could lead to more information about each cell's role in the tissue or culture being studied.

Of the available methods for amplifying mRNA for use in gene expression experiments, most require a larger mRNA sample than would be found in a single cell or a very small number of cells (most cells contain about 0.1 pg of mRNA), or would result in a length bias in the amplified material.[1] The Eberwine process transcribes double-stranded cDNA (produced from the original mRNA sample) into antisense-RNA (aRNA), amplifying the original sample approximately 10^3-10^4 fold per reaction without length bias.[2] However, this reaction becomes less efficient at cDNA template concentrations under 0.5 ng/□ L (10 ng in 20 □ L). To address this problem, we have created a microfluidic device to perform the Eberwine process using a column of 6 µm polystyrene beads, on which the mRNA can be isolated and immobilized, and cDNA reverse transcribed. Microfluidic devices were chosen for this application because higher concentrations of template cDNA can be achieved due to the small volume of beads (1-5 nL) when compared to test tubes (≈10 µl), thereby allowing the enzymes used in the process to perform optimally. The channels of the device contain sieve valves, which retain the beads while allowing the liquid reagents to pass through. This simple "flow through" design allows beads with RNA bound to them to be loaded and held in place by the valve, and then reagents flown over. Also, a single device contains 9 parallel channels, allowing multiple amplification reactions to be performed on the same device.

We began with on-chip processing of relatively large total RNA samples (10-100 ng) to demonstrate that full Eberwine processing can be run on a microfluidic chip. Smaller sample sizes near the single-cell level (about 100 pg of total RNA) were then processed to determine limits of amplification. Through all steps, both on-chip and benchtop processing are compared to determine which method gives higher gene expression coverage.

References:

1. FB Dean, et al. *PNAS*, 2002, 99, 5261-5266
2. R van Gelder, et al. *PNAS*, 1990, 87, 1663-1667

"Why Has an Answer to the LBA Problem Been Such a Mathematical Problem?"
Amy Hudson

This talk encompasses a history of how the linear bounded automata (LBA) problem sprung up among linguists, mathematicians, and computer scientists and is important enough in those fields that many people have tried to work on the problem without getting an answer. The LBA problem has still not been solved, whereas the similar four-color problem for maps has been.

A linear bounded automaton is a machine that has (1) a tape made of cells holding letters from a finite alphabet, and (2) a head that will read or write to one cell at a time and can be moved to any other state on the tape. You can also view the LBA as a Turing Machine with a finite tape length. Noam Chomsky, the famous linguist and philosopher, created a hierarchy ranking for syntax in languages, in which he labels the LBA as Type 1, being able to recognize a context sensitive grammar. Similar to, but more limited than, a Turing Machine, linear bounded automata are more accurately reflective of modern computers if the problem could be solved.

The LBA problem is that it is unknown whether nondeterministic linear bounded automata are more powerful than ordinary ones. The discovery, or at least evolution, of this problem may bring innovation in how programs are developed with regards to their language and exactly how much information they will be able to communicate given their finite tape. Many people have tried to answer the problem, with a few making progress in defining and partially solving the LBA problem; and some of these findings will be mentioned.

Edge-Roughness Modeling of Magnetic Nanostructures
Shifra Katz

In recent times, there has been considerable research conducted in current-induced switching of nano-scale magnetoresistive random access memory (MRAM) devices. The interest stems from the fact that spin-polarized MRAM is viewed as the future of non-volatile, high density, memory storage devices. At present, the fabrication of these devices uses electron-beam lithography to create magnetic nanostructures from various Co-Fe-B compositions. Such a process, naturally, leaves behind some characteristic edge roughness on the fabricated devices.

Using Object Oriented Micro-Magnetic Framework (OOMMF), developed at NIST, we modeled the spin-transferred switching properties of Co-Fe-B-like ellipsoids with sinusoidal edge roughness. In three series of simulations, we correlate the effect of edge roughness, ellipse aspect ratio, and tunneling current magnitude, respectively, with the time required to switch an element from an "on" state to an "off" state. In simulating these nano-elements, the recently published edge correction algorithm [1] has been vigorously tested and subsequently employed.

This research has a myriad of applications in the next generation of memory storage. With a deeper understanding of the behavior of magnetic nanostructures, we hope to facilitate the commercial production of the cheaper, faster, and smaller, spin-polarized MRAM device.

[1] M. J. Donahue and R. D. McMichael, Magnetics, IEEE Transactions on **43** (6), 2878-2880 (2007).

Combinatorial Synthesis and Characterization of TaCN Composition Spread Metal Gate Electrodes on HfO_2 for Advanced Gate Stacks

Hilary Lane

Traditional complement metal oxide semiconductor (CMOS) devices incorporated polycrystalline silicon (poly-Si) as the metal gate. This material, however, has lead to many problems, including scaling issues, Boron dopant diffusion, and poly-Si depletion. Furthermore, the selection of a new gate substitute has proven to be a complicated one. Criteria for an appropriate substitute lie on quality of interface with the oxide layer, electrical characteristics, and thermal stability.

Combinatorial methodology is ideal in solving these issues. It lets scientists conveniently synthesize a large collection of compositionally varying materials using the same conditions at one time. This is so monumental because previous efforts to explore new materials used the "one composition at a time" approach, which is extremely time consuming.

The goal of this research is to exhibit the effectiveness of combinatorial techniques in revealing the electrical and physical properties of the metal gate: TaCN on a high-κ dielectric (HfO_2). The metal gate is created as a composition spread "library" via a sputtering system, equipped with a moving shutter. The shutter allows for the formation of alternating TaN and CN wedges. Through a stainless steel shadow mask with hundreds of small openings, (150 μm diameter) we are able to generate hundreds of in-situ metal-oxide-semiconductor capacitors (MOSCAPS).

Rutherford backscattering spectroscopy (RBS) was used to determine the stoichiometry of the TaCN libraries. Scanning x-ray microdiffraction was used to determine microstructure. This revealed polycrystalline and amorphous structures for TaN and CN, respectively. Finally, a semi-automated probe station measured equivalent oxide thickness (EOT) and flat band voltage (V_{fb}) from hundreds of MOSCAPS. This allows for extraction of work functions (Φ_m).

The Effect of Processing on the Magnetic and Structural Properties of Magnetite Nanoparticles

Christine Lau

In general, when cancer cells experience a temperature greater than forty-two degrees Celsius for an appropriate amount of time, they die. On the other hand, healthy tissues do not experience the same damage until the temperature reaches forty-five degrees Celsius. This provides the basis for using magnetic nanoparticles in hyperthermia treatments for cancer. Though this idea has been around since the late 1950s, it has only been in the last decade that technological advancements finally allowed scientists to take steps towards making this treatment possible. The main mechanism behind hyperthermia treatments comes from the fact that magnetic nanoparticles generate heat when they are placed in an alternating magnetic field. For a successful cancer treatment, there must be a sufficient number of nanoparticles in the tumor, each generating enough heat to raise the temperature locally without affecting the surrounding healthy tissue. The nanoparticles studied here are comprised of magnetite (Fe_3O_4) cores that undergo a five-stage processing procedure, coating them in organic

material for both colloidal stability and biological tagging capabilities. Samples of varying sizes and from each processing stage were collected so that the effects of the procedure on the particles' magnetic properties and lattice parameters could be better understood. Using a SQUID magnetometer, hysteresis loops of all the samples were measured, and analysis showed that the magnetic properties of the particles stay consistent in the last two stages of processing but vary in the initial stages. Investigations of the magnetite nanoparticles' crystal structures were pursued using powder x-ray diffraction techniques. The results of this analysis reveal interesting systematic trends in the lattice spacing that also appear to correlate with processing parameters. This information will be used to start defining processing and structure property relationships in magnetite nanoparticles.

Study and Test the Performance of a Nanopositioner Controller Filter Compensator
Donna Le

The Precision Meso/Micro Systems for Nanomanufacturing project currently being conducted at NIST seeks to decrease the cost of nano-manufacturing by reducing the size of equipment and establishing high yield, parallel nano-manufacturing. This project features a MEMS micro-scale nanopositioning stage, a high precision device that is moved by bent-beam thermal actuators. To understand the actuator bandwidth and determine the effects of resonance on the device's motion, the frequency response of the stage is measured and analyzed. This data is critical to the mechanism's performance because it determines the fastest rate at which the nanopositioning stage can move without exciting resonant oscillations.

The objective of this project is to increase the working bandwidth of the device while still maintaining as close as possible uniform frequency response. Research was conducted on simple RC controller compensators and how they may be used to improve the frequency response of the nanopositioner controller system. Several simple RC circuits were designed. The most favorable circuits were fabricated and then connected to the existing controller and nanopositioning stage for testing. Their frequency responses were measured to determine which compensator circuit produced the best results. The most successful circuit significantly increased the device's bandwidth from about 42 Hz to above 90 Hz. Therefore, the addition of this compensator to the current controller improves its performance greatly.

Chemical Characterization of the Degradation of Poly-3-hexlthiophene (P3HT)
Timothy Lee

The discovery of conducting polymers in the 1970s and the modern demand for alternative energy has spurred research on polymer photovoltaics for electrical energy production. Polymer photovoltaics are of great interest because of their light weight and potential for cheap mass-production. Polymers with the ability to transform light into electrical energy can be easily dissolved in a gamut of solvents and deposited onto substrates by a variety of methods, including spin-coating, ink jetting, screen printing, and doctor blading, to create a thin-film conducting layer. Researchers are currently investing areas such as low power conversion efficiencies and short effective lifespans.

This study sought to analyze the photo- and thermal- chemical changes for poly-3-hexylthiophene (P3HT), a conducting polymer commonly used in polymer photovoltaic devices. Samples with P3HT films of varying thickness were created by spin-coating a dilute P3HT solution onto IR transparent double-sided polished silicon wafers, silicon wafers with gold films, and silicon wafers with silver films. The samples on double-sided polished silicon had either silver or titanium deposited on top to create substrate-polymer-metal arrangements and were heated on a hot plate. The substrate-metal-polymer samples were subjected to photo-degradation in ambient air at room temperature. Polarized backside reflection absorption infrared spectroscopy (pb-RAIRS) was used to obtain FTIR (Fourier Transform Infrared Spectroscopy) spectra of the polymer layers over time. The resulting spectra were compared to analyze trends in degradation time, degradation type, film thickness, and metal.

Characterization of Z-Axis Non-Linearity in a CD-AFM Scanner

Song Li

The goal of this SURF project was to characterize the non-linearity in the z-axis response of a critical dimension atomic force microscope (CD-AFM). CD-AFMs are instruments that can scan surface topography at the nanometer to micrometer scale and generate three dimensional images. Typically, these instruments employ piezoelectrically-actuated flexure translation stages to achieve three-axis rectilinear motion with low straightness and angular errors. In metrology-grade instruments, capacitance gauge displacement sensors are normally used to measure the displacement movement of the tip as it is scanned over the surface.

Although not inherently traceable, capacitance gauges can be readily calibrated and usually have good reproducibility. Capacitance sensors also have a high degree of linearity in their response to motion. However, for metrology applications in which an analysis of measurement uncertainty is required, it is necessary to characterize the level of non-linearity in the capacitance gauge response.

The most common method of characterizing the non-linearity of the z-axis in any type of AFM is to measure a step height at different positions within the range of the instrument. However, in this project we focused on an alternate method which involves scanning a tilted surface to produce a height change that is approximately linear with respect to lateral displacement. In this manner, our goal was to extract a ‘signature’ of the z-axis non-linearity.

A special holder was designed having sloped pockets with tilts of 3º, 5º, 7º and 9º into which we inserted a very smooth silicon chip for scanning with our CD-AFM. The use of multiple angles was important to understanding potential errors in our methodology. During data acquisition, we also used different locations on the chip and different orientations to separate the various contributions to our observations.

In this presentation, we will present a summary of our observations and our conclusions about the magnitude of the z-axis non-linearity.

Quantitative Performance Evaluation of Navigation Solutions for Mobile Robots
Keddy Liu

The necessity and demand for robotics, including with the manufacturing sector and the Urban Search and Rescue sector, is increasing globally because of the practicality of this technology. Robots are beneficial to society since they are capable of accomplishing various mundane tasks with high levels of accuracy and are able to operate in environments that prove very hazardous for humans. In order to safely integrate this technology into existing industries and other situations, it is a very important, but challenging, task to characterize the performance of these machines in any given setting. When evaluating these unmanned autonomous vehicles, various testing environments and settings must be utilized in order to thoroughly analyze the robot's ability to locate and navigate itself within the realm. Past research efforts around the world have been mostly qualitative, and there is no single agreed-upon quantitative means to test this autonomous unmanned technology. NIST has a long standing effort in the development of de facto testing standards and evaluation methods that allow researchers to quantitatively assess the performance of this technology and better understand each system's capabilities and limitations.

I am contributing to this project by using various open source software libraries and tools in developing a Java-based GUI (graphical user interface) application to help researchers quantitatively assess the performance of the robot being observed in a given testing scenario. This software application will stream and plot live data from the test subject and the test environment. It will allow the researcher to view the errors in real-time in order to better understand the limitations in the robot's navigation system. This is done by displaying a map of the test environment with the vehicle's true trajectory determined by external measurements of the vehicle's position, a plot of the vehicle's estimated trajectory determined by the its own sensory perceptions, and plots displaying the errors between the robot's true trajectory and its estimated trajectory. To help further assess the robot's ability to locate and navigate itself, the application will display an approximation map of the environment generated by readings from the robots on board laser range scanner, as well as other various displays and graphs. This interactive graphics-based application will contribute to this large, ongoing study by giving researchers a visual means to quantify the performance of their robotic test subjects in any given experimental scenario.

A ZigBee Implementation of the IEEE 1451.5 Smart Sensor Network
George Luo

Industry advancements in wireless and microelectronics technology now permit wireless transducers of increasing complexity and decreasing cost, size, and power consumption. The IEEE 1451 family of network transducers is crafted to take advantage of these recent advancements and provide a framework for “smart” sensors, called Transducer Interface Modules (TIM) that can communicate their own identity and capabilities upon startup to their wireless network partners, the Network Capable Application Processor (NCAP). From the NCAP a user will then be able to access or distribute sensor data as they wish. The IEEE 1451.5 branch of this family focuses on wireless transducers in particular and is designed to use existing,

popular wireless communication protocols, such as WiFi, Bluetooth, and ZigBee, for networking sensors.

The ZigBee is an industry-developed wireless communication protocol based on the IEEE 802.15.4 standard optimized for low-power, low-bandwidth wireless networks (often across transmitters operated by embedded microcontrollers). As many potential sensors and actuators fall in this range, it is of obvious advantage to adapt this protocol for use with IEEE 1451.5. This project is focused on the implementation of IEEE 1451.5 with-ZigBee in the C programming language. The platform used for this development is the Ember Corporation's EM250 Development Kit.

Fabrication of NanoPatterns by Nanoimprint Lithography

Devon MacNeill

The common goal for nanofabrication is high through-put, high fidelity and low cost; but traditional methods are limited by high cost, slow production methods, and optics. Light diffraction and scattering hinders traditional lithographic techniques, which use photons and electrons to alter the properties of the resist.

Nanoimprint lithography is a potential high resolution, high through-put alternative to traditional top down methods. This method is based on mechanical deformation of a resist material under high pressure and at high temperature. It is not limited by optics, like traditional lithographic techniques, so it can produce structures less than 32 nanometers. The reusable mold makes this process high throughput and can create large area patterns, on the order of square centimeters.

The objective of this project is to create a master mold with sub-100 nm structures. The mold was developed with nanoimprint lithography techniques. Thermal nanoimprint resist material was spin cast onto a four inch silicon wafer. Then the resist material was imprinted in the Nanofab with an original mold of defined surface grating. Highly anisotropic reactive ion etching (RIE) was used to transfer the grating pattern to the silicon wafer. The first reactive ion etch trial resulted in successful pattern transfer, but low pattern height. Measurements of the grating, via scanning electron microscopy (SEM), allowed for revision and optimization of the reactive ion etch recipe to achieve greater pattern height for later samples.

The mold will be completed by depositing a uniform thin film onto the pattern with low pressure chemical vapor deposition. This allows for the alteration of the pattern dimensions through variation of the film thickness.

This research will contribute to the development of cost effective processes to fabricate large area nanoimprint molds of sub-100 nanometer pitch size. The prepared mold can be utilized to investigate the nanoimprinted pattern stability and crosslinking density of ultraviolet nanoimprint resist as a function of pitch size.

Thermal Imaging Cameras: Testing and Validation of the Standard
Stephanie Martin

Thermal imaging cameras (TICs) are becoming a valuable tool for the fire service. Fire fighters can use these thermal cameras to rescue people in a smoke-filled room or find the heat source that caused the fire. In industry there are many types of thermal cameras, each is different and has varying performance levels. Therefore, a national performance standard is currently being written with the National Fire Protection Association that addresses design robustness and image quality. This standard ensures the safety, effectiveness, and utility of the fire service in their job, no matter which brand of thermal camera they use.

But how good is good enough? What is the minimum performance required for each area of image quality that allows fire fighters to use the thermal cameras effectively and accurately? Perception tests were performed at Night Vision Lab, where trained fire fighters were asked to identify a fire hazard in thermal images that were incrementally degraded in noise, contrast, brightness, and sharpness. From this data, minimum performance levels can be assigned to the tests in the standard. The thermal cameras will be objectively tested by certification organizations and the results compared with the minimum performance levels to determine compliance with the standard.

There are two general categories in which each thermal camera is tested: durability, eg., temperature stress, immersion/leakage, vibration, impact-acceleration, corrosion, heat resistance, heat and flames; and image quality, e.g., contrast, effective temperature range, spatial resolution, non-uniformity, and thermal sensitivity. The image quality test methods have been determined and are in the process of being validated through extensive testing. The primary focus of this work is validation of the image quality test methods.

Use of a Computational Fluid Dynamics Model for Fire Protection in Nuclear Power Plants
Alexander Mont

The Fire Dynamics Simulator (FDS) is a computer program that uses Computational Fluid Dynamics (CFD) models to simulate the growth and spread of fires. Because CFD models track relevant features of the space (such as temperature and soot density) over a grid of cells spanning the entire region, they can produce much more detailed and accurate results than previous fire models, known as zone models, which only divide regions up into a much smaller number of zones, such as a bottom and a top layer of a room. Hence, CFD models have been used in more and more applications in recent years. The NRC (Nuclear Regulatory Commission) is currently in the process of developing guidelines for the use of fire models, including CFD models, for fire risk assessment in nuclear power plants (NPPs). We have put together a set of sample scenarios based on fire scenarios commonly considered for NPPs and have run them with several different models, including FDS and existing zone models. We show that FDS and zone models can produce markedly different results for the same scenario, demonstrating that FDS can be used to identify fire hazards not detected by other zone models. This work will be incorporated into an NRC publication that will serve as a “user's guide” for fire protection engineering in NPPs.

Singled-Walled Carbon Nanotube Dispersions: A Study of Various Surfactants for Selectivity and Stability
Peter Niarhos

Single-Walled Carbon Nanotubes (SWCNTs) have many promising applications in today's nanotechnology due to their superior predicted optical, thermal and electrical conducting, and mechanical properties. However, in order to fully realize these potentials they must be separated and purified. SWCNTs are characterized by three criteria: length, chirality (diameter and angular rotation), and its helical rotation direction. Current synthesis techniques form heterogeneous bundles aggregates of SWCNTs of all different types. This diminishes the superior properties that make SWCNTs desirable. One method of separation is through dispersion in aqueous solvents using chemical surfactants. Dispersing in an aqueous medium is also advantageous because it makes it easier to manipulate SWCNTs. Two separate investigations were conducted to measure the dispersive abilities of various surfactants.

Porphines are highly conjugated heterocyclic molecules often forming the foundations of many natural dyes. Porphyrins are the family of dyes derived from the porphine base structure. Porphyrins have been found to be effective SWCNT dispersing agents. A recent study used a synthetic porphyrin-like molecule to selectively disperse right-handed or left-handed SWCNTs. However, a complex synthesis process was required to produce this synthetic molecule. We wanted to look at natural porphyrin derivatives to see if there was similar helical selectivity. We used naturally chiral porphyrin derivatives to disperse SWCNTs and used UV-Vis-NIR spectroscopy to analyze them. Qualitative comparisons and some quantitative studies were conducted to compare dispersion quality and debundling capacity. Work is currently being conducted to determine any helical selectivity.

One family of surfactants used was single-strand DNA (ssDNA) oligomers. Short-length ssDNA are known to effectively disperse SWCNTs through a wrapping model. One hypothesis is that ssDNA may form duplex-strand complexes. We performed a DNA denaturing study to examine this hypothesis. We dispersed SWCNTs in A_{30}, C_{30}, T_{30}, GT_{30}, and AC_{30}, and measured its binding efficiency. Dialysis was performed on the solutions to remove any excess free ssDNA that would interfere with the study. The ssDNA-SWCNT complexes were then heated and analyzed through UV-Vis-NIR spectroscopy to measure changes in solution quality that could be attributed to DNA denaturing.

Compartment Fire Experiments for Validation of Advanced Computer Models
Kelly Opert

The purpose of an ISO 9705 compartment fire is to simulate a fire in a room. The configuration is very desirable due to the numerous applications of the information retrieved from the fires. Because of this, it has become somewhat universal for the validation of numerical fire models. Many previous experiments have looked at the global parameters of these compartment fires. However, recent advances in modeling capabilities require more detailed and spatially resolve chemical species and thermal measurements in a room to promote further model development and provide more rigorous model validation. Recently a series of full scale compartment fire experiments were conducted at the NIST large fire lab

(LFL). As part of an ongoing effort to better understand what occurs within a compartment fire, the radiative heat flux environment was analyzed. The analysis of the thermal radiation environment provides information on how much soot is being produced inside the room. This information is used for correcting temperature measurements and provides new data to modelers to create a more accurate picture of the internal environment of the room.

Characterizing the Assembly of HIV-1 Gag Protein on a Model Membrane Surface
Sidhushree Raghunandan

The Gag protein has been identified as a prominent factor in the assembly of the HIV-1 virus. Gag is a multi-domain protein composed of five structured domains and four flexible linkers. Viral formation begins with the expression of Gag in the cellular cytoplasm and then targeting of the protein to the cell membrane where assembly occurs. Experimental evidence in vitro shows the protein is relatively compact in solution [J. Mol. Biol. 2007 (365) p. 812]. However, in vivo studies of virus like particles (VLPs) show Gag to be fully extended [Current Biology, 1997 (7) p.729]. This change in structure is required and favored for virus formation. The results of those experiments have motivated two main areas of study.

The first area focuses on characterizing the solution structure of the protein. The significant variability in protein conformation is due to the linker regions. Previous small angle neutron scattering (SANS) data on partial protein constructs containing at least one linker region was gathered. The initial SANS analysis showed these constructs to be compact with a radius of gyration below 35 Å. A more detailed atomistic modeling of the SANS data was performed with the program SASSIE. SASSIE allowed us to generate multiple protein conformations by varying the dihedral angles of the linker regions. SANS profiles from the computed structures were compared with the experimental data and density plots of the best-fit conformations were generated.

Because viral assembly occurs on the membrane surface, the second area explores the formation of model membranes on silicon wafers. Methods of lipid bi-layer formation including rapid solvent exchange, vesicle fusion, and the Langmuir-Blodgetry, each with advantages and disadvantages, were explored. Neutron reflectivity measurements were used to characterize the structure and completeness of the lipid bi-layer formed by each method.

Eventually the Gag protein will be introduced to these bio-mimetic membranes and will allow us to actively study the interaction of the protein with not only the lipid bi-layer but to other Gag proteins and viral proteins as well. By discovering properties intrinsic to the Gag protein that are closely associated with VLP formation, we can examine how to inhibit protein extension and prevent the spread of the HIV virus.

Examining the Reliability of the BANG3-PRO Gel as a Three Dimensional Dosimeter
Scott Robertson

Radiation has become a mainstream part of modern day medicine, with applications ranging from radiological imaging to radiation therapy. As such, there has been an ever-growing need for a reliable three dimensional dosimeter to accurately measure doses that patients are exposed

to. This will provide a better understanding of the radioactive sources used in treating tumors, specifically regarding brachytherapy procedures, and will ultimately lead to more precise radiation therapy practices.

We have studied several properties of the new BANG3-PRO gel kit to determine its reliability as a 3D dosimeter. The gel kit was melted in a heat bath, and a copper(II) sulfate catalyst and an L-ascorbic acid solution were added to remove the oxygen from the sensitive gel. They were then poured into different 200mL acrylic cylinders and allowed to harden for 48 hours. Once solidified, the gels were exposed to a well-calibrated $^{90}Sr/^{90}Y$ beta source for varied amounts of time, causing monomers within the gel to polymerize and produce a visible recording of the radiation. The gels could then be placed in a computed tomography (CT) scanner, which recorded the dose response for analysis.

Using this data, a calibration curve was created plotting the dose response of the gel as a function of the applied dose. Then, another gel was irradiated several different times to explore the response of the gel to an accumulated dose, which we found to correlate very closely to our calibration. Finally, temperature effects were examined for gels that had been refrigerated prior to irradiation. It was determined that if the gel was kept below 24°C to prevent melting or softening, then temperature differences had a negligible effect on the gel response.

Expanding e-FITS with Java

Cameron Rose

The e-FITS project involves the development of a web page to provide a user-friendly environment in which the end-user can generate numeric values, tables, graphs, and random numbers for various probability distributions. The current implementation uses the Common Gateway Interface (CGI) and Perl to generate the outputs by running the Dataplot graphed data analysis program on the server machine. This implementation is impractical for public use of the website due to the heavy load placed upon the web server if many processes are invoked, so my particular portion of the project is to assist in the implementation of the e-FITS user interface in Java. A Java applet runs solely on the personal machine of the user, and additionally, is compatible with many different operating systems using Java Virtual Machine. Many of the Location-Scale probability distributions were implemented previously, so I am expanding the functionality of the Java portion of the web page to encompass many of the One-Shape Parameter-Location-Scale distributions, and enhancing the functionality of the Location-Scale distributions.

Implementation of Armstrong's Particle Correction Algorithms in the NIST DTSA-II Microanalysis Software Package

Mark Sailey

Scanning electron microscopy (SEM) with energy dispersive spectrometry (EDS) is a powerful form of nondestructive chemical analysis. Although microanalysis is a thoroughly established field, there are still many limitations and areas for improvement, especially in the field of particle analysis. Particle analysis has many important applications, so improvements will greatly benefit

fields as diverse as air pollution, geology, forensic chemistry, and materials research, among others. To address the issues specific to particle analysis, such as electrons passing through the particle and complex 3-dimensional x-ray absorption path lengths, a series of experimentally derived corrections were proposed by John T. Armstrong (Electron Probe Quantification, K. F. J. Heinrich and D. E. Newbury, eds., Plenum Press, New York, 261-315). The main purpose of the project was to implement Armstrong's corrective algorithms in DTSA-II, a software toolset developed at NIST for electron beam x-ray microanalysis, and then evaluate them against Monte Carlo simulations. This presentation will cover the basic premises and procedures of SEM/EDS, the differences between bulk and particle analysis, and an overview and evaluation of Armstrong's correction algorithms.

Development of a Graphical Interface for Monte Carlo Simulations of Magnetic Crystals
Thomas Sarvey

In condensed matter physics, we are often faced with the challenge of understanding the magnetic properties of real materials. While the phenomena of magnetism have been known for millennia, the physics behind it is still the subject of intense study. The origins of magnetism lie in quantum mechanics. Atoms consist of neutrons, protons, and electrons. It is the electrons which are responsible for magnetism. Electrons have two types of angular momentum. One is the well known “orbital” angular momentum which arises from the motion of the electron about the nucleus. The other is known as “spin” and has its origins in the marriage of relativity and quantum mechanics.

Crystalline solids are made up of regular arrays of atoms. The magnetic properties of these materials are determined by the pattern of spin alignment upon these lattices. These spin configurations are determined by the interactions between the spins in the lattice which arise from the interplay of Coulomb repulsion between the electrons and the Pauli Exclusion Principle. For insulators, we can use the Heisenberg model which only considers pair-wise interactions between spins. If we construct a model of the pattern of interactions upon a lattice, we can then find the most likely spin configurations by minimizing the total energy of the system using a Monte Carlo method.

In this project, we created a program to automate this tedious process through a friendly user interface. We first generate a 3D model of the crystallographic structure using the symmetry of the lattice. Similarly, interactions and the respective matrices describing them are entered and translated or transformed throughout the lattice. Using a Monte Carlo algorithm, we then find the ground state spin configuration of the system. In the future, we will consider excitations above the ground state. The automation of these tasks will allow researchers to more easily explore a variety of models for fitting their data.

Measuring Security Risk of Networks Using Attack Graphs
Roshan Shah

Because computers have become a critical resource for information storage at various enterprises, network security has become a very important issue. More precisely, enterprises need to know the degree to which a network is secure. Previous studies were directed towards

the qualitative nature such as how to protect the network, while this research is focused on quantifying the risk associated with the network. Quantifying is done using the device of Attack Graphs. An Attack Graph generates various attack paths that an attacker can take to break into a network. Now, probabilities are also integrated into these Attack Graphs. These probabilities are derived from the CVSS (Common Vulnerability Scoring System) exploit scores taken from the NVD (National Vulnerability Database). CVSS provides an open framework for communicating the characteristics and impact of IT vulnerabilities. Since these exploit scores are in the range of 0 to 10, the corresponding probability of that score is obtained by dividing the exploit score by 10. Then while propagating through the graph, conjunctive and disjunctive relationships of these probabilities are used, and at the end we produce a numerical score. This research hasn't yet discovered whether this numerical score is, in fact, descriptive. We continue to research the actual level of security of the network. Furthermore, the implementation for this research was done in Java, and an open-source Graphical User Interface tool called GraphViz was used for displaying the attack graph.

Cell Response to Surface Roughness of Dental Composites

Kathy Tang

As photopolymerized methacrylate-based polymers have been increasingly used as dental restorations, the effects of critical material properties, such as degree of conversion, filler content, and roughness, on the biological response must be studied. A combinatorial platform was developed to test multiple properties on a single sample. Previous studies using these test platforms revealed that cell response varied with the composition, degree of conversion, and roughness of the dental composite. The test platform used had both a conversion and roughness gradient.

In order to separate the effects of degree of conversion and roughness, the objective of this study is to evaluate cell response on composites varying in surface roughness. Samples of similar degree of conversion but varying surface roughness were prepared using two approaches. The first approach utilized the combinatorial platform to fabricate dimethacrylate-based composites with varying filler content and a continuous roughness gradient. The second approach consisted of individual samples polished to different degrees of roughness using grit paper. The materials were characterized to evaluate degree of conversion, surface roughness, and surface hydrophobicity. Using Fourier transform infrared spectroscropy, the degree of conversion was confirmed to be similar on all samples and ranged from 68 % to 78 %. This degree of conversion range has been previously shown to have no significant effect on cell response. The profilometer confirmed a roughness gradient on the combinatorial platform and different roughness on the individual samples. Water contact angle measurements were obtained using the goniometer. While the roughness gradient demonstrated an increase in hydrophobicity towards the rough end, the individual samples exhibited a slight decrease in hydrophobicity on rougher samples.

After the material characterization, the samples were sterilized, and MC3T3-E1 pre-osteoblasts and RAW264.7 macrophages were cultured on them for 24 h before fixing and staining. Using an epifluorescent microscope for cell characterization, the cell viability, cell density, and cell spreading were imaged and quantified. Preliminary results show that

although cell viability is high on both the combinatorial platforms and the individual samples regardless of the surface roughness, the cell density and spreading varied.

The results of this study will be compared to the previous study in order to better understand the role of surface roughness in dental composites and the corresponding biological response.

Modulus Influences on Moisture-Induced Adhesion Loss
Nicholas Wagman

Many adhesive joints undergo dramatic loss in adhesion once the environmental relative humidity (RH) exceeds a critical value. Moisture induced adhesion loss is a major concern for numerous industries ranging from microelectronics to aerospace. A significant number of studies have focused on understanding mechanisms of moisture induced adhesion loss. However, the studies thus far have been limited to glassy polymers, but the understanding of the variation of interfacial moisture distribution with moduli of the adhesive and its direct correlation with the adhesion strength across the interface would be of great importance. This has significant practical implications, particularly in developing a better understanding of the interaction between water molecules and adhesive/substrate system. In addition, this knowledge is of particular importance in developing service life prediction models without resorting to extensive and long term testing.

The aim of this overall study, therefore, is to investigate modulus influences on moisture-induced adhesion loss. A series of homologous poly(alkyl methacrylates) with a range of modulus were chosen for study due to (a) the wide range of moduli available by simply changing the alkyl chain length and (b) the minor difference in chemistry to avoid ambiguity in the results due to chemical differences.

Significant deterioration in adhesion occurs at a critical RH. Prior research for this study involving poly(methyl methacrylate) (PMMA) and poly(butyl methacrylate) (PBMA) has postulated that adhesion loss above the critical RH value occurs due to the dual action of bulk swelling of the adhesive and deterioration of adhesive strength at the interface through moisture accumulation. The extent of bulk swelling, and hence swelling induced stresses, may be governed by the modulus of each adhesive.

The aim of the present study is to further elucidate the fundamental mechanisms of adhesion loss at a critical RH by examining the effect of modulus on the adhesion loss. The adhesive used for this study was poly(ethyl methacrylate) or PEMA. The study involves preconditioning bulk polymers and adhesive joints at various relative humidities. A fracture mechanics approach using a shaft-loaded blister test (a constant displacement-rate test) was employed to measure the adhesive fracture energy (G_c) at the interface. Attenuated total reflectance-Fourier transform infrared spectrometry (ATR-FTIR) was used to examine the fractured surfaces to accurately determine the loci of joint failure (interfacial or within the adhesive). Water sorption isotherm measurement for the bulk adhesives will also be made to characterize the bulk swelling.

An Introduction to Optical Tweezers
Andrew Ward

"Optical tweezing," as using a single-beam gradient-force optical trap has come to be called, is a method of manipulating micro and nanoparticles that has wide applications in physics, biology and nanotechnology.

Optical tweezers are in essence just a laser beam with a steep intensity gradient. A dielectric particle in the beam will scatter light and consequently feel a force: because the momentum of the light has changed, the momentum of the particle must change as well. The varying intensity of the beam is such that the force actually traps that particle. If the beam can then be moved, so too can the particle.

This talk is an introduction to optical tweezing, beginning with a brief history. Then the physics—simple in concept if not in practice—are discussed, particularly in the limiting cases of ray optics for large particles and dielectric response for small particles. The talk also explores the optical tweezers setup that NIST's Nanoscale Metrology Group employs as well as its goal of precisely manipulating smaller and smaller objects in three dimensions. Finally, a sampling of the uses of tweezing is given, including trapping single atoms, making precise physical and biological measurements, and nanofabrication.

Improving Measurement and Automation Features of an Electricity Reference Standard
Minghui Yang

The Radian RD-33 is useful as a portable Electricity reference standard with a high degree of accuracy. It can be calibrated against a more accurate stationary reference standard, and in turn be used to calibrate power meters in the field. Currently, measurements and calibration using this device can be done using vendor provided software. While functional, the software lacks several key features that could improve calibration times, efficiency, and accuracy, such as automated real time data acquisition, storage of measurement data, data processing, and comparisons between measurements of taken with different devices. New software is developed using LabView with these features to improve the functionality of this device.

University of Puerto Rico

The Applicability of a P(r) Inversion Method
Raiza Cortes

The Distributed Data Analysis for Neutron Scattering Experiment (DANSE) is a software development project for materials science. Part of the project is to develop tools for the Small Angle Neutron Scattering (SANS) technique where radiation is elastically scattered by a sample and the resulting scattering pattern is analyzed to provide information about size, shape and orientation of some component of a sample.

A SANS measurement will produce *I(Q)*, the scattering intensity distribution as a function of the momentum transfer Q. A technique used for fitting SANS data is the *P(r)* inversion technique

which gives the probability distribution of distances between any two points in the system. The pair-correlation function *P(r)* is related to *I(Q)* by a Fourier transform. The *P(r)* inversion technique is done by expanding *P(r)* with a set of base functions. A regularization term is also added to stabilize the result in the *P(r)* inversion technique.

Our study involved validating the technique by evaluating *P(r)* for simulated *I(Q)* data for which the *P(r)* distribution was known. A simulation program was used to generate *P(r)* and *I(Q)* for various sample geometries. It was possible to generate an algorithm to determine how many terms are necessary in the *P(r)* expansion to obtain a reliable result. Comparing the output of the technique to the simulated distribution, it was also possible to predict the size of the regularization term. We also tried to determine the types of systems that the technique is good for and how sensitive the technique is to the maximum length of the system. Results found with SANS data taken at the NCNR will also be presented.

Characterization of Graphene Ribbons from Liquid Exfoliation of Graphite
Paul Fuentes-Martinez

The study of graphene, a single layer of carbon atoms bound together, is becoming a growing international area of research interest, due to its presumed mechanical, thermal, electrical and optical properties and possible practical applications. Since its discovery in 2004, by physicists from the University of Manchester, graphene has been rigorously investigated as this innovative material was expected not to exist in nature because in its free state it is unstable with respect to the formation of curved structures such as buckyball, nanotubes and 3D diamond and graphite. These structural instabilities have resulted in dedicated efforts in the field of material science focused on procuring thinner and thinner layers of graphite, approaching nano-particulate scale, or growing epitaxial graphene on surfaces for later removal and incorporation into variety of applications.

This ongoing research project is focusing on the optical and electric properties of graphene ribbons and the corresponding larger networks. We explored ultrasonic agitation bath as an initial step towards mechanical exfoliation of graphite into individual graphene sheets. Graphite flakes having an average size of 45 μm were dispersed in isopropanol at concentration of 1mg/ml. Then the liquid suspensions were sorted by ultracentrifugation method at 21000 RPM for 10 minutes. This procedure separates the suspended particles by size, where graphene ribbons are located on top while larger particulates concentrate on the bottom of the test tube. We selected ribbons from the top fraction by depositing it onto a nanoporous membrane, via a vacuum filtration process. The optical properties of the deposited films were analyzed by measuring the diffuse reflectance spectra and compared them with the transmittance of the fractionated liquid suspensions using a UV-Vis-NIR spectrophotometer. These spectra can be used to identify and characterize free charge carriers present in individualized graphene sheets. In order to determine the electrical conductivity properties, the membrane was sputter coated with gold electrodes, and the impedance at different frequency was measured using an impedance analyzer.

Measurement of SRM 2461 Standard Casings Using a Nanofocus Confocal Microscope
Stephanie Montalvo-Delgado

When a bullet or casing is recovered from a crime scene, the evidence is entered into a nationwide database using the IBIS (Integrated Ballistic Identification System) system. This system uses image capture and image analysis technology to generate a profile. Examiners from various laboratories around the nation including the Bureau of Alcohol, Tobacco, Firearms and Explosives (ATF) and the Federal Bureau of Investigation (FBI) use the IBIS machines to compare firearm related evidence stored in their database. When a new signature is entered in one of the laboratories, the system searches the existing database for a match. The problem is that each laboratory uses its own individual quality control bullet and casing for the calibration of their IBIS. Therefore, it is essential to establish one traceable measurement standard for all the labs to use. The National Institute of Standards and Technology (NIST) have developed Standard Reference Material (SRM) 2460/2461 bullets and casings to be used as a reference standard for instrument calibrations at these crime laboratories. The SRM2461 casings are produced through electro formation using a fired master casing. The 3D topography of the replicated casings are generated using the Nanofocus Confocal Microscope. To guarantee the same surface topographic in all of the replicated standard casings, the decay factor of the replication process needs to be tested. Using the cross correlation function (CCF_{max}) and a NIST proposed parameter called the topography difference (D_s), the casings can be correlated for accuracy. The replicated casings are expected to have CCF_{max} values higher than 95 % when compared to the master. This demonstrates reproducibility for the manufacturing process and the measurement system.

High Resistivity Measurement at High Temperatures for Solar Probes
Angelica Muniz-Mercado

The surface and volume resistivity measurements are being implemented using a test fixture. The purpose of the test fixture is to ensure a fixed measurement configuration to obtain consistent results. Volume resistivity is the electrical resistance through a one-centimeter cube of insulating material and is expressed in ohm-centimeters. Surface resistivity is the electrical resistance between two electrodes on the surface of an insulating material and is expressed in ohms. Because of NIST expertise in high resistance measurements and characterization of materials, we started testing with high resistive materials with known parameters to then determine the feasibility of the measurement process as well as the confidence of the test fixture. After we determine the viability of the project, NIST will build a high temperature test fixture to measure the high resistance materials at high temperatures (1000 °C).

This project is related to a Solar Probe mission to one of the last unexplored regions of the solar system, the Sun's corona. The thermal protection system (TPS), protecting the payload from the extreme solar heating, will be constructed of the electrical insulator alumina (Al_2O_3) or other advanced materials. Also, at high temperatures alumina can be a thermally conductive material. Surface and volume resisitivity measurements will be used to determine the temperature dependent change in resistivity insulating materials which effects the charging of the TPS. This project will be considered as a future collaboration between NIST, NASA, and The Johns Hopkins University Applied Physics Laboratory (JHU-APL). The mission will answer

fundamental scientific questions about the heating of the Sun's corona and the acceleration of solar wind.

Principal Components Analysis and Singular Value Decomposition for Automated Angle Measurements
Axel Y. Rivera Rodriguez

Angles are an important element in measurements. They can determine the size of a polygon or the height of a building; they can improve details of simulations, etc. An angle is formed by two vectors. However, sometimes these vectors consist of a large number of dimensions. Many of these dimensions may be unimportant. For this reason algorithms exist that reduce the vector's dimensions. Also these algorithms help to get the most important information from the vectors. Two of these algorithms are: Principal Components Analysis and Singular Value Decomposition. This project studies these algorithms from the mathematical and computer science points of view and implements them to do angle measurements in two dimensions. The results show that when these routines were used on noisy vectors that form angles, the new angles have small differences from the original ones.

University of Rochester

Standardizing Voltage Characteristic Measurements of Electroshock Weapons
Daniel Green

The growing popularity of TASER®s and other electroshock weapons (ESWs) among law enforcement agencies, as well as several recent ESW-related deaths, has raised concern regarding the danger associated with the high voltage output of ESWs. Existing research has paid little attention to accurately measuring the voltage and current characteristics of an ESW's output. [1] This research can be improved by establishing standardized measurement and uncertainty analysis practices for use in characterizing the high voltage output of ESWs. This project investigates voltage measurement methods using a high voltage capacitive voltage divider and an electro-optic method based on the Pockels effect.

To accurately measure high voltage ESW output using a standard oscilloscope, a probe must be used to attenuate the output to a level within the oscilloscope's operating range. Previous research has assumed the high voltage probes used had a constant attenuation over the bandwidth of the ESW pulse [1]. More accurate voltage measurements can be obtained by characterizing the frequency response of the probe and then deconvolving it from the output measured through the probe. The high voltage probe tested in this project is found to have an attenuating factor up to 10% lower than claimed over the bandwidth of the ESW output, while the manufacturer claims <1.5% accuracy in this frequency range. The accuracy of ESW output voltage measurement is increased significantly by performing deconvolution instead of ignoring the frequency response of the probe.

An optical method of measuring the voltage characteristics of an ESW's output is advantageous because the measurement instrumentation is isolated from the electric noise

produced by high voltage sparks and discharges occurring inside the ESW. Several optical materials with birefringence affected by surrounding electric fields are used to change the polarization of incident laser light by an amount proportional to the applied electric field. The change in polarization is measured by the relative intensity of orthogonal polarization states and can be related to the voltage between the two electrodes of an ESW creating the electric field.

****Disclaimer****

Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST.

[1] 'PSDB Evaluation of Taser Devices', T.J. Donnelly, K. Douse, M. Gardner and D.I. Wilkinson, PSDB Publication 9/02.

University of San Diego

Through-Barrier Radar Detection and Imaging

Emmett Perl

The ability to detect and image objects through various non-metallic materials has many applications to law enforcement, emergency response, and the military. With recent advances in technology, the ability of through-barrier radar systems to detect objects or people hidden behind visual obstructions has improved. However, there are many challenges that must be overcome before through-barrier radar can reach its full potential. No standard has been developed to evaluate these systems and universal metrics are required. For this reason, we are developing a standard test method to characterize these systems. We acquired a Constant Look Radar System, centered around 3.6 GHz ($\lambda \approx 83$mm), with through-barrier capabilities to carry out our tests. We also designed and built a test apparatus to simulate the Doppler and micro-Doppler radar returns of a standing or walking person. This device allows us to control the vibration (frequency and displacement) of a 20 cm × 20 cm square aluminum plate. By aiming our radar system toward the aluminum plate, we are able to distinctly see its micro-Doppler signature.

Over the course of the study, we have carried out a number of tests on our radar system. To find the minimum signal that the radar could detect, we varied the displacement of the plate. We found that the radar could pick up a vibration as small as 20 micrometers across a distance of 4 meters (~13 feet). Then, by varying the frequency of vibration, we were able to determine the frequency response of our radar system. We found that the sensitivity of our system varies predictably across its range of Doppler frequencies. We have recently started testing the ability of our system to detect these displacements through walls by measuring the signal attenuation caused by various construction materials. So far, we have found that the loss in signal through masonry block is around 15 dB, and the loss through concrete is around 28 dB, which is consistent with previous NIST studies on the propagation properties of these materials. We are currently testing our system with other building materials to characterize its ability to penetrate a variety of walls. As the project continues, we will begin to add variables, such as changing the angle of incidence or combining different walls, in order to simulate a real world situation.

University of Texas, Austin

Nanocapacitance Measurement
Chong Jiang

The goal of the nanocapacitance measurement project is to investigate methods of measuring sub-picofarad (pF) capacitors, with the eventual goal of attofarad resolution. Capacitance is an important characteristic for many novel semiconductor devices – such as nanotube-based field-effect transistors – yet these nanostructures have capacitances that are not readily measurable today. My involvement in this project this summer has consisted of four main parts, each involving the creation, test, and analysis of a method for sub-pF capacitance measurement.

The first of these consisted of setting up a constant-voltage-charging capacitance measurement board. We created a LabVIEW-based data acquisition and control scheme in order to automate the operation of the board. This setup now measures capacitors using differential mode, and has ~1 femtofarad (fF) resolution.

Next, we considered alternative approaches to capacitance measurement. One such method is to use a constant-current-charging circuit, and we designed a prototype circuit based on this idea. This board is still being fabricated, but we expect ~10fF resolution.

Another approach we investigated is based on the RC time-constant. The application of a voltage step to a capacitor and a resistor in series results in an exponential decay of voltage at the intermediate node versus time. By using an analog to digital converter to sample the voltage, and fitting the resultant waveform to an exponential curve, we were able to extract capacitance with ~1fF resolution.

The final, and largest, component of my work this summer involved the measurement of a series of chips, each with several hundred capacitors, with capacitances ranging from 0.4fF to 1pF. Using a commercial capacitance meter, we obtained capacitance vs. voltage (C-V) curves for metal-oxide-semiconductor (MOS) and metal-insulator-metal (MIM) capacitors on five chips. We were then able to examine the fit between measured and theoretical values (accuracy of ~5fF), as well as determine the resolution of our measurements for the same capacitor on the same chip (~0.5fF), equivalent capacitors on the same chip (~5fF), and the same capacitor on different chips (~5fF). This not only confirmed the design of these chips, but also yields a benchmark for which future methods for very small capacitance measurement can be compared against.

University of Texas, Pan American

Surface Chemistry Parameters of Environmental Isolates of Bacillus Thuringiensis Spores
Ike Muniez, Jr.

The aim of this study was to determine how a spore's unique surface characteristics and the media it was grown on might play a role in the surface chemistry of different morphological strains of *Bacillus thuringiensis.* Six strains of BT were grown on PGSM media and ten strains (includes the first six plus four new ones) were grown in CCY media. Strains were chosen based

on their morphology; certain strains contain filaments and others possess unusual crystals resembling caps or tails. One strain, BT 2-56, possesses an internal crystal which apparently could be lost when grown on different media (PGSM), and has filaments attached. Another strain, BT 3-14, has a long tail like structure which is presumably an exosporium or long crystal and BT 1-54 possesses similar features.

Initial quantification of spores is necessary to determine if the purity and concentration of each sample is sufficient to perform analytical surface chemistry experiments. Phase contrast microscopy was used to count spores on haemocytometers. Colony forming units (cfu), an indication of viability, were also counted by performing serial dilutions and spreading different concentration levels on LB agar plates. These values were compared with those obtained with phase contrast to check for consistency, purity, and viability. A purity of at least 95% and a concentration of $1x10^8$ cfu/ml was required to ensure that further measurements were on spores not contaminating debris.

Comprehensive understanding of a spore's surface chemistry including hydrophobicity and electrophoretic mobility can help draw conclusions on how spores will interact in the environment and with other spores in a suspension. Hydrophobicity was calculated using the Young-Dupré equation by utilizing contact angle measurements taken with a goniometer. Filter membrane spore-covered surfaces were prepared with a filtration apparatus. Three solvents, milliQ water, Formamide, and Diiodomethane, were applied to the membrane mounted bacterial spores and the contact angle was measured. The contact angle measurements of BT 2-56, BT 1-54 another strain called BT 1-14 showed significant variation between the two growth media used, which resulted in a noticeable difference in their hydrophobicity values. The mobility recorded for strain BT 3-14 was significantly lower than what was seen for other strains on both media used, indicating that its morphology might have played a role. Electrophoretic mobility readings were obtained using a Zeta PALS Zeta Potential Analyzer with spores washed and suspended in MOPS pH 7 buffer.

This work enhances our understanding of the role of spore morphology and surface chemistry in influencing the fate and transport in environment, terrestrial or aquatic. Such measurements have impact on food processing and packaging, environmental effectiveness of insecticides and simulant selection for biohazard threats.

University of Wisconsin, Stout

Nano-Scale Milling with a Helium Ion Microscope
Jarod Feight

The Gallium LMIS (Liquid Metal Ion Source) FIB (Focused Ion Beam) is a versatile tool capable of utilizing ion milling to perform tasks which require physical modifications on the nano-scale. The FIB has been the choice tool for multiple applications ranging from TEM (Transmission Electron Microscope) sample preparation to semiconductor repair and manufacturing. Even though the FIB has generated excellent results continuously since its inception, due to physical limitations the FIB is not suitable for applications requiring mills

smaller than a few hundred nanometers. Recently a new ion microscope, the HIM (Helium Ion Microscope), was released as a new imaging and metrology tool theoretically capable of generating an increased depth of field, lower energy spread, and smaller spot size than traditional electron microscopes. Even though the tool was originally designed to improve imaging and metrology processes, the HIM may potentially be viable as a nano-scale milling devices. The small spot size and low energy spread points to the HIMs potential for milling at even smaller sizes than the FIB. We aim to show this by attempting to mill 100nm gold particles with both the FIB and the HIM. Theoretically the HIM should be able to outperform the FIB by being able to mill on a smaller scale, thus expanding the capabilities of the HIM and improving a users ability to precisely mill on the nano-scale.

Virginia Polytechnic Institute and State University

Triplet Correlations in Magnetic Flux Line Lattices Within Elemental Type II Superconductors

Matthew Glazer

Type II superconductors, some of which are considered high-temperature superconductors, have a mixed magnetic state at certain temperatures and magnetic fields. In the mixed state, magnetic fields can penetrate a superconductor to a certain depth. Due to the quantized nature of magnetic fields, these fields form discrete flux lines within an array of superconducting electron vortices. These flux lines and arrays of superconducting electron vortices vary with magnetic field and temperature. All penetrating magnetic fields disappear below a second transition temperature. In order to investigate the structure of the arrays of vortices, and ultimately the locations of individual flux lines, Small Angle Neutron Scattering (SANS) can be used to determine the structure factor of the vortex array. Using a reverse Monte Carlo (RMC) computational approach, we can discover the actual structure and position of the vortex lattice within a superconductor.

Once the positions of individual vortices within the superconductor have been obtained, correlation functions can be calculated to describe these vortices. Correlation functions are statistical measures of displacement, orientation, density or other properties within a structure. These correlation functions can be generalized into theories describing interactions between the vortex lattice, externally applied magnetic fields and temperature. These correlation functions are typically calculated using pairs of vortices. However more information and perhaps different interactions can be described by comparing triplets of vortices.

For my project, I created a program to describe triplet correlations within a perfect crystal of niobium slightly above absolute zero with zero magnetic field. The program then compares the correlations from the perfect vortex lattice to that of a single crystal of niobium at 2.6 K and an applied field of 200 mT, which was generated using an RMC approach. Currently, it is uncertain whether or not triplet correlations are nontrivial. By analyzing triplet correlations, we hope to better understand the nature of Type II superconductors and more accurately describe phenomena within the superconducting mixed state.

Prototype for Simulation-Based Testing of Shop Floor Scheduling

Brian Mayer

The goal of the Simulation-based Manufacturing Interoperability Standards and Testing program is to create a Virtual Manufacturing Environment that simulates a machining job shop in order to test manufacturing software applications. This will consist of three integrated levels, machine specific simulations, shop floor simulations and supply chain simulations. This project focuses on the modeling and simulation of the shop floor.

Scheduling a shop floor is critical, and it is not an exaggeration to say that effective and timely scheduling can be the difference between success and failure. Discrete Event Simulation (DES) has become a widely used technique to predict and ultimately improve the performance of manufacturing systems. In particular, DES is often used in capacity planning, to evaluate order release policies, and to evaluate dispatching policies. Currently simulation modeling takes time and effort. In addition, companies usually do not have resources adequately trained to build simulation models of their facility from scratch. To address this problem a simulation prototype to evaluate a job-shop schedule has been developed.

The prototype created incorporates a template format that allows companies to generate a model specific to their facility. The simulation is data-driven. Input data in Excel format is used to populate the model. The shop-specific model needs the schedule or production list as a simulation input. It simulates delays and randomness to create a much more realistic production schedule than the given schedule. The model outputs the simulated production times and job metrics into a report file. To create various scenarios, different schedules can be input or the user can choose different dispatching rules for the simulation. Key performance indicators, such as average makespan, work-in-process, and number of tardy jobs, are outputted to compare the scenarios and determine the best possible schedule for the shop. The same model can later be used to determine the best schedule for other chosen time periods.

The model can cover many different job-shop situations and sizes. A company does not have to spend time learning simulation techniques or developing a model from scratch. All they need to do is to provide the data. Once created there is no need to update the model unless changes need to be made.

Most importantly the template can be easily re-used by many companies to create their own specific model and then evaluate as many schedules for as many different time periods as necessary, to maximize the company's production and efficiency with minimal time, effort, and training. WARNING - Any shop can use this template.

Washington University in St. Louis

Building a Scanning Kelvin Force Microscope Feedback Loop
Nathan Shemonski

Simple methods of Scanning Kelvin Force Microscopy (SKFM) can be performed using a standard Atomic Force Microscope (AFM). These methods include open loop and amplitude modulation (AM) SKFM. Although these methods are useful, the resolutions of their images are less than desirable. Open loop SKFM does not give the cantilever the sensitivity required for high resolution imaging, and AM SKFM results in a smeared image due to its dependence on capacitance and not the gradient of capacitance. Other more advanced methods, such as frequency modulation, may not be possible with the standard equipment due to some of the signals being fully internal to the system.

Using a cheap (~$2,500) digital signal processing (DSP) board, a function generator, a lock-in amplifier, and a summing op-amp, a feedback loop can be built to perform all the signal processing external to the AFM. By tapping into the raw cantilever response signal, and applying the AC and DC biases between the AFM tip and the sample directly, full control over the signals can be achieved and higher resolution imaging should be possible.

Other possibilities include taking advantage of the onboard FPGA chip. A standard hardware image for the FPGA comes with the DSP board, but with some modifications it may be possible to put some of the external devices such as the lock-in amplifier and the summing op-amp inside the FPGA.

Wellesley College

Evaluation of the Effects of Cocktail Composition and Instrument Dependence on the Activity Determination of ^{63}Ni by Liquid-Scintillation-Based Efficiency Tracing with ^{3}He Standards
Willa Freedman

Efficiency tracing by liquid scintillation (LS) spectrometry with ^{3}H standards is one of the more powerful tools used for radionuclidic metrology by the NIST Radioactivity Group, namely for the activity determination of nuclides that decay by pure beta emission. The current method for efficiency tracing, as developed by NIST and CIEMAT (Centro de Investigaciones Energeticas Medioambientales y Technologicas), is a protocol that is used to determine the LS detection efficiencies for the radionuclide that is to be traced (under known, varying quench conditions) by following the experimentally-determined LS efficiencies for a set of closely-matched cocktails of a ^{3}H standard. Model-based calculated efficiencies for the two sets of cocktails are linked through a "figure of merit" parameter *M* that is used to characterize the quenching and overall detection efficiency for the LS counting instrument. Two codes are currently used at NIST for performing these calculations: EFFY4, developed by Garcia-Torano at CIEMAT; and CN2003, develop by Gunther at the Physikalisch Technische Bundesanstalt (PTB) in Germany. If the efficiency tracing method is valid, then the functional relationship between two sets of matched

cocktails should be independent of both composition of the LS cocktails as well as the specific LS counter that is used for the measurements. Previous research at NIST suggests that this may not be true for low and medium-energy betas emitters. Experiments, using ^{63}Ni traced against ^{3}H standards, were designed to evaluate the efficacy of the model and calculational codes under conditions of varying cocktail composition and in three different commercial LS counters. Variations in cocktail composition included changes in the cocktail's aqueous fraction and in ionic content, as well as the use of scintillation fluids based on four different solvents. The three instruments used for the measurements are known to have considerably different operating characteristics (low-energy threshold, deadtime, linear vs. logarithmic energy binning, etc.). The wide variations in cocktail composition and instrument characteristics should prove to be a robust test of the efficacy of the method for ^{63}Ni and other medium energy beta emitters.

Western New England College

Motion Behavior of a Stagger-Tuned Piezoelectric Shaker
Alexander Boutin

Piezoelectric shakers are instruments used to calibrate accelerometers at frequencies in the range of 3-25 kHz. They usually consist of several piezoelectric and alumina cylinders mounted end-to-end in such a fashion that sinusoidal motion along a single axis is achieved over the necessary frequency range. Sufficient surface displacement and minimal surface distortion are important factors in providing an accurate calibration. The purpose of this project was to create a software model of a piezoelectric shaker to predict the characteristics of its motion. An accurate software model would allow the shakers to be constructed with the optimal materials and dimensions. A tungsten carbide base and two piezoelectric disks were fastened together with epoxy to serve as the actual physical model. Tests were performed to observe the surface motion of the physical model over the frequency range of 1-40 kHz using miniature accelerometers placed at specific locations and through the use of a scanning vibrometer setup. The model was replicated in a FEA software package using the same dimensions and material properties from the physical model. The surface motion of both the physical and software models were compared in terms of their response over the 1–40 kHz frequency range.

Microscopic Robotics: Characterization of How They Move
Kathryn Purdum

This talk will discuss microscopic robots that are less than 100 micrometers long in their largest dimension and are micro fabricated using semiconductor processing techniques. Since these robots are so small they may be used for applications current technology cannot be used for, such as the manipulation of nanoparticles and single atoms, or as surgical instruments for the dispersal of clots found in arteries.

The goal of this project is to characterize the motion of the microscopic robots using advanced metrology tools. Fluorescent microscopy will be used to measure the size of a single step the robot takes, which is theorized to be 15 nm. Strobed interferometric microscopy will be used to measure the height of the robots along with their three-dimensional movement in response to

changes. These changes include the dielectric the field is constructed of, the roughness of the surface, and the various signal parameters.

Whitman College

Protein Adsorption Affects Osteoblast-Glass Adhesion Strength as Measured by Colloidal Probe Atomic Force Microscopy
Jackson Cahn

One of the most important properties of a potential biomaterial, such as a drug-delivery device, an implant, or a surgical tool, is the degree to which tissues adhere to it. Atomic force microscopy is a powerful technique for investigating the adhesion between a single cell and a potential biomaterial, because of its high sensitivity. By gluing a sphere (diameter 20µm-50µm) of the test material to the cantilever of the microscope, the adhesion measurements can be tailored to investigate a number of different materials.

The adhesion data obtained by this method can vary significantly based on the contamination of the sphere by proteins and other biomolecules adsorbed from the cell-culture medium or remaining attached due to previous contact with cells. Under most conditions, as the sphere becomes contaminated with biomolecules, the adhesion decreases markedly until the sphere is completely contaminated. Investigations were carried out to determine the nature and magnitude of this decrease and the controlling factors. Measurements recorded in a culture medium lacking in extracellular proteins took significantly longer to become fully contaminated, as did those using extremely hydrophobic dichlorodimethylsilane-treated spheres. However, hydrophobic glass spheres in a protein-containing medium showed an increase in adhesive strength when contaminated with protein.

Additionally, two methods for cleaning spheres, a sodium dodecyl sulfate (SDS) detergent and/or etching with low-pressure radio-frequency-generated oxygen plasma, were investigated to determine whether they restored the adhesion of the spheres to a state comparable to unused spheres, thereby allowing reuse of prepared cantilevers. These results will also be discussed.

Worcester Polytechnic Institute

Developing Virtual Fire Fighter Trainers
Timothy Lontz

Fire fighters must fight fires in order to improve their fire fighting skills. While fighting fires is dangerous, fire fighter training can be hazardous as well. In the past, fire fighter training has consisted primarily of physically based methods. It has become apparent that new methods for fire fighter training can take advantage of recent technological advancements. The purpose of this project was to demonstrate fire behavior in a safe environment, namely, on the computer using fire modeling and visualization tools developed by NIST before fire fighters encounter dangerous fire situations in real life. This fire fighting training tool was developed for use as a

supplement to live fire fighter training, rather than stand alone use. A variety of fire scenarios were modeled and visualized using the NIST developed software, Fire Dynamics Simulator (FDS) and Smokeview. Each of the fire scenarios created with FDS and Smokeview were modeled true to form, meaning that the physical dimensions of the buildings and specifications of the devices used by fire fighters were imported accurately into the computer models. FDS created the simulations needed while Smokeview provided a visual representation of the simulations and results. After the simulations were created, DVDs were produced which included the various fire scenarios allowing a fire fighter the ability to interact with the simulations and animations from the relative safety of a couch.

New Measurement Technique for Characterizing the Anisotropyof Brachytherapy Seeds
Long Tong

The National Institute of Standards and Technology (NIST) provides the calibration standards for brachytherapy seeds, encapsulated radioactive sources that provide a safe and quick alternative treatment for malignant tumors, through the use of the Wide-Angle Free-Air Chamber (WAFAC) and a spectrometer which are used to measure the air-kerma strength and anisotropy of these sources, respectively. We characterized the anisotropy of I-125 and Pd-103 sources, the most widely used brachytherapy seeds for the treatment of prostate cancer, through the use of a spectrometer and explored the possibility of performing similar measurements using three different ionization chambers; a well-ionization chamber commonly found in most clinics, a spherical ionization chamber, and a cylindrical ionization chamber. Ionization current versus distance measurements were performed for each seed/chamber combination to analyze the effect of scattering and attenuation on the chamber signal due to the air medium. The results of the measurements were then used to select the optimal position to begin the anisotropy measurements. The seeds were rotated clockwise every 5 degrees while within 30 degrees from the zero position and then 15 degrees thereafter until they had rotated a full 360 degrees. Similar to the procedure of normalizing the air-kerma strength calculated from the energy spectrum measured per angle for each seed, the current measured per angle for each seed/chamber combination was also normalized in a way that allowed a comparison of values between the air-kerma strength analyzed from the spectrometer and the current measured from the ionization chambers. By comparing the anisotropy graphs obtained from the spectrometer and three ionization chambers for the I-125 source a direct correspondence between the air-kerma strength obtained from analyzing the spectrometry data and the ionization currents is observed for all chambers. A similar conclusion can also be drawn for the Pd-103 source for the anisotropy graphs obtained from the spectrometer and all three ionization chambers. The practical applications of these results include the possibility of replacing the anisotropy measurements of incoming sources using a spectrometer with an ionization chamber which would dramatically decrease the time spent by NIST on performing quality assurance (QA) tests for each seed. In addition, clinics can now perform their own anisotropy measurements of these sources as an added layer of QA which would give medical physicists and radiation oncologists an added level of confidence when planning and treating prostate cancer patients with brachytherapy seeds.

- Intentionally Blank -

APPENDIX A. QUICK CROSS-REFERENCE – SURF 2008

STUDENT	UNIVERSITY	TALK TITLE	OU
Behm, Nathan	American University	Using Magneto-Optical Trapped Lithium Atoms to Create a Versatile FIB	CNST
Kelleher, Brian	American University	Rate Dependent Magnetization Reversal in Thin Co/Pt Multilayer Films	MSEL/NCNR
Madison, Benjamin	Appalachian State University	Characterization of Femtosecond Laser Frequency Comb and a Micro-Channel Plate (MCP) Detector for High Resolution Atomic Spectroscopy	PL
Durnford, Andrew	California Institute of Technology	Simulating Diffusion from Laser-Excited Gold-Coated Silica Nanoparticles	MSEL/NCNR
Vu, Kennedy-Kiet Tuan	California State University Fresno	Fate and Behavior of TiO_2 Nanoparticles in the Natural Environment	CSTL
Bunker, David	Carnegie Mellon University	Materials Informatics Tools and Crystallographic Databases	MSEL/NCNR
Greer, Benjamin	Carnegie Mellon University	Terahertz Spectroscopy and Modeling of Biological Molecules in Reverse Micelles	PL
Shih, Jennifer	Carnegie Mellon University	SANS-USANS Investigation of Magnetic Nanoparticles Chaining in Polymer Epoxy Nanocomposites	MSEL/NCNR
Devine, Brittany	Centre College	Measuring User Experience in Large Simulated Networks	ITL
Miller, Lauren	Clemson University	Influence of Temperature on the Molecular Conformation in Gold-Monolayer-Semiconductor Structure	EEEL
Anderson, Justin	Colorado School of Mines	Theory of Quantum Corrals on Graphene	PL
Fosu, George	Colorado State University Pueblo	Validation of the SysML Tools and Specifications	MEL
Bolz, Brian	Cornell University	Controlled Electrostatic Deposition of Graphene	CNST
Huang, Eric	Cornell University	Microwave and Radio-Frequency Addressing of Bose-Einstein Condensate	PL
Ligda, Jonathan	Cornell University	Mechanically Exfoliated Graphene	CNST
Wen, Yanan (Henry)	Cornell University	Single Molecule Studies on Membrane Protein Using Hydrosomes and Optical Trapping	PL
Johnson, Joshua	Florida Gulf Coast University	Development of Static and Dynamic Stability Test Standards for a Load Carrying Device	MEL
Nowak, Stephen	Franciscan University Steubenville	Simulating CO Pollution Across the Indoor/Outdoor Interface	BFRL
Naudus, Philip	George Mason University	Gamma-Gamma Coincidence Detection	PL
Forney, Anne Marie	Gettysburg College	Examination of the B3 Dosimeter Temperature-Dose Response Dependence	PL
Rakholia, Akash	Harvey Mudd College	Reverse Monte Carlo Refinements of Local Structure Using Atomic Pair-Distribution Functions and EXAFS	MSEL/NCNR
Cahill, Alex	Haverford College	Refining the Fine Structure Constant: Theoretical Calculations of Fine Structure Splittings in Highly Ionized Atoms	PL
Winogradoff, David	Haverford College	Neutron Optics and the Beam-Stop Problem	MSEL/NCNR
Stauffer, Hilary	Hood College	Combinatorial Pulsed Laser Deposition of Functional Oxides	MSEL/NCNR
Walton, Eric	Hood College	High-Fidelity Simulation Environment for Testing Virtual Robots	MEL

STUDENT	UNIVERSITY	TALK TITLE	OU
Abbott, Lauren	Indiana University of Pennsylvania	Quantum Mechanics and the Mystery of Life: Quantifying DNA's Interactions	PL
Juhnke, Bethany	Iowa State University	Assessing Cell Morphology and Adhesion of a Small Library of Tyrosine-Derived Polycarbonates	MSEL/NCNR
Barker, Lydia	James Madison University	Optimizing Standard Addition Design for Minimal Uncertainty	CSTL
Berry, David	James Madison University	Determination of Toxic Metals at Trace Levels in SRM 955c Caprine Blood by Isotope Dilution Inductively Coupled Mass Spectrometry	CSTL
Ng, Tiffany	Johns Hopkins University	Preparation and Characterization of a New Tethered Bilayer Lipid Membrane (TBLM) Model Membrane System	MSEL/NCNR
Schultz, Justin	Juniata College	Development of an Axicon MOT for Rubidium Atoms	PL
Sabol, Joseph	Lehigh University	Microwave Methods Generating CdSe/ZnS Nanostructures	MSEL/NCNR
Schneider, Lisa	Loyola College of Maryland	External Calibration of a Camera and Laser Range Finder	MEL
Ngai, Tammy	Massachusetts Institute of Technology	Standardizing Base Metric Scoring for the National Vulnerabilities Database Operations Team and Other Users of the Common Vulnerabilities Scoring System	ITL
Parker, Beatrice	Massachusetts Institute of Technology	Contributions to the Electronic Kilogram Experiment: Measuring the Acceleration of Gravity and Configuring a Motion Control System	EEEL
Bonnen, Tyler	Miami Dade College	The Morphology of C_{60}/Pentacene Heterojunctions	CSTL
Palacios, Sebastian	Miami Dade College	Interoperability of Building-Related CAD Applications	BFRL
Vega, Jonathan	Miami Dade College	Time-of-Flight Laser Scanners and 3D Modeling	BFRL
Manders, Jesse	Miami University Ohio	An Atom-by-Atom Approach to Alzheimer's: Coordination in Metal-Peptide Complexes	CSTL
Workman, Kevin	Millersville University of Pennsylvania	Using Video Games to Improve Visual Analytical Software for Digital Natives	ITL
Yilma, Semme	Montgomery College	Modeling of a Reinforced Concrete Portal Frame Under Fire	BFRL
Wroge, Christine	Mount Saint Mary's University	ρ-Aminophenyl Phosphoryl Choline Purification of C-Reactive Protein for Development of a Mass Spectral Internal Standard	CSTL
Taylor, Courtney	North Carolina State University	Design of a Detection Calibration System for Use in the Neutron Lifetime Project	PL
Schalch, Jacob	Oberlin College	Understanding Hydrogen Adsorption in Carbon-Templated Zeolites	MSEL/NCNR
Brockett, Adam	Pennsylvania State University	Ontological and User Interface Development for the Urban Search and Rescue Robotics Program	MEL
Chang, Matthew	Pennsylvania State University	An Atom Thick: Graphene Based Quantum Hall Resistance Standard	EEEL
Ebert, Matthew	Pennsylvania State University	Two-Photon Microscopy	PL
Neal, Adam	Pennsylvania State University	Process for In-House Soldering of Printed Circuit Boards	EEEL
Bouis, Craig	Purdue University	Characterization of the UV Degradation of Photocatalytic Nanoparticle-Filled Polymers	BFRL
Gibney, Joseph	Rensselaer Polytechnic Institute	Modeling Holey Fibers	PL

STUDENT	UNIVERSITY	TALK TITLE	OU
Kutten, Johannes	Rensselaer Polytechnic Institute	Measuring the Effect of Cytotoxic Compounds Using an Engineered Reporter Cell Line	CSTL
Timmerman, Laura	Rice University	Toward Monodispersity of Single-Walled Carbon Nanotubes via Ultracentrifugation	MSEL/NCNR
Minutillo, Nicholas	Saint Joseph's University	The Silk Purse from the Pig's Ear – Optimization of a Prototype Detector for Large Area Radionuclide Contaminated Urban Material Characterization	PL
Bowers, Patrick	Saint Mary's College of Maryland	2D vs. 3D Measurement of HER2 FISH Bioimaging in a Cell	CSTL
DeSavage, Sara	Saint Mary's College of Maryland	Characterization of a Medical Imaging Camera for Improved Color Contrast of Human Tissues	PL
Mooney, Martin	Saint Mary's College of Maryland	The Effect of the Floor on Thermoplastic Melt Spread Rate in a Fire	BFRL
Tebbe, Amelia	Saint Mary's College of Maryland	Estimating Volumes of Simulated Lung Cancers by B-Spline Modeling	ITL
Reimonenq, Wade	Southern University and A&M College	Efficiency of 35S Promoter PCR Assays for Quantitation of Biotech Maize	CSTL
White, Theodore	State University of New York Binghamton	First Order Reversal Curve Measurements of Magnetic Tunnel Junctions	PL
MacArthur, James	Swarthmore College	Using Interference Lithography to Create Magnetic Nano-Stripes	CNST
Johnson, Tessa	Tulane University	Probing the Underlying Physics of Graphene with Raman Spectroscopy	PL
Ly, Nhieli	University of California Irvine	Influence of Nanoparticles on Short-Term and Long-Term Performances of Polymeric Materials	BFRL
Rowell, Griffin	University of California Santa Barbara	The Normalization of Alanine Dosimeter Films	PL
Lambarqui, Amine	University of District of Columbia	Microfluidic Chips and Microwave-PCR for DNA Amplification	EEEL
Tierney, Kevin	University of Florida	Diagramming the Phase Relations of the CeO_2-Nd_2O_3-Sm_2O_3 System	MSEL/NCNR
Torres, Jr., Carlos Manuel	University of Florida	Green's Functions, Scattering Effects, Impurities…Oh My! Predicting the Behavior of Electrons Confined to Quantum Structures	CNST
Kuruvilla, Sibu	University of Illinois Urbana-Champaign	Modeling of Nanotube Separation in Field Flow Fractionation	MSEL/NCNR
Payson, Grady	University of Iowa	Metric Evaluation and Report Generation for the NIST 2008 Metrics for Machine Translation Challenge (Metrics MATR)	ITL
Aguilar, Izath	University of Maryland Baltimore County	Molecular Electronic Devices	EEEL
Fertig, Derek	University of Maryland Baltimore County	Water Calorimetry and Heat Transport	PL
Jackson, Brandi	University of Maryland Baltimore County	Characterization of Local Mechanical Properties in Epoxy Nanocomposites	BFRL
Jeong, Jeong-O	University of Maryland Baltimore County	Development of Software Tools for Extracting Model Parameters of SiC Power Diodes	EEEL
Schuldenfrei, Andrew	University of Maryland Baltimore County	Observations of the Oxidation of Pentacene Thin Films in Air by Photoluminescence Spectroscopy	CSTL
Serova, Nadezhda	University of Maryland Baltimore County	Non-Linear Polymer Film Thickness Gradients Through Flow Coating	MSEL/NCNR

STUDENT	UNIVERSITY	TALK TITLE	OU
Shurupoff, Kimberly	University of Maryland Baltimore County	Large Building Evacuation	BFRL
Sims, Christopher	University of Maryland Baltimore County	Fundamental Interaction Mechanisms of Engineered Nanomaterials with DNA	CSTL
Spiegler, Julian	University of Maryland Baltimore County	An Energy Model of the IAQVG Test House	BFRL
Taylor, Malcolm	University of Maryland Baltimore County	Parallel Covering Array Generation: The Future of Combinatorial Testing	ITL
Birenbaum, Jeffrey	University of Maryland College Park	Optimizing the Nano-Manufacturing of Crystalline Single Electron Transistors	PL
Biser, Dustin	University of Maryland College Park	Development of an Optical Waveform Generator Using Digital Micromirror Devices	PL
Buzek, Olivia	University of Maryland College Park	Inclusion of Parallel Vectors in FiPy	MSEL/NCNR
Cho, Suehyun	University of Maryland College Park	Cheerios Gone Micro!	CNST
Dorsey, Shauna	University of Maryland College Park	Using X-ray Microcomputed Tomography to Assess Cell Adhesion and Proliferation in Polymer Scaffolds	MSEL/NCNR
Feric, Marina	University of Maryland College Park	Manipulating Microstructure to Achieve High Performance Organic Thin Film Transistors	EEEL
Franson, Nicholas	University of Maryland College Park	Flow Table Reference Material	BFRL
Gorbashev, Aleksandr	University of Maryland College Park	Robot Sensor Evaluation and Calibration	MEL
He, Christine	University of Maryland College Park	Facilitating Structure-Based Drug Design: Updating the HIV Structural Database	CSTL
Howell, Marc	University of Maryland College Park	Using Microfluidic Devices to Amplify Small mRNA Samples	CSTL
Hudson, Amy	University of Maryland College Park	"Why Has an Answer to the LBA Problem Been Such a Mathematical Problem?"	ITL
Katz, Shifra	University of Maryland College Park	Edge-Roughness Modeling of Magnetic Nanostructures	MSEL/NCNR
Lane, Hilary	University of Maryland College Park	Combinatorial Synthesis and Characterization of TaCN Composition Spread Metal Gate Electrodes on HfO_2 for Advanced Gate Stacks	MSEL/NCNR
Lau, Christine	University of Maryland College Park	The Effect of Processing on the Magnetic and Structural Properties of Magnetite Nanoparticles	MSEL/NCNR
Le, Donna	University of Maryland College Park	Study and Test the Performance of a Nanopositioner Controller Filter Compensator	MEL
Lee, Timothy	University of Maryland College Park	Chemical Characterization of the Degradation of Poly-3-hexlthiophene (P3HT)	MSEL/NCNR
Li, Song	University of Maryland College Park	Characterization of Z-Axis Non-Linearity in a CD-AFM Scanner	MEL
Liu, Keddy	University of Maryland College Park	Quantitative Performance Evaluation of Navigation Solutions for Mobile Robots	MEL
Luo, George	University of Maryland College Park	A ZigBee Implementation of the IEEE 1451.5 Smart Sensor Network	MEL
MacNeill, Devon	University of Maryland College Park	Fabrication of NanoPatterns by Nanoimprint Lithography	MSEL/NCNR
Martin, Stephanie	University of Maryland College Park	Thermal Imaging Cameras: Testing and Validation of the Standard	BFRL

STUDENT	UNIVERSITY	TALK TITLE	OU
Mont, Alexander	University of Maryland College Park	Use of a Computational Fluid Dynamics Model for Fire Protection in Nuclear Power Plants	BFRL
Niarhos, Peter	University of Maryland College Park	Single-Walled Carbon Nanotube Dispersions: A Study of Various Surfactants for Selectivity and Stability	BFRL
Opert, Kelly	University of Maryland College Park	Compartment Fire Experiments for Validation of Advanced Computer Models	BFRL
Raghunandan, Sindhushree	University of Maryland College Park	Characterizing the Assembly of HIV-1 Gag Protein on a Model Membrane Surface	MSEL/NCNR
Robertson, Scott	University of Maryland College Park	Examining the Reliability of the BANG3-PRO Gel as a Three Dimensional Dosimeter	PL
Rose, Cameron	University of Maryland College Park	Expanding e-FITS with Java	ITL
Sailey, Mark	University of Maryland College Park	Implementation of Armstrong's Particle Correction Algorithms in the NIST DTSA-II Microanalysis Software Package	CSTL
Sarvey, Thomas	University of Maryland College Park	Development of a Graphical Interface for Monte Carlo Simulations of Magnetic Crystals	MSEL/NCNR
Shah, Roshan	University of Maryland College Park	Measuring Security Risk of Networks Using Attack Graphs	ITL
Tang, Kathy	University of Maryland College Park	Cell Response to Surface Roughness of Dental Composites	MSEL/NCNR
Wagman, Nicholas	University of Maryland College Park	Modulus Influences on Moisture-Induced Adhesion Loss	BFRL
Ward, Andrew	University of Maryland College Park	An Introduction to Optical Tweezers	MEL/TS
Yang, Minghui	University of Maryland College Park	Improving Measurement and Automation Features of a Electricity Reference Standard	EEEL
Rivera Rodriguez, Axel Y.	University of Puerto Rico Humacao	Principal Components Analysis & Singular Value Decomposition for Automated Angle Measurements	ITL
Fuentes-Martinez, Paul	University of Puerto Rico Inter American University	Characterization of Graphene Ribbons from Liquid Exfoliation of Graphite	MSEL/NCNR
Cortes, Raiza	University of Puerto Rico Mayaguez	The Applicability of a *P(r)* Inversion Method	MSEL/NCNR
Muniz-Mercado, Angelica	University of Puerto Rico Mayaguez	High Resistivity Measurement at High Temperatures for Solar Probes	EEEL
Montalvo-Delgado, Stephanie	University of Puerto Rico Rio Piedras	Measurement of SRM 2461 Standard Casings Using a Nanofocus Confocal Microscope	MEL
Green, Daniel	University of Rochester	Standardizing Voltage Characteristic Measurements of Electroshock Weapons	EEEL
Perl, Emmett	University of San Diego	Through-Barrier Radar Detection and Imaging	EEEL
Jiang, Chong	University of Texas Austin	Nanocapacitance Measurement	EEEL
Muniez, Jr., Ike	University of Texas Pan American	Surface Chemistry Parameters of Environmental Isolates of *Bacillus Thuringiensis* Spores	CSTL
Feight, Jarod	University of Wisconsin Stout	Nano-Scale Milling with a Helium Ion Microscope	MEL
Glazer, Matthew	Virginia Polytechnic Institute and State University	Triplet Correlations in Magnetic Flux Line Lattices within Elemental Type II Superconductors	MSEL/NCNR
Mayer, Brian	Virginia Polytechnic Institute and State University	Prototype for Simulation-Based Testing of Shop Floor Scheduling	MEL
Shemonski, Nathan	Washington University St. Louis	Building a Scanning Kelvin Force Microscope Feedback Loop	EEEL

STUDENT	UNIVERSITY	TALK TITLE	OU
Freedman, Willa	Wellesley College	Evaluation of the Effects of Cocktail Composition and Instrument Dependence on the Activity Determination of ^{63}Ni by Liquid-Scintillation-Based Efficiency Tracing with ^{3}He Standards	PL
Boutin, Alexander	Western New England College	Motion Behavior of a Stagger-Tuned Piezoelectric Shaker	MEL
Purdum, Kathryn	Western New England College	Microscopic Robotics: Characterization of How They Move	EEEL
Cahn, Jackson	Whitman College	Protein Adsorption Affects Osteoblast-Glass Adhesion Strength as Measured by Colloidal Probe Atomic Force Microscopy	MSEL/NCNR
Lontz, Timothy	Worcester Polytechnic Institute	Developing Virtual Fire Fighter Trainers	BFRL
Tong, Long	Worcester Polytechnic Institute	New Measurement Technique for Characterizing the Anisotropy of Brachytherapy Seeds	PL

- THE END -

http://www.nist.surf.gov/surf2.htm