2011 SURF

summer undergraduate research fellowship

PROGRAM AND ACTIVITIES

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2011 SURF Summer Seminars and Tours

May 23 — First official work day and orientation for SURF Session I students

June 2 — Dr. Elizabeth Strychalski
NIST Material Measurement Laboratory, Biochemical Science Division

Nanoslinky: DNA Molecules Descending a Nanofluidic Staircase

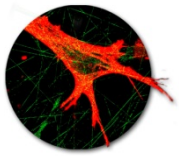
Systems seek to increase their disorder, or entropy. We introduce a method called "entropophoresis" that exploits this tendency to control the otherwise random motion of DNA molecules in a fluid. When squeezed into a nanoscale channel shaped like a staircase, a DNA molecule moved analogously to a Slinky walking down a flight of stairs. While a Slinky is driven by momentum and gravity, the DNA "Nanoslinky" diffused across each step and stepped down to increase its entropy. Entropoporesis enabled an automated and multiplexed study by widefield Epifluorescence microscopy of the change in DNA size between strong and moderate nanofluidic slitlike confinement.

June 2 — ***Laser Safety Training***

Josh Hadler from the Optoelectronics Division provided laser safety training for all staff, associates, and students.

June 9 — Dr. Kaushik Chatterjee
NIST Material Measurement Laboratory, Polymers Division

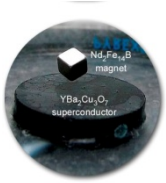
Engineering Tissues at NIST



The field of tissue engineering has the potential to revolutionize healthcare through regeneration and repair of damaged tissues and organs in the human body. Combining engineering principles with fundamental knowledge of biological, chemical and physical sciences, tissues are being engineered from cells seeded in a three-dimensional structure often known as a tissue scaffold. This talk will present an overview of the current strategies in this field. Also described will be the work of the Biomaterials Group at NIST to develop high-throughput screening technologies and reference scaffolds to systematically measure cell-scaffold interactions towards accelerating the pace of tissue engineering research.

June 16 Robert M. Briber
Professor and Chair, Department of Materials Science and Engineering,
University of Maryland, College Park

Materials for the Future



The field of materials science and engineering sits at the boundary between the disciplines of physics, chemistry and engineering. Advances in materials have been the precursors of new technologies and future developments in materials will be the building blocks of continued technological innovation. The talk will provide an introduction to the field and gave examples of many advanced materials through hands-on demonstrations and audience participation.

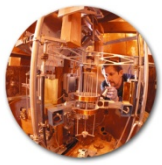
June 23 Dr. Gretchen Campbell
NIST Physical Measurement Laboratory, Atomic Physics Division

Time Keeping with Ultracold Atoms

Precise timekeeping is important for a number of everyday applications. Precise clocks are used for synchronizing telecom networks and GPS. They are also essential for navigation and for communicating with deep-space probes and rovers. It is predicted that with even higher precision, clocks will lead to new types of gravity sensors, and will allow for the testing of fundamental physical laws. Currently the most precise clocks are made with cesium atoms, where microwave radiation is used to probe and measure an atomic resonance. At NIST researchers are working to develop new atomic clocks, which use optical light to proe ultra-cold alkaline-earth atoms. By using higher frequency optical light instead of microwaves, the clocks divide time into smaller units, offering record precisioin. In these clocks, atoms are held very tightly in optical lattices. The lattice is formed by standing waves of intense laser light. By carefully controlling the environment and interactions between the atoms, optical frequency standards have recently surpassed the accuracy of the best cesium clocks. With their current accuracy, the clocks would neither gain nor loe a second in more than 200 million years.

July 7

The Electronic Kilogram and the Planck Constant and The Next Generation E-Kilogram

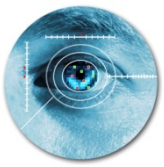


The Electronic Kilogram project uses a mass balance and induction coil in a background magnetic field. The mechanical

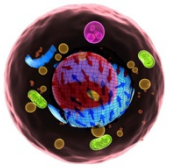
force of gravity on a mass reference is balanced against an electromagnetic force generated with current in the coil, as in a linear electric motor. When the same coil is moved to generate voltage, as in an electric generator, the voltage to velocity radio provides an effective calibration of the magnetic field. From these measurements, mechanical power watt units are measured relative to electrical power units, and the result, the fundamental Planck constant, is measured. The electronic standards that go into the measurement are atomic clock time and frequency, laser length, Josephson effect voltage, and quantum Hall resistance. A kilogram mass reference is a standard traceable to the one and only defining artifact in a vault in Paris. Since this measurement involves electronic standards and fundamental physical constants, in the near future the definition of kilogram units of mass will be changed to one using the watt balance method as a new electronic mass standard.

July 14 Vincent Stanford
NIST Information Technology Laboratory, Information Access Division

Distributed Sensor Data Acquisition and Pattern Recognition



July 21 Professor Brian Paegel
Scripps Research Institute



Total Synthesis of a Cell

In pursuit of a total synthesis of the cell, chemical and enzymatic routes to small-molecule metabolites, oligonucleotides, genes, peptides and proteins abound, but there are no elegant synthetic strategies for accessing the lipid bilayer envelope. In fact, among the molecular milieu of the cell, the various membranous structures are uniformly elusive targets. Our laboratory is exploring rational, controlled routes to bilayer synthesis that is driven by microfluidic technology. Our microfluidic phase transfer strategies have proven successful in the synthesis of uniform giant unilamellar vesicles, and set the stage for assembling more complex cellular structures, such as the double bilayers found in the nuclear envelope, or the iconic bilamellar assembly of the eukaryotic cell.

August 2 Final presentations by SURF students moderated by invited guests.

August 2 Lunch: SURF Directors and special invited guests.

August 3 Final presentations by SURF students moderated by invited guests.

August 4 Final presentations by SURF students moderated by invited guests.

August 5 Last day for SURF students and farewell pizza party.

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2011 SURF Summer Activities

It's difficult when you're in a new city and starting a new job. Many of the NIST Gaithersburg SURF students find themselves in the same boat and thus forge bonds that may last a lifetime. A number of the students also come back for a couple years so they're more than willing to help the new students with the benefit of their experience. They work together AND play together. In fact, to make life easier NIST SURF Director Lisa Fronczek created a Facebook group just for the SURFers called "NIST SURF 2011 – Gaithersburg.

SURF BBQ – NIST Picnic Grove

The SURF Directors' continued the tradition of welcoming the SURF students with a BBQ at the NIST Picnic Grove. The Directors' provide burgers/dogs, fruit, chips, and dessert. The students showed up and did what they do best – eat and have fun – music, Frisbees, footballs, etc.

Bubble Tea

At least once a week number of the SURFers would head to a nearby bubble tea shop to indulge in their favorite tea.

For the first-timers, ordering a Bubble Tea can be an event. The tea is likely to be in pastel colors of pink, green or yellow. The unique ingredient of Bubble Tea is the tapioca pearls . About the size of pearls or small marbles, they have a consistency like gummy candy (soft and chewy). Being heavier than the drink they tend to always stay near the bottom of the glass. These drinks are usually served in large see-through plastic containers with an extra-wide straw to sip these jumbo pearls. Just sucking on the translucent straw creates a show, with pearls floating up in succession. Children like to blow the balls out from the straw to shoot at targets or at each other. Some people find the tapioca balls bizarre and repelling. If you try it and like it - you'll crave the drink and never look at coffee the same way again!

The Bubble Tea craze has been huge in Taiwan and other parts of Southeast Asia for the last 15 years. In fact, Bubble Tea has taken Taiwan by storm over the past decade. The drink originally started as a childhood treat in Taiwan in the late 1980's at small tea stands in front of the schoolhouses. Teenagers and elementary school children looked forward to their after school tea. Tapioca pearls are made mostly from tapioca starch. Someone came up with the idea of adding tapioca pearls as a bit of novelty, and the idea spread. This created a new fad of adding tapioca pearls into the children's favorite tea drinks.

July 4th in the Nation's Capital

Photo © Capitol Concerts

Many of our 153 SURF students are out of the area and were given a chance to see the celebration that takes place in our Nation's Capital, with Washington, DC museums and the U.S. Capitol in the background. Whether you were young, old, local, or all the way from Puerto Rico, who could pass up the chance to mark 31 spectacular years featuring the most dazzling display of fireworks anywhere in the Nation. Many people arrive early (public access starts at 10 a.m.) to stake out their seats/blankets on the lawn for the festivities. There were plenty of activities during the whole day to keep the whole family busy. The fireworks were captured by 18 TV cameras stationed around Washington, DC. OK SURFers, we hope you were behaving because you never know if you were being photographed.

2011 SURF T-Shirt Design

T-shirts are always a popular way to remember where you've been, i.e., trip to Hawaii, from a concert of your favorite band, but what's even better — design your very own souvenir T-shirt from your summer at NIST. Unlike the run of the mill T-shirts from the abovementioned venues, these T-shirts are designed by a group of fellow SURFers. Again this year's group was very industrious, designing two T-shirts. In addition to the main T-shirt," they designed a shirt similar to Letterman's "Top Ten" only this was NIST's "Top Ten." All the fashion conscious, be it SURF student, scientific advisors, or administrative staff, are seen sporting the latest design across the 578 acre NIST campus. It also lets all those students at their home university know where *they* were during the summer!

NIST Summer Institute for Middle School Science Teachers

The 5th NIST Summer Institute for Middle School Science Teachers was held from July 18 – 29, 2011. The workshop sponsored 20 teachers from Maryland, Virginia, North Carolina, South Carolina, Illinois, and Washington, DC.

The Summer Institute is a collaboration between NIST and local school districts, is an innovative combination of hands-on activities, lectures, tours, and visits with scientists in their laboratories. Designed to coordinate with the middle school curriculum, the teachers are provided with resources and instructional tools for teaching math and science, with an emphasis on measurement science used at NIST. Led entirely by NIST scientists, the Summer Institute translates the cutting-edge research done in the laboratory to activities designed to be carried out in the classroom. Networking among the scientists and teachers provide long-term resources through the on-going relationships for the teachers and their students. Since the SURFers were working on interesting projects they were asked to help in the project. It's important for the SURFers to learn to explain what they are doing to others. This made them great examples for the teachers. It's a small world out there – maybe they got to connect with a science teacher from years ago – something I'm sure all the teachers would like to have happen in the future!

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.

Books, Bears & Bonnets, Inc.

NIST has a Volunteer Club that often does work for a charity called Books, Bears, & Bonnets. This organization creates care packages that include a book, a stuffed animal, and hats for cancer patients of all ages. Periodically they ask the NIST group to help assemble parts of the baskets (e.g., pencils, notepads cards, a letter about their organization, and sometimes books). When the SURFers showed up to offer their support, they had everything assembled in half the normal time the meeting runs. Ah, it makes your heart feel good to donate a whimsical gift box to bring smiles to children and adults fighting cancer.

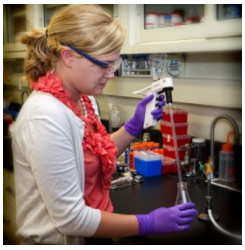
The Future of a Scientist

Dr. Katharine Gebbie, Director of the NIST Physical Measurement Laboratory, offered to speak with any interested SURFers one-on-one about their future career plans. The Physical Measurement Laboratory initiated the SURF program back in 1993 with a group of only 20 students. This year we had over 150 students participating.

SURFer Selected as *Washington Post* Federal Player

Federal Player of the Week: NIST Intern working to prevent cavities and promote healthy teeth

By Partnership for Public Service, Published: August 1, 2011



Since her first dental appointment, 19-year old Courtney Keeler has been fascinated with teeth and the science behind keeping them healthy.

Keeler has now channeled this curiosity as a 2011 Summer Undergraduate Research Fellow (SURF) at the National Institute of Standards and Technology (NIST). As a fellow, she has been contributing to ongoing research on a dental materials project under the guidance of a NIST scientist.

"I feel like a real scientist. You go to school, you grow and have science fairs and now I am here actually contributing to the scientific world and effectively making a difference," Keeler said. "I am able to make contributions to science that will help more than just me."

According to the Centers for Disease Control and Prevention, more than 40 percent of children ages five to 17 as well as most adults have tooth decay. To treat this disease, dentists are increasingly using polymeric materials in dental fillings. Keeler said that most of these composites must eventually be replaced due to recurrent decay from oral bacteria. The goal of the NIST research is to provide measurement methods and reference materials to facilitate the rational design of polymeric dental materials, thus enabling improvements in their clinical performance.

Recent NIST studies have shown that the chemicals that leak out of dental materials can alter the growth of bacteria. To help determine which chemicals are primarily responsible for altered bacterial growth, Keeler has been in the lab everyday preparing solutions of the individual chemicals, adding them to the bacteria and measuring the bacteria response.

Through Keeler's research, she believes that dental materials can be better understood and become more effective at maintaining oral health.

Knitting Circle

Knitting isn't just for elderly ladies. If you came by Summerfield Suites Hotel every Tuesday and Thursday from 7:30 – 9:00 p.m., you would have seen a group of *young* people in the SURF Knitting Circle enjoying a fun and relaxing hobby after a day of working away in their labs. Unfortunately, many people are plagued with knitting anxiety, intimidated by the many kinds of stitches, yarns, and loops they've heard and read about. Fortunately, knitting really isn't all that hard to learn once you have a few of the basics down. SURFers aren't afraid to give anything a try…at least once.

Tour of White House and U.S. Capitol Building

It's not every day 153 SURFers get to visit The White House and the U.S. Capitol Building. It takes some work and organization and the SURFers are excellent at both. They were lucky enough to be granted a tour.

For more than 200 years, the White House has been more than just the home of the Presidents and their families. Throughout the world, it is recognized as the symbol of the President, of the President's administration, and of the United States.

Rebel Race Maryland/DC 2011

Are you sick of the same routine every week? Hmmmm…. suppose there were some SURFers who answered yes to that question. Unleash your inner rebel: ditch the coat and tie and free yourself from the daily grind and enjoy the mud!

Rebel Race is a weekend get-away for athletes that want to run a military style 5k or 15k and then party like there's no tomorrow! — it's the most adrenaline rushing obstacle run ever!

The Rebel Race Series is designed for people feeling the urge to tackle intense obstacles. From start to finish, Rebel Race's military style obstacles will have you dashing, barricade-climbing, mud-crawling, rope-swinging and fire-jumping. Our grueling course forces each rebel to test their physical toughness and mental endurance. Cross the finish line and bask in the glory with tons of beer, food, live entertainment, and many new friends covered in mud. Earn the bragging rights!

Whether you were running, watching, or camping, it was a weekend you'll never forget!

Drag Racing

It seems our SURFers are into everything, including drag racing. SURFers Chris Choi and Lo-Hua Yuan came to cheer Nathan on to winning. It was their first time at a drag race. Nathan Jacobson was racing his car on Saturday, July 23rd at the Mason Dixon Raceway in Hagerstown, MD. The Mason Dixon Dragway is a ¼ mile NHRA dragstrip. Nathan made it down to the semi-finals and then lost by .006 of a second. It was super close, in distance about 6 inches. Who knew that there is a lot of math involved in drag racing, – reaction times, elapse times, and acceleration, just to list a few. In the end everyone enjoyed themselves and understood how to analyze a run based on the time slip and left with a new outlook on the mathematics involved in drag racing – it's more than just "putting the pedal to the metal" as the saying goes. The picture above is Nathan's 1972 Volvo 1800es that he raced.

Trips

The SURFers all get together and make trips to places in the area they may not normally have a chance to visit.

Cedar Point Amusement Park, OH

People throughout the entire world know about it. It's the number one rated amusement park on the planet. It's also the second oldest park in North America near the beautiful, sandy Lake Erie beach. In 1870 Cedar Point first opened as a public bathing beach. The history of thrill rides at Cedar Point began in 1892 with the introduction of the peninsula's first roller coaster, the Switchback Railway. The addition of the 25-foot-tall, 10-mph scream machine would forever shape the future of Cedar Point. In 2003 Cedar Point shocks thrill-seekers yet again with the debut of the 420-foot-tall, 120-mph Top Thrill Dragster – making Cedar Point home of the tallest and fastest roller coaster in the world. Maverick was voted the best new attraction in 2007 by readers of *Amusement Today*, a leading amusment industry publication.

Ocean City, MD

Ocean City, Maryland's beaches are perfect for swimming and sunning. For surfing or fishing. For kayaking or canoeing. During the summer, there are free family activities six nights a week, including concerts, bonfires, movies - even a beach Olympics! Sounds great for a large group of SURFers who are always $$ conscious and getting the most they can out of the summer near the Washington Metropolitan area.

SURF Farewell Pizza Party

Every year the SURF Directors treat the students to a farewell pizza (50 of them) party. Again this year the SURF T-shirt committee made a few dollars profit selling the summer's hottest fashion item – the SURF 2011 (your choice of two) T-shirts. Luckily for their fellow SURFers, the T-shirt committee put that extra money into treating everyone to Rita's Ice -- pizza and dessert, what's not to love.

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Student Abstracts
2011 SURF Program

Agnes Scott College

The Effect of Tethering on the Glass Transition Temperature In Thin Polymer Films
Christine Franzel

For polymers, the glass transition temperature (T_g) is the temperature at which the polymer shifts from a brittle, glassy state to a soft, rubbery state. At the T_g, many fundamental physical and mechanical properties such as the coefficient of thermal expansion show sudden changes. Thus, the T_g is an important property for technological applications of polymers. Studies have found that when polymer chains are under confinement, the T_g deviates from that of the polymer in bulk. Polymer brushes represent one type of confining architecture in which polymer chains are grafted at one end to a surface or an interface. When the grafting density is high, chains stretch away from the surface due to steric effects, forming a highly confined system. Polymer brushes have many potential applications in fields such as microelectronics, biomedicine, and drug delivery. As such, the behavior of the T_g of polymer brushes represents an important point of interest in polymer science, yet inconsistencies in the literature have shown differing T_g trends with changes in properties such as brush thickness.

This project seeks to measure the T_g of thin, high grafting density (~0.5 chains/nm) polystyrene (PS) brushes of varying thicknesses as well as PS brushes swollen with low molecular weight (2200 g/mol) PS chains using x-ray reflectivity. The T_g of 12 nm, 20 nm, 31 nm, and 67 nm thick brushes are measured and the results are compared to those found in the literature for sparsely grafted chains and ungrafted chains. When the 67 nm thick brush is coated with a layer of 24 nm thick, 2.2 kg/mol chains in such a way that the short chains completely penetrate into the brush, the T_g of the film is lower compared to that of the pure brush.

Appalachian State University

Surface Topography Analyses for Images of Firing Pin Impressions Acquired via Confocal Microscopy
John Villanova

United States firearms examiners utilize the Integrated Ballistics Identification System (IBIS) to assist in firearm identification by comparing a reference cartridge case or bullet image to images in a large database. Once a list of possible matches is formed, a firearm examiner must compare each possible match to the cartridge case in question. By looking at tool marks left on a cartridge case including breech face impressions, ejector marks, and firing pin impressions, an experienced examiner may be able to make an identification in a still highly subjective process.

The surface and microform metrology group at the National Institute of Standards and Technology (NIST) has developed a correlator program that quantitatively measures the similarity between two tool mark topographies using the areal cross-correlation function (ACCF). With images acquired from a confocal microscope as its input, the program preprocesses the data by identifying and masking outliers

and interpolating through drop-out points according to a list of parameters. It then filters out waviness and class characteristics to leave primarily individual characteristics of the tool mark for comparison. The De Kinder cartridge case collection was previously used as a performance test for the IBIS. We investigated the unexpectedly low ACCF scores of matching pairs of cartridge case images from a sample of the De Kinder cartridge case collection. By optimizing the set of parameters, we achieved significantly higher ACCF scores and greater separation between the matching and non-matching distributions of scores, which would be of particular importance for the accurate use of a ballistics database in firearm identification based on surface topography measurement.

Arizona State University

Iconic Conductivity in Gadolinium and Praseodymium Doped and Co-Doped Cerias for Solid Oxide Fuel Cell

William Bowman

Rare-earth doped cerias (CeO_2) are potential candidate materials for intermediate temperature (500 °C to 700 °C) solid-oxide-fuel-cell (IT-SOFC) electrolytes. Cerias doped with aliovalent dopants have been found to possess high oxygen-ion conductivity in the intermediate temperature range (500 °C to 700 °C). Dholabhai et al [1,2] have used density functional theory (DFT) and a kinetic Monte Carlo model to investigate the variation in ion conductivity with dopant concentrations for single crystal Pr- and Gd-doped and co-doped cerias. We have employed a spray drying technique to prepare a series of Pr and Gd doped and co-doped cerias with compositions close to the optimum values suggested by the DFT study. A precision impedance analyzer probe station has been outfitted with a high temperature button heater capable of reaching 1000 °C in air in order to conduct in-situ ionic conductivity measurements via impedance spectroscopy. Experimental ionic conductivity measurements performed over the intermediate temperature range (400 °C to 800 °C) will be presented for binary and tertiary ceria compositions as well as pure ceria specimens. For validation of technique, identical precision impedance measurements have been done on commercially available yttria-stabilized (YSZ) zirconia samples of known ionic conductivity. YSZ electrolytes are currently being employed in commercial high temperature SOFCs.

1. P. P. Dholabhai, J. B. Adams, P. Crozier, R. Sharma, "Oxygen vacancy migration in ceria and Pr-doped ceria: A DFT+*U* study," *The Journal of Chemical Physics*, vol. 132, Mar. 2010.

2. P. P. Dholabhai, J. B. Adams, P. Crozier, R. Sharma, "A density functional study of defect migration in gadolinium doped ceria," *Physical Chemistry Chemical Physics*, no. 12, May 2010; pp. 7904-7910.

Organic Photovoltaic Devices: Band Gap Engineering

Alena Matusevich

In this presentation I will talk about thin film organic photovoltaic (OPV) devices and discuss how band gap engineering was used to systematically very the electrical and electrical-optical properties of specially designed test structures. Metrology was developed to understand the impact of such engineering on the extrinsic device characteristics. Specifically, we inserted nanometer scale organic semiconductor film between the bulk hetero junction layer and the cathode. The insertion of a neat, planer film was used to restrict the directional flow of photo generated charge carriers allowing electrical characterization methods to be developed to better understand device physics and the influence on the electrical-optical properties for the band gap engineered test structures.

Oxidatively Induced DNA Damage Analysis of Shrimp Exposed to Conditions Resembling Those of the Deepwateer Horizon Oil Spill

Varun Patel

Since 1950s, there has been more than sixty deliberate or accidental oil spills with approximately twenty major oil spills worldwide. The exposure of marine organisms to crude oil results in extensive mortality due to acute toxic effects. However, there have been relatively few studies measuring the chronic effects of crude oil on marine life. At the same time, there have been no previous studies on toxicity of dispersants such as corexit. Previous studies indicate that oil exposure has a genotoxic and mutagenic effect on aquatic organisms such as by causing DNA strand breaks and adducts, increase of micronuclei, absence of micronuclei in erythrocytes, and induction of erythrocytic nuclear abnormalities. Most of these studies have utilized flow cytometry and/or the Comet assay to quantify the extent of DNA damage. Although these techniques are widely used in DNA damage analysis, both techniques have inherent disadvantages. Therefore, in this short-term project, DNA of shrimp in mesocosms exposed to one of four conditions (control, oil, corexit, and oil plus corexit) were analyzed using gas chromatography/mass spectrometry/mass spectrometry. This technique promises confirmation of the lesion's identity and provides quantitative data on each individual lesion that is traceable to high-purity reference standards using isotope-dilution mass spectrometry. Each group of shrimp was exposed for 2, 7, 14, or 30 days. Current results from the shrimp exposed for 2 and 7 days indicate a lack of oxidatively-induced DNA damage for shrimp exposed under these conditions, while the 14 and 30 day data points are still being analyzed.

Brigham Young University

Mitigation of Set Time Delays in High-VolumeFly Ash Cement Pastes through Fine Limestone Additions

Lisa Gurney

The sustainability movement has renewed interest in reducing cement content in concrete mixtures in order to reduce the carbon footprint of concrete manufacturing and to reduce production costs. One approach is to decrease the amount of Portland cement in concrete by replacing a portion of it with fly ash (often up to 50%). Fly ash is a byproduct of coal combustion and the majority of fly ash produced ends up in landfills. Portland cement – fly ash mixtures generally have very good long term strength and durability, but often suffer from problems at early ages, including retardation of the cement hydration reactions, setting time delays, and lower early age strengths. Other powders have previously been investigated that can be added to these mixtures to mitigate such negative characteristics, and calcium carbonate (limestone) has shown some promise.

In this project, fine limestone (including nano particle-sized limestone) additions to cement – fly ash mixtures were investigated in order to optimize the cement – fly ash – limestone ratio and evaluate the effect of limestone particle size on the cement hydration reaction and set times. It was found that decreasing the particle size of the limestone from 3 μm to 120 nm significantly reduced the set times of the pastes investigated and that similar set times were observed between 100 % cement paste and mixes that replaced up to 45 % of the cement with a fly ash/limestone blend.

Carnegie Mellon University

Tight-Binding Analysis of Twisted Graphene Bilayers
Christopher Baldwin

Graphene, a two-dimensional hexagonal carbon lattice, has of late become a material of immense scientific interest, largely due to its remarkable electronic properties. Electrons in solids are described by the bands of their allowed energy values and the gaps between those bands, and graphene is characterized by a lack of separation between the highest-filled and lowest-unfilled bands. This makes it a semiconductor with notably high electron mobility, suggesting numerous potential applications in the electronics industry. One of the primary means of producing graphene, and the most promising for commercial production, is by heating a SiC wafer to temperatures at which the Si sublimates. The resulting carbon layers are rotationally disordered, in the sense that no pattern exists in the relative twist angles of adjacent layers. The collective structure is termed "few-layer graphene", and its electronic behavior is not yet fully understood.

Here, we present an analysis of bilayer graphene system in which the two layers have been rotated relative to each other by an arbitrary angle. One of the main ways of calculating a material's electronic structure is by assuming that the electrons are held close to atoms and simplifying the material's Schrodinger Equation accordingly. Such a method is referred to as "tight-binding". By implementing a simple model of the bond strength between atoms in different layers, we've extended the tight-binding analysis of a single graphene layer to that of an arbitrarily twisted graphene bilayer. The results give us a more complete picture of how few-layer graphene structures behave, and help us to understand the experimental results obtained by groups at NIST and elsewhere.Here, we present an analysis of bilayer graphene system in which the two layers have been rotated relative to each other by an arbitrary angle. One of the main ways of calculating a material's electronic structure is by assuming that the electrons are held close to atoms and simplifying the material's Schrodinger Equation accordingly. Such a method is referred to as "tight-binding". By implementing a simple model of the bond strength between atoms in different layers, we've extended the tight-binding analysis of a single graphene layer to that of an arbitrarily twisted graphene bilayer. The results give us a more complete picture of how few-layer graphene structures behave, and help us to understand the experimental results obtained by groups at NIST and elsewhere.

Interferometer for the Measurement of a MEMS Device in an SEM
Matthew Swisher

The goal of the project is to setup and confirm the operation of an interferometer for measuring the motion of a micro-electro-mechanical system (MEMS) device in a vacuum as well as in ambient conditions.

The first part of the project was setting up the feedback control for the interferometer setup. This enables the setup to fix the wavelength of the light so that overall drift does not affect the measurements obtained using the interferometer.

One of the issues with the initial setup is that it can only measure the device in ambient conditions. To solve this problem the setup will be modified so that the measurement arm of the interferometer will travel through fiber to the location of the measurement. This will enable the interferometer to measure MEMS devices inside of the vacuum of the SEM.

The operation of the setup will be tested using piezo actuators and MEMS devices vibrating at known frequencies with known displacements. The measured distances and the known distances are then compared to confirm the operations of the interferometer. Additionally a Fabry-Perot cavity may be added to try and improve the signal to noise ratio of the measurements.

Photoinduced Magnetization in Prussian Blue Analogue Tri-Layer Films
Brian Zakrzewski

Functional materials with physical properties that are tunable by external stimuli have the potential to be used in a number of technological applications. Being able to change properties such as conductivity, magnetization, and even molecular structure with easily controllable stimuli like temperature, pressure or light is an exciting prospect. The development of these materials requires an understanding of the fundamental mechanisms governing their behavior. Our experiment is focused on two specific materials that share a face centered cubic Prussian blue analogue (PBA) structure, a cobalt hexacyanoferrate (CoFe) that displays photoinduced magnetization up to 20 K, and a nickel hexacyanochromate (NiCr) that shows pressure dependent magnetization up to 70 K. The goal of our experiment is to examine a combination of these two materials in a trilayered NiCr-CoFe-NiCr heterostructure, where ~200 nm layers are synthesized one on top of the other, with one CoFe layer between two of NiCr. This structure displays photoinduced magnetic tunability and long range magnetic order at temperatures higher than that of CoFe alone. The hypothesized mechanism for the observed properties of the trilayered film involves a photoinduced structural change in the CoFe layer which increases the overall volume of the layer. This places stress on the NiCr layers, which induces a change in the magnetization because the NiCr layers have pressure dependent tunability.

A number of different methods are used to probe these NiCr-CoFe-NiCr heterostructures. Fourier transform infrared (FTIR) spectroscopy is used with a cryogenic apparatus to examine the vibrational modes of the structures before and after illumination at low temperature. X-ray diffraction (XRD) measurements are utilized at room temperature to determine the long-range structure. Extended X-ray absorption fine structure (EXAFS) spectroscopy is also used, in order to determine the local structure. To characterize the magnetization, a superconducting quantum interference device (SQUID) is used. The data obtained from the measurements mentioned above are then analyzed in concert to determine the validity of this hypothesis.

City College of New York

Characterization of the Effect of Thermal Cycling on the Signal Integrity of Interconnect Structures Used in 3D Integrated Circuits
Annas Afzal

The reliability and performance of microelectronic devices are only as good as the interconnects that link the transistors between them. Good interconnects allow electric signals to flow freely in a circuit with very limited impedance. This allows for high speed and quick response of microchips. However, microelectronic devices are subjected to fluctuating temperature conditions during their operational lifetime, which adversely affects their signal propagation fidelity. Therefore, this project takes a look at the relationship between repeated temperature cycling and the signal integrity of interconnects in microelectronic circuits. We study this relationship on two types of interconnects: back-end-of-line (BEOL) and through-silicon via's (TSV). BEOL consists of metal lines embedded in a dielectric and are used to wire transistors together. TSV's are a new type of interconnect that are being heavily researched for its role in 3D stacking of chips. We simulate the real world conditions by applying repeated temperature cycling at various maximum temperatures, and with the aid of an RF network analyzer, we extract the reflection and transmission signal characteristics of the interconnects. The mean-time-to-

failure (MTTF) of the interconnects were determined upon their breakdown. This is followed by a failure analysis study to determine the cause of failure and the predominant failure mechanism.

Massive Parallel Long-Term Reliability
Kaly Fon

As technology advances and we submerge into the world of nanoelectronics, we need to ensure the reliability of semiconductor devices because of the impact that it has over society's daily lives. Reliability is the ability of a system to perform a specified function for a stated period of time, which should be measured with large statistics. The current set up for measuring Time Dependent Dielectric Breakdown (TDDB) for semiconductor devices operates using a large rack of equipment and it can only test a limited amount of devices at a time. Because of this, we need to find a method to test hundreds of devices at a time and miniaturize the test set up. Therefore, we designed and implemented an embedded system to test TDDB in MOSFETs and SiC devices. This project seeks to simplify measuring tasks implementing a Printed Circuit Board (PCB) that is operated by a PIC microcontroller. The board is capable of capturing a vast data stream from a probe array of semiconductor devices and saving them in a database, resulting in an overall test capability of hundreds of devices. The microcontroller communicates to the other components of the board through I2C protocol and via USB to the computer. MPLAB was used to develop the firmware of the microcontroller, establishing communication with the different components of the board and making sure that the PCB is recognized by the computer. A software application was programmed within Microsoft Visual C++ to design the user interface that communicates with the system.

Web Application Development on Computer Security Metadata
Errol Markland

The Computer Security Division (CSD) at NIST-ITL releases many publications and reports to provide information about and to enhance standardized methods of security practices. While the wealth of information available is a substantial resource to anyone, the information is essentially unstructured. Unstructured information refers to information which is meaningful in of itself, but is not practical for automatic machine processing. The purpose of this project is to create an application that will analyze these unstructured documents and generate structured metadata pertaining to how each publication relates to other publications. In this web application, we will generate an interface that will show the user all relations and dependencies between the publications. This will demonstrate how changes in a particular publication will affect other publications maintained by CSD. Using the Java Programming Language, the Apache Unstructured Information Management Architecture (UIMA) framework, and the Stanford Natural Language Processing (NLP) Library at its core, the application will be capable to generating annotations that explicitly state the relations or dependencies that a publication may hold against a pool of publications. Storing all annotations in a persistent SQL Relational Database or a semantic RDF triple-store data model, the application will also be capable of processing new publications on the fly to determine how they relate to existing publications in CSD.

College of William and Mary

Constructing a Cryogenic Dipper for Tunneling Magnetoresistance Measurements of Cross-Wired Devices
Ethan Lowery

Tunneling magnetoresistance is a characteristic of magnetic tunnel junctions (MTJs) and describes the quantum tunneling probability of electrons through the insulating barrier between two thin film ferromagnets. The relative orientation of the magnetic moments of the ferromagnetic layers [parallel or

anti-parallel] is important in determining the resistance of the magnetic tunnel junctions. Our MTJs are composed of an insulating aluminum oxide barrier between cobalt electrodes grown in a cross-wired geometry on a silicon oxide chip and we can change the relative magnetic moment orientation of the electrodes with an applied external magnetic field. I designed and constructed a cryogenic dipping apparatus onto which we can mount our chips in order to carry out these resistance measurements. The dipper is a 70 cm hollow steel pipe with a top flange adapter fitted to our liquid helium dewar and a 25 cm printed circuit board mounted at the base of the dipper with a low profile 24-pin DIP and chip mount inside a superconducting solenoid. The design allows us to submerge the chip and solenoid in liquid helium and to determine with 4-point measurements the resistance of each MTJ in magnetic fields as great as 2 tesla and at temperatures as low as 2 kelvin. These measurements will allow us to determine how the tunneling magnetoresistance is affected in different magnetic field and temperature environments and to even further investigate spin dependent electron transport in magnetic nanostructures.

Probing the Validity of Theoretical Models for Predicting Vibrational Spectra of Alanine and Its Polypeptides
Kyle Zora

Alanine is the smallest of the 20 standard amino acids that compose all proteins in the human body. Due to its prevalence in biology and its structural simplicity, alanine continues to be the focus of many theoretical and experimental investigations in order to provide a solid foundation on which to base more complex studies. Identifying the fundamental vibrational modes of a molecule is an informative diagnostic of its structure. During this project, the vibrational energy levels of alanine and its polypeptides, including di- and tri-alanine, were predicted using classical and quantum mechanical methods and compared with experiment, focusing on the low frequency (10-200 cm-1) region of the electromagnetic spectrum. Density functional theory (DFT), a readily available quantum mechanical method, was chosen as the main computational method to evaluate. DFT invokes approximations based on the electron density that allow it to be computationally cheaper than other methods, but often less accurate because of the incomplete treatment of intermolecular interactions. A comprehensive examination of the available DFT methods was compared with classical models as well as experimental results. The calculations were performed modeling multiple states of the molecule, such as gas phase, aqueous solutions with varying amounts of water, and as a crystal by including periodic boundary conditions to better match the experimental data that was collected. Both Raman and infrared (IR) spectroscopies were used to obtain the vibrational spectra of alanine and its complexes through the range of states studied. By comparing the outputs from the different DFT models with the output from classical calculations and experimental results, we hope to quantify the validity of the DFT models, and to define the extent to which they can be used to predict low-frequency vibrational spectra.

Colorado School of Mines

Reactor Software Upgrades and Analysis of Test Stand Behavior
Joshua Johnson

The NIST Center for Neutron Research (NCNR) operates a 20 MW nuclear reactor as a source for various neutron based experiments. To accommodate the high demand of neutron beam time, the NCNR is in the process of being expanded with a new guide hall and four new neutron beam guides. This expansion shutdown also provides an excellent opportunity to upgrade existing reactor systems. One system, the reactor control room, faces obsolescence as older analog components are no longer produced or are in limited supply. The upgrade to digital interfaces necessitates an update of procedures concerning reactor health, namely, annual scram tests and withdrawal and insertion tests. The objective of the summer was to ensure that these tests could be performed with ease using a LabVIEW based computer program.

The rate of fission events in the NCNR reactor is controlled via four cadmium control rods referred to as shim arms; raising the arms increases the rate of reaction and lowering the arms decreases the rate of reaction. In case of any abnormal activity (radiation output spike, loss of site power, etc.) all of the shim arms must be fully lowered as quickly as possible. The current operating license for the reactor states that shim arms must be inserted five degrees within the first 240 ms of a scram event.

The LabVIEW software developed for this summer project is designed to measure the time for five degrees of scram insertion and also measure the total amount of time required to fully insert and withdraw the control rods under normal control. The programs are designed to be robust and simple to use for reactor operators. LabVIEW instrument interface libraries allow most of the test devices used to be set up programmatically.

In addition, the NCNR has a shim arm test stand used for prototyping new control systems before they are to be used in the reactor. Another data acquisition program was developed for the test stand to ensure the prototype shim system behaves similarly to the reactor shim system. Over many trials we were able to compare a mathematical model of the control system response to actual test data acquired.

Persistent Currents in a Rotating Toroidal BEC

Bryce Robbins

Following the discovery of Bose-Einstein condensation (BEC), both theoretical and experimental interests in superfluidity coupled with technological advancements in guiding cold atoms have afforded physicists the tools to probe and utilize the various phenomena exhibited by quantum fluids. Their remarkable properties make them useful for building ultracold atomic gas analogs of modern day electronics and in particular, extremely sensitive detectors such as superconducting quantum interference devices (SQUIDS). These ultra-precise detectors have applications ranging from biological and medical practices (MRI), monitoring seismic activity, geothermal energy surveying, and quantum computing.

The field of "atomtronics," or using atoms to build electronic devices, is still in its adolescent stages. Recent experiments, however, demonstrate maturity in the field with the first realization of a closed-loop atom circuit. By optically trapping ultra-cold atoms in a multiply-connected toroidal geometry and exciting quantized rotational modes of the condensate, persistent super-fluid flow was observed for periods long enough (≈ 40 s) to thoroughly study the stability of the superfluid current. For a homogeneous system, at a critical velocity equal to the speed of sound, the superfluidity of the condensate is impaired due to dissipation. The inhomogeneity of a real system, however, leads to vortex-like lowest energy excitations. This leads to dissipation well below the speed of sound as was observed experimentally. By injecting a blue-detuned laser beam into the condensate as a stationary impurity, the critical velocity can be tuned allowing direct control of the current around the loop and a significant step toward realizing an atomic SQUID analog.

In the context of Gross-Pitaevskii theory, we seek to study the existence of superfluid current around an optically trapped rotating BEC and compare it to recent experimental findings. By tuning the strength of a repulsive stationary optical barrier and controlling the rotational excitations of the condensate, we simulate the dynamics of the system and look for vortex-antivortex excitations as a signature of dissipation. We present our findings and a theoretical model for the effects of this barrier on the condensate.

Optical Femtocalorimeter
Tristan Storz

The thermal and kinetic properties of nanomaterials are necessary for the development and commercialization of devices with nanoscale structures. Measuring these properties requires a non-invasive tool that can detect extremely small quantities (femtograms) in very short time scales (microseconds). The current electrical nanocalorimeters are limited in these aspects. The proposed optical femtocalorimeter utilizes a non-contact design to measure samples on bilayer cantilevers within the necessary scales needed for nanomaterials. A high-power pulsed laser acts as a heater, while a low-power laser measures the deflection angle of the cantilever. The experimental setup uses two cantilevers: one as a reference and one for the sample. Cantilevers of different geometries were modeled using finite element analysis software (COMSOL) to model how the system will respond to the high energy optical power in microsecond time scales. Due to the small cantilevers having a high resonant frequency (several MHz), specialized avalanche photodiodes (APD) are characterized to determine the optimal spot size and optical power for measuring tiny fluctuations in the deflection angle at high frequencies.

Frequency Conversion Through Four-Wave Mixing Bragg Scattering
Bryce Thurston

Optical frequency conversion has important applications in quantum information processing and low light level detection. In the former, it can be used to connect disparate quantum systems that use photons for coupling but operate at different energies, provided that the conversion process maintains the quantum properties of the light states being manipulated. In the latter, it can be used to detect light in challenging wavelength detection bands by converting it to regions in which high performance detectors are available.

One method to achieve frequency conversion is through four-wave mixing. Four-wave mixing is a third order non-linear optical process that produces an idler wave from two pump waves and a signal. This happens through different processes such as modulation interaction, phase conjugation, and Bragg scattering. Modulation interaction and phase conjugation both involve power transfer from the pump waves to the signal and idler waves, which allows for the amplification of signals, but also results in the amplification of noise. Bragg scattering is different from these two in that it results in power being transferred directly from the signal to the idler wave without amplifying noise. It thus allows for frequency conversion in which the quantum properties of light are preserved. This in principle meets the criteria for the applications described above.

To achieve frequency conversion by means of Bragg scattering, we look to utilize the nonlinear optical properties of nanofabricated silicon nitride waveguides. Numerical, finite element method simulations are performed to analyze waveguides with geometries of varying thickness and width at a variety of wave frequencies. The results of the simulations are evaluated to determine phase-mismatch, conversion efficiency, and dispersion for a wide range of pump and signal setups. Optimal waveguide geometries, to obtain high efficiency frequency conversion from the signal wave to the idler wave over a large frequency bandwidth, are determined.

Spatial Uniformity of a Three-Element Optical Trap Detector
Brenden Villars

A single photodiode used for the detection of light is known to have poor spatial uniformity and detection efficiency due to variations in the reflectivity at the surface of the detector. An optical trap detector addresses these issues using a system of three photodiodes to “trap” the reflected light. These photodiodes are arranged in a geometry that causes any reflected light from the first photodiode to sequentially hit the

other two. The reflection from the third photodiode, which is normal to the path, travels back along the same path offering two more chances for the light to be absorbed. The signal from the optical trap detector is the sum of the outputs from the three photodiodes.

Previous measurements of the spatial uniformity of an optical trap detector found that the response of the detector varies less than 0.1% as a function of position [1]. That measurement was limited by the noise of the instrumentation used. The goal of this project is to reduce the noise experienced in this spatial uniformity measurement so that a more precise analysis may be performed. Ultimately, we expect to establish a variation of less than 0.01% in the response of the trap detector as a function of position.

[1] Lehman J., Cromer C. "Optical Trap Detector for Calibration of Optical Fiber Powermeters: Coupling Efficiency" Applied Optics. Vol.41, No.31 2002

Columbia University

Chirped-Pulse Terahertz Spectroscopy for Broadband Trace Gas Sensing
Jonathan Orthwein

Spectroscopy in the terahertz region is a highly sensitive technique for the detection of important molecules in many emerging fields of scientific research. As such, a newly devised broadband trace gas sensor based on chirp-pulse terahertz spectroscopy has been created in order to allow for extremely fast and accurate measurements of these gases to be taken. In the wake of its initial demonstrations, our mission has been to improve upon its speed and accuracy through modifications to the data processing techniques involved in the system.

The sensor relies on newly developed solid state sources and heterodyne detectors to generate and detect short chirped-pulses in the terahertz frequency range to polarize gas molecules and then record their decay emission (free induction decay or FID) in zero background (i.e., THz source power turned off). In our attempts to improve the sensor, our primary concern is to acquire the best line shapes in the frequency domain with the highest signal to noise ratios possible. To eliminate noise, we apply various windowing functions to the time-domain signal before Fourier transforming to the frequency domain to minimize spectral leakage. Alongside this, to improve line shapes, time delays in data acquisition and the non-linear sweep rate of the chirped pulse are taken into account to correct the phase of the signal's component frequencies, which allows for the extraction of the pure absorption spectrum (imaginary component of the FFT). Here, I present the improvements made by such techniques in achieving greater accuracy and precision as well as future plans for further improvements.

Converse College

pH Dependent Kinetics of Ion Channel Formation of Bacillus Anthracis Protective Antigen 63 (PA63)
Julianne Casil

Bacillus anthracis is the bacteria responsible for the disease Anthrax. Protective Antigen (PA63) from *Bacillus anthracis* can be utilized to learn more about its structure and to develop bio-sensors to detect *Bacillus anthracis*. To achieve this, it is important to understand the chemical kinetics of how it attacks a cell membrane. PA63 insertion as a biological nanopore into a lipid bi-layer membrane is observable by measuring the change in current over time. The pH of the solvent electrolyte solution affects the amount of PA63 aggregated in solution, and thus the amount available to form pores. Prior work using Small Angle Neutron Scattering suggests that as the solution becomes more acidic PA63 aggregates. The rate of insertion was observed as a function of pH, and the data gathered maybe utilized to help model the rate of

insertion of PA63 in a membrane. From the rate of current change, information regarding the concentration of PA63 channels in the membrane as a function of time can be determined and directly related to the overall rate of the insertion reaction. Besides the number of available pores, pH also affects the rate at which the reaction takes place; increasing the rate as pH decreases. It has been observed that the optimal pH for the insertion and aggregation kinetics is pH 6.6, leading to the greatest quantity of pores inserted into the membrane.

Cornell University

Layer by Layer Self Assembly on Soft Foams: Reduced Foam Flammability Using Nanoparticle Filled Coatings
Christopher Choi

Soft furnishing manufacturers use fire blocking barrier fabrics to comply with newly proposed national flammability regulations. Without these barriers, the foam cores in these products won't meet flammability requirements; however, these barrier fabrics increase the manufacturers' cost. Layer- by-layer assembly (LbL) is an innovative, cost-effective way to apply thin polymer coatings containing nanoparticles to improve the flammability of polyurethane foam used in soft furnishing.

Using electrostatic attraction, alternating charged polymer layers are deposited onto the surface of a substrate – building up polymer "armor" one polymer monolayer at a time. LbL deposition process is very simple and intuitive, and it is able to tune the thickness of the coating down to a nanometer scale. The durability, ease of construction, and customizability of these polymer coatings make them an appealing technology for many applications, including fire performance. The goal of this project is to understand how to engineer nanoparticle filled (e.g., carbon nanotube, carbon nanofiber, nanosilver, and clay) armor reduces the flammability of foam, and to develop the test standard to measure the release of nanoparticle due to stresses.

My task in this project has been to develop and characterize the LbL assembly coating procedure on foam substrates. Part of this included analyzing the release of nanoparticles used to perform toxicology studies on the nanoparticle composites being used to treat the foam. Additionally, I began studying and characterizing coatings using silver nanoparticles that may have antimicrobial applications.

FHS-LAB: A GUI for Simulating Structural Behavior Subjected to Fire
Daniel Lu

Current research in the field of structural fire engineering has focused on the modeling of three different but interrelated phenomena: fire development and growth, heat transfer in structures, and structural response to elevated temperatures. Numerous approaches have been developed to model each phenomena or stage, yet very few tools have been developed to analyze how well such models can work together as a whole. This talk will focus on a graphical user interface (GUI) software that integrates simulations of fire development, heat transfer, and structural response. The GUI will report a structure's behavior in selected fire conditions. More importantly, the GUI allows users to choose from a selection of models for the three stages. For instance, when choosing a fire growth model, users can select from preset time-temperature curves to more complex models such as the Consolidated Model of Fire and Smoke Transport (CFAST) and Fire Dynamics Simulator (FDS). The user can switch between fire growth models for the same building compartments. The talk will also go over the process of designing the GUI and discuss its potential uses for engineers and researchers.

Electron Spin Resonance
Jun Ma

Electron spin resonance (ESR) is a technique used to find unpaired electrons and impurities in chemical species. The basic concepts of ESR are very similar to that of nuclear magnetic resonance (NMR). The main difference between the two is that electron spins are excited in ESR as opposed to nuclei spins in NMR. This technique is crucial for identifying the atomic structures of defect/impurities, providing valuable information about the material. The ESR signal is in general extremely small. A bridge technique is commonly used to enhance the detection sensitivity. The microwave is split into two arms – one arm bounce off the sample while the other does not. Both arms are converted to direct current (DC) by diode detectors. A differential detection between the two arms allows the signal to be extracted. It is very important that the two arms are perfectly balanced in the absence of a signal, allowing extremely high gain amplification of the signal. Due to the imperfection of real components and detectors, the two arms are usually not balanced. Worse, this imbalance is dependent of the microwave frequency which must be swept during the experiment. Such imbalance limits the amplifier setting and the ability to detect the signal. Thus the project is to design an electronic circuit that forces the two arms into perfect balance at all frequencies while not affecting the desired signal which is modulated at 100 kHz.

Two main solutions have been chosen to solve the problem. Both solutions use circuit feedback loops that autonomously equalize signal 1 to the value of signal 2 for frequencies much lower than 100 kHz while allowing the 100 kHz signal passes through unchanged. The first solution uses an NMOS transistor to attenuate one of the signals to equalize the two signals. The NMOS transistor acts as a nonlinear voltage controlled resistor in a simple voltage-divider network. The control response is exponential when we look at R vs. V_G, resulting in very quick corrections. The second solution uses only op-amps, basic circuit components, and the summing circuit technique. The control response is completely linear, resulting in a simpler control analysis, but slower corrections.

With either implementation in place, ESR can be performed with great accuracy and speed. Impurities can be analyzed closely without interference between the manufacturing discrepancies between the two photon energy sensors.

Davidson College

Dealloyed $Pt_{100-x-y}Co_xNi_y$
Demetrios Pagnonis

A significant obstacle in the development of fuel cell technology is the cost and performance of the Pt catalyst for the oxygen reduction reaction (ORR). Pt alloys with transition metals (M), such as Co, Fe, Ni, and Cu, and a Pt_3M stoichiometry have been shown to produce a shift in the d-band center that generates more active sites for oxygen adsorption by reduced interaction with oxide intermediates. The result of which is reduced Pt loading from both alloying and increased ORR activity. Among the various transition metals alloys, Pt_3Ni and Pt_3Co have been shown to be the most active.

In this work we have studied the catalytic behavior and structure of a ternary alloy, $Pt_{100-x-y}Co_xNi_y$. The films were deposited by underpotential assisted electrodeposition, in which the transition metals co-deposited at potentials more positive than that required for pure Ni and Co or those that typically impose kinetic limitations. Applied potential and electrolyte concentration were utilized to tune film composition and structure. The Pt content increased monolithically as deposition potential decreased, while the Co and Ni followed anomalous codeposition at more negative potentials. The films were activated by dealloying or removal of the transition metals, creating a variety of Pt-rich nanoporous morphologies, as shown by electron microscopy. The $Pt_{100-x-y}Co_xNi_y$ catalysts were examined using a

rotating disk electrode to find the kinetic activity and surface area of each composition. M-rich films displayed the highest specific activity and electrochemically active surface area with $PtCo_5Ni_2$ being the most active, exhibiting a specific activity three times greater than that of Pt.

DePauw University

Circuit Synthesis for Cryptographic Applications
Catherine Baker

Currently there is no method that can find the optimal circuit for every possible function. There are a variety of heuristics available to create good circuits, but when compared to the circuits created by the circuit minimization team, these heuristics find inferior circuits. An optimal circuit can be defined in a variety of ways: small number of AND gates, small number of total gates, small depth, etc. Circuits may not optimize all of these factors and thus there can be a variety of best circuits depending on the needs of the user. This project focused on finding circuits with a small depth and with a small number of AND gates.

By reducing the depth of the circuit, you can increase the performance of the circuit. There are two programs that can be used to reduce the depth of the circuits. One program reduces the depth of the circuit while keeping the same number of gates. But in some cases a circuit can end up having only one or two gates at the final depth. In this case, adding a few gates may reduce the depth further. In these cases, it is best to try the second depth reducing program as well. The second depth reducing program adds gates in order to reduce the depth of a gate that would otherwise be irreducible. In some cases this will allow the circuit to reduce its overall depth further and in other cases it will not. These programs were able to be modified to get better results. By modifying which gates the program would try to reduce the depth of, a circuit that was originally reduced from depth 10 to depth 9 was able to be reduced to depth 7.

The other project was reducing the number of AND gates in a circuit. There are 65536 circuits that have four inputs and one output. The goal was to show that all of these circuits can be created using a maximum of three AND gates without requiring an extremely large number of XOR gates. By running simulations on a circuit building program, the goal is to determine how many circuits can be built with a maximum of three AND gates and seven gates total.

Duke University

Shelf Life Study of Silver Nanoparticles
Anne Rohlfing

Due to the increasing amount of consumer products containing silver nanoparticles (AgNPs), there has been a growing volume of studies conducted to investigate the environmental and toxicological impacts of AgNPs, as well as other potential applications. However, there is limited research on the aging, or shelf life, of AgNP suspensions after synthesis, which could have a dramatic effect on the results of these studies as they are carried out over weeks, months or years. Therefore, the aim of our work is to monitor the transformations that occur after AgNP suspensions are synthesized and while they are stored until use for either scientific or manufacturing purposes. The matrix of variables studied includes light exposure, dissolved oxygen content, temperature, silver concentration, type of nanoparticle coating, and the ratio of coating to silver. Combinations of these variables have resulted in 66 experiments completed or currently underway with additional experiments planned. Results of these studies all include UV/vis spectroscopy to monitor the typical absorbance spectra of AgNPs, indicating the possibility for aggregation and/or dissolution. Dynamic light scattering (DLS) has revealed statistically significant increases and decreases

in average particle size. On select samples, X-ray photoelectron spectroscopy (XPS) and x-ray diffraction (XRD) results will be examined for information on chemical changes and crystallinity, respectively. Based on the recent UV/vis and DLS data, we have found that storage conditions can have a great impact on the stability of AgNP suspensions over time.

Eastern Kentucky University

Verification and Modeling of Results from Nuclear Power Plant Control Room Fire Tests

Jerrod Hegwood

In 1985, Factory Mutual Research Corporation (FRMC) conducted a series of 25 full scale control room fire tests for the Nuclear Regulatory Commission (NRC) at Sandia National Laboratories (SNL) in Albuquerque, New Mexico, USA. The purpose of these tests was to provide data on fire behavior and fire characteristics within the test control room, and to provide a basis for operational regulations of nuclear power plants. As of this date, only three of the 25 test data sets were analyzed in detail, with regards to fire modeling. It is the task of the NIST Engineering Laboratory to analyze the data from the remaining 22 tests and generate fire models to determine the validity of the test results. The validity of the fire test data is tested by using it as input to a computer based fire model program. The results of running each test through the computer based fire model, and comparing the results to those of the original tests, determine the validity of the test(s) performed in 1985.

Modeling Smoke in Room-Scale Fires

Timothy Lenhof

The number one cause of death from fires is smoke inhalation, due to the toxic gases that it contains. Being able to predict the composition of smoke and how much people are exposed to it can increase life safety and allow better design of fire protection systems. This project contributes to this effort in two ways. Using the Computational Fluid Dynamics (CFD) model Fire Dynamics Simulator (FDS), we first tested the design of an actual hands on experiment that will be used to predict how much toxic gas could be emitted if typical items like furniture are involved in a fire. We found that proposed design changes could substantially alter the fluid flow in the experiment. We also found that a proposed design for a gas mixing chamber would adequately mix the gases before they entered the experiment. In the second part of the project, using FDS we modeled two side by side hotel rooms with an attached corridor. In this model a simulated wastebasket fire was used to initiate a room-scale fire. This model demonstrates the transport of smoke and toxic gases to the non-fire room, which would be dangerous if it was occupied. It will also be used to calculate the potential exposure for people who would try to leave the room, travel down the smoke-filled corridor, and exit the building.

Fayetville State University

Microscopic Analysis of Synthesized Mixed-Phase Atmospheric Particles

Reid Gunn

Aerosols affect climate change by altering the radiative properties of the atmosphere [1]. The effects of aerosols are complex and difficult to model due to highly variable bulk compositions, atmospheric residence times, and morphologies [2]. The typical net cooling effect of aerosols is due to their ability to scatter light and cause an increase in Earth's albedo. However, anthropogenic aerosols contain light-absorbing carbonaceous compounds in addition to light-scattering sulfates. Absorbing aerosols can warm the atmosphere while cooling the surface of the Earth, creating a flattened vertical temperature profile that affects the hydrologic cycle [3].

Fuller et al modeled optical properties for particles with a light-absorbing soot phase and a light-scattering shell. Variations in optical properties were studied in terms of the morphology and composition of soot. Specific absorption significantly increased in particles with concentric soot inclusions due to a light focusing effect by the scattering phase [4].

Atmospheric particles containing a light-absorbing carbon phase and a light-scattering metal phase were synthesized by combusting isooctane fuel containing titanium tetrachloride (Xaiofei Ma, UMD/NIST). Synthesis produced titanium dioxide particles containing black carbon inclusions and surface-adhering grains. The morphology and amounts of titanium, carbon, and oxygen contained in particle populations were characterized using automated particle analysis with a scanning electron microscope (SEM). Individual particles were further examined using SEM and focused ion beam techniques.

Size, shape, and composition of these mixed-phase particles were characterized in order for future research to produce a reference material to aid in climate change research and the calibration of aerosol optical property measurements.

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George Washington University

Transformative Applications: Using Android-Powered Smartphones to Enhance Soldier Operations

Shelly Bagchi

The Transformative Applications program is a DARPA (Defense Advanced Research Projects Agency) initiative that aims to develop smartphone applications for soldiers to aid their military operations, particularly in Afghanistan. These applications, developed for the Android mobile operating system, aim to give the soldiers easily accessible resources to augment their tasks. The types of applications include map imagery, geo-location operations, map annotation, tactical ground reporting, and language & translation aids, among others.

The NIST team's niche in this project is to act as independent, third-party testers for the hand-held devices and applications. A NIST tester attempts to evaluate each application by finding bugs, determining where enhancements can be made and making judgments as to the usability of the application's features. These findings are reported back to the application developers, who make the necessary fixes and improvements. The new versions of the applications are then sent back to the NIST team for further testing.

My role on the NIST project team was that of an applications tester. My focus was on the main maps application and its various sub-features, which include map drawing, GPS (global positioning system) tracking and tactical ground reporting. This involved repetitively using the application to determine any flaws, a procedure known as regression testing. I also suggested many improvements to the applications and saw them implemented in later versions.

Software Improvement of Visualization Tools for Video Analytic Evaluations

Michelle Cano

VidAT, a prototype Perl tool developed by NIST, is used to check the accuracy of systems that detect and track objects in video data. Visually mapping the detection and tracking on the video can assist in verifying the precision of the system-generated output with the ground truth annotations. Bounding boxes, object identification labels, and optional snail trails used for object tracking are added to video data based on information provided in a tracking log file produced by the CLEARDTScorer. Each bounding box is color coded to indicate the box type and score received by the CLEARDTScorer. To make the required annotations to the video data, the VidAT tool implements elements of the FFmpeg library to extract each frame of the video as a single image, overlay additions to individual images, and regenerate the video data from the modified images.

In an effort to greatly reduce execution time and remove the costly steps of image extraction, editing, and regeneration, a new filter has been developed for the FFmpeg library to achieve the results of the VidAT tool as FFmpeg is processing the video data. This filter collects information from a text file generated by the VidAT tool which is used to overlay the bounding boxes and labels directly within the video data. Linearly interpolated transformations can also be added to the resulting video data for any frames without references in the CLEARDTScorer tracking log. Integrating the video additions in the FFmpeg processing of the video data has significantly improved execution time and eliminated the need for image extraction and manipulation, resulting in a version of the VidAT analysis technique that is more convenient and user-friendly.

Hemoglobin Saturation as Expressed by its Absorbance Curve

Hailey Cunningham

Hemoglobin is the main oxygen carrier in the body and oxygen saturation of hemoglobin is a good indicator of tissue oxygenation. A method of determining whether hemoglobin is oxygenated or not is through spectrometry. Hemoglobin in its two forms, carrying oxygen and not carrying oxygen, has two different absorbance curves. The oxygen carrying form of hemoglobin has an absorbance curve with two humps at 540 and 580 nm respectively. The deoxygenated form of hemoglobin has one wider hump centered around 550 nm. These two distinct curves represent the 100% and the 0% of oxygen saturation in the hemoglobin respectively. My research this summer has centered around correlating the absorbance waveforms for hemoglobin at the intermediate points of oxygen saturation with the actual concentration of oxygen.

The goal was to be able take the absorbance spectra of the hemoglobin at different oxygen concentrations. For this the hemoglobin had to be fully deoxygenated and reoxygenated several times without destroying the hemoglobin. It was therefore important to find a way to remove the oxygen from the hemoglobin quickly while keeping the hemoglobin intact. After experimenting with several deoxygenation methods, we chose to use sodium hydrosulfite, an oxygen scavenger, in very small quantities to deoxygenate the hemoglobin. The matter of reoxygenation turned out to be simple due to hemoglobin's high affinity for oxygen. The hemoglobin would naturally reoxygenate from the headspace in a sealed container relatively quickly. To speed the process up, it was possible to bubble gas containing oxygen through the hemoglobin to reoxygenate as well.

To get the corresponding oxygen concentration in the solution, a separate oxygen probe was used. This allowed the spectral data and the oxygen concentration data to be taken at specific times to see how the spectra changed with the concentration of oxygen in the solution. This data could then be analyzed to find out if the intermediate spectra of hemoglobin are linear combinations of the oxygenated and

deoxygenated forms. The overall objective of this study is to validate the use of hemoglobin spectra in measuring oxygenation level in tissue.

Georgia Southern University

Prototyping Method for Bragg-Type Atom Interferometers
Brandon Benton

We present a method for rapid prototyping of new Bragg ultra–cold atom interferometer (AI) designs useful for assessing the performance of such interferometers. The method simulates the overall effect on the condensate wave function in a given AI design using two separate elements. These are (1) modeling the effect of a Bragg pulse on the wave function and (2) approximating the evolution of the wave function during the intervals between the pulses. The actual sequence of these pulses and intervals is then followed to determine the approximate final wave function from which the interference pattern can be predicted. The exact evolution between pulses is assumed to be governed by the Gross–Pitaevskii (GP) equation whose solution is approximated using a Lagrangian Variational Method to facilitate rapid prototyping. The method presented here is an extension of an earlier one that was used to analyze the results of an experiment [J.E. Simsarian, et al., Phys. Rev. Lett. 83, 2040 (2000)], where the phase of a Bose–Einstein condensate was measured using a Mach– Zehnder–type Bragg AI. We have developed both 1D and 3D versions of this method and we have determined their validity by comparing their predicted interference patterns with those obtained by numerical integration of the 1D GP equation and with the results of the above experiment. We find excellent agreement between the 1D interference patterns predicted by this method and those found by the GP equation. We show that we can reproduce all of the results of that experiment without recourse to an ad hoc velocity–kick correction needed by the earlier method, including some experimental results that the earlier model did not predict. We also found that this method provides estimates of final interference patterns at least four orders–of–magnitude faster than direct numerical solution of the GP equation.

Hamilton College

Analysis of aCORN Data
J. Elliott Adelman

The aCORN experiment represents an attempt to measure the electron-antineutrino correlation coefficient (or “little a”) of free neutron decay to an improved level of precision. Last winter, the aCORN apparatus collected several terabytes of preliminary decay data both as a check of overall system health and as a tool to improve experiment design. After improvements to existing analysis software and the energy calibration algorithm, the examination of the outstanding data allowed for the determination of preliminary values for little a, as well as estimates of signal to noise ratios, for data sets run under differing apparatus settings. These results will allow future incarnations of the experiment to optimize these parameters, so as to reduce the effects of systematic errors and facilitate the project’s goal of improving the precision of measurements of little a.

Harvard College

Determining Switching Mechanisms and Switching Field Distributions in Bit-Patterned Media
Robert Boling

It was proposed that storage densities in hard-drives can increase if conventional granular media are replaced by bit-patterned media (BPM). In traditional magnetic media, many magnetic grains correspond

to one bit. In BPM, magnetic nanodots are organized periodically, and each dot corresponds to one bit. Co/Pd multilayer is a perpendicular magnetic material that is promising for BPM, and patterned nanodots of this material are therefore the subject of this work. The switching mechanisms of bit patterned media have recently been of concern, especially the angular dependence of fields required to nucleate or to propagate reversed domains. Additionally, while switching field distributions (SFD) of different configurations of nanodot ensembles have been reported, few have investigated the intrinsic SFD in single nanodots. This research has two foci: (1) clarifying the switching mechanism in Co/Pd multilayer nanodots when the reversal field is applied at near in-plane angle and (2) decoupling the intrinsic SFD due to individual nanodots from the average SFD measured from a nanodot ensemble.

1. H.J. Richter et al., Recording potential of bit-patterned media, Applied Physics Letters 88, 222512(2006)
2. B.C. Stripe et al., Magnetic recording at 1.5 Pb/m^2 using an integrated plasmonic antenna, Nature Photonics 90,10.1038 (2010)

Harvey Mudd College

USARSim: A High-Fidelity Simulation of Robotics

Taylor Brent

The USARSim project (Unified System for Automation and Robot Simulation) aims to develop high-fidelity, physics-based simulations that can be used to aid research in the field of robotics. The powerful Unreal game engine provides a free simulation environment that when combined with open source modifications may be used to achieve this goal. The existence of USARSim makes it possible for third-parties who do not have access to expensive robots to do robotics testing.

Over the summer, my work focused on achieving more realistic physics by investigating different methods of simulation as well as working on shifting from an older platform (Unreal Tournament 3) to a newer and more accessible platform (Unreal Development Kit – UDK). To achieve better physics, a complete overhaul of the way robots are simulated was required, including remaking both the physical models and the operating code. This talk will describe a few aspects of the upgrade and the improvements that have been made to USARSim.

Band Alignment Study Using Internal Photoemission: Applications to Metal-Gate / High-k Dielectric / Semiconductor Interfaces

Hong Sio

As transistors shrink in size, an active search is ongoing for high-k dielectric and metal gate materials for the next generation of Metal-Oxide-Semiconductor (MOS) device. The electronic performances of these devices strongly depend on how the electronic band structures are formed and aligned at their interfaces. Internal Photoemission Spectroscopy (IPE) is an elegant method to extrapolate barrier heights at the heterojunctions of MOS device by measuring the photocurrent across the device as a function of incident photon energy.

In particular, my project this summer aims to improve the accuracy of IPE barrier height determination by correcting for the wavelength-dependent attenuation, interference, and multiple reflections of the incident photon flux as it travels through the MOS structure. The thickness and complex refraction index of each film layer are measured with Spectroscopic Ellipsometry (SE), and then the transfer matrix method is applied to obtain the transmission coefficients throughout the MOS device. As expected, the magnitude of this correction on the final barrier height is small, but not necessarily negligible depending on optical properties of the film layers. Results are presented for the InP-Al_2O_3-Al and the InP-HfO_2-Al system.

Hood College

Improving Electronic Health Record (HER) Usability, Research, and the Communication Effort
Andrea Haines

Health IT has become a priority around the nation as the use of technology to electronically access and exchange health information has increased. NIST's efforts are focused on establishing secure, usable, and testable health IT information and communication systems. Two important objectives of this project were to raise awareness of the field of health IT and to open channels of communication and collaboration to better understand and define/create guidelines and testing methods for usability.

To foster communication and collaboration, NIST is pursuing new channels of social media to inform the general public about its activities in health IT by creating an explanatory animated video that will highlight NIST's roles. To further advance the communication effort, a team developed a NIST Health IT Usability TWiki to allow the community to provide input and feedback about the efforts to develop Electronic Health Records (EHRs) usability evaluation protocol.

To further efforts in the usability of EHRs, a recent workshop titled "A Community-Building Workshop: Measuring, Evaluating and Improving the Usability of Electronic Health Records" allowed attendees to provide constructive technical feedback directly to NIST about the proposed evaluation methods for usability of EHRs. A team was then able to organize, conduct, and provide comments/responses.

We created a template for a proposed data-sheet for logging data collection in proposed usability testing protocol. In order to create this template, we examined best-practices in usability and human-factors studies and completed extensive research in an attempt to identify the end-user of an EHR. This template includes the demographics, backgrounds, and questionnaires for potential usability testing participants, a screening process to select end-users of EHR systems, and data collection sheets on user-performance and experience interacting and using EHRs.

Creation of an Evaluation Interface for Human Assessments of Machine Translations
Jennifer Hill

The NIST Open Machine Translation (OpenMT) Evaluation series is responsible for coordinating formal open evaluations of existing text-to-text machine translation technology. The project is designed to support research in, and measure advancements in the state of the art of, technologies for translating text between natural human languages by providing reliable, standardized quality assessments of system translations.

Translation performance is measured for quality using both computed metrics and human assessments. While automatic measurements excel at providing consistent, objective assessments, human judgments remain the most reliable form of semantic and contextual evaluation. In order to minimize subjectivity in these man-made judgments, several different human evaluation methods are currently being researched.

The goal of this project was to create a graphical user interface (GUI) to be used by human assessors for judging the quality of system translations. The GUI provides human judges with a simple, clean, efficient method of performing both semantic adequacy and preference-based assessments of system translations compared to human-translated references. The interface is designed for ease of use and maximal useful feedback while minimizing the potential for human bias.

Access Control Policy Tool (ACPT)
Nathan Jacobson

The National Institute of Standards and Technology (NIST) is currently developing a prototype of the Access Control Policy Tool (ACPT) system. This system allows users to create computer security model(s) based on the attributes of subjects, resources and actions from a computing environment. The ACPT user will be able to create policy models: Attribute Based Access Control (ABAC), Multilevel Security Model (MLS) or Workflow. The system will then validate/test any user specified security properties against the previously created policy/model with the NuSMV Model Checker and the NIST's combinatorial testing tools. The focus of my project was to start the software testing phase of the ACPT in order to make sure all of the features work properly. This phase is crucial for testing the verification and test functionalities of the software and getting accurate results. Along with testing ACPT, I designed a user manual for future users. I also helped layout some of the new features for the graphical user interface (GUI) of the ACPT. One facet of my project involves researching new features for the next updated version by investigating other related access control systems.

Jackson State University

Measuring the Efficacy of Ligand Displacement of Gold Nanoparticles – Applications in Nanomedicine
Melanie Shelton

The "separate-and-analyze" approach (i.e., removing surface-bound functional ligands from nanoparticles and solubilizing them prior to analysis) is widely used for characterizing molecular conjugation. Ligand displacement is typically employed for the separation step, but the uncertainty of recovery efficiency (i.e., the fraction of released versus residual ligands) can be a significant concern, possibly limiting the capacity for quantification of results.

In this study, we apply a toolbox characterization approach to better understand the efficiency of the ligand displacement process. Characterization methods include dynamic light scattering, electrospray-differential mobility analysis, and attenuated total reflectance-Fourier transform infrared spectroscopy. Thiolated polyethylene glycol (SH-PEG) and bovine serum albumin (BSA) conjugated to gold nanoparticles (AuNPs) are chosen as our model system because of the relevance to cancer therapeutics. Because of their small size (avoiding steric hindrance effects), dithiothreitol (DTT) is used for displacement of ligands. Combining information related to changes in physical dimensions and spectroscopic signals, we quantify adsorption of DTT, desorption of SH-PEG and BSA, and then draw conclusions regarding efficacy of the ligand displacement process. The complementary characterization methods demonstrated here can be used as a prototype approach to quantitatively study the removal efficiency of other types of conjugated ligands, such as other proteins or deoxyribonucleic acid.

James Madison University

Tether Lipid Molecules for High Precision Metrologyof Integral Proteins
Fay Crawshaw

The study of proteins and their function is important because of the vital role proteins have in life. Integral membrane proteins (IMPs) are found in bilayer lipid membranes and are the "gate-keepers" of material or chemical signals into and out of cells/organelles. Studying IMPs in their native bilayers would be ideal because the IMPs would be in their native conformations for structure-function studies; however, this is difficult because of the complexity of the system. Tethered bilayer membranes (tBLMs) are an

attractive and much simpler alternative that places a bilayer environment next to a surface for the application of surface science metrology, such as neutron reflectometry, and other experiments, such as electrochemical redox experiments. Lipidic anchor molecules are a part of these tBLMs. Previously prepared lipidic anchors at NIST had two identical alkyl segments. My talk will outline progress on a project consisting of two parts (a) synthesizing a molecule with two different alkyl chains because it will more closely resemble those found in nature and (b) working to optimize previous reactions in order to find the most effective and successful procedures. Using different leaving groups, i.e., mesylates, we have raised yields of difficult substitution reactions to ~80%. In addition, I will discuss results related to strategies for the preparation of lipidic anchor molecules with more than one anchor-bond. Such molecules are desirable as they should add stability to the resultant tBLMs.

Novel Methods for Remote Sensing Bassed on DIAL
Eric Vess

As part of the Greenhouse Gas Initiative we have set out to develop new and innovative methodologies for the range resolved concentration measurement of greenhouse gases. Differential Absorption LIDAR (DIAL) is a well established measurement technique which can perform range resolved concentration measurements up to several kilometers away with a range resolution of a few tens of meters. This technique is historically accomplished by setting a single frequency of near-IR light on a desired absorption transition, and counting the backscattered photons as the light pulse travels through the atmosphere. This step is repeated with the laser tuned off the absorption transition and the derivative of the log ratio yields the range resolved absorption measurement.

We have designed a system which uses an Electro Optic Modulator (EOM) to add multiple sideband frequencies to the center frequency of the laser which allows a transition to be characterized instantaneously. The linewidth of a CO_2 absorption at 6242 cm^{-1} is approximately 0.0133 cm^{-1} (4GHz), this transition was probed both on and off resonance simultaneously. Detection was accomplished by using two heterodyne detectors, the return signal was beat with a LO on an avalanche photodiode. A portion of the outgoing signal, before going through the sample, was picked off and beat against the LO on an InGaAs photodiode to generate a reference signal needed for normalization. Testing of this prototype system was accomplished by absorption spectroscopy using optical transmittance/absorbance over a distance of a few meters under various concentrations of CO_2. Further experiments and applications will be discussed in light of these developments.

Johns Hopkins University

A Statistical Approach to EDS Peak Identification: A Proof of Concept
Howie Joress

Energy dispersive X-ray spectrometry (EDS) has become a mainstream scientific technique; many of the scanning electron microscopes (SEM's) in commercial, academic and government labs across the country and the world are equipped with an EDS detector. Nearly all software packages for the analysis of EDS spectra have an automatic peak identification tool. With the widespread use of EDS, automatic peak identification has become a well utilized and relied upon feature. Unfortunately, there are a variety of peak identification errors that typically occur when using the automatic peak identification function on most currently available software. If not corrected, this could threaten the credibility of EDS microanalysis as an accurate elemental analysis method. These blunders are due to the reliance upon matching a single channel at the peak maximum to a known characteristic X-ray line.

Here we propose and provide proof of concept for a technique that utilizes statistical methods to analyze entire spectra rather than a single channel for determining the elements present in a sample. We have

demonstrated the feasibility of this approach by demonstrating that we can distinguish between particularly difficult element combinations, chosen for their misidentification potential (e.g. Pb and PbS and $MgBr_2$ and Mg_xAl_y), by using principal component analysis (PCA). We have shown this using both simulated data as well as experimental data. We have also developed simple artificial neural networks that are capable of reading EDS spectra and providing a Boolean solution as to the presence of a limited class of elements within the sample. Based on this work we believe it is possible to create a neural network capable of returning a solution for any element found in EDS spectra.

Juniata College

Optimizing the Sputtering Parameters for Permalloy Thin Films to Minimize Surface Roughness
Theresa Ginley

The spatial resolution by which the surface structure of a thin film can be determined by neutron reflectometry is limited by the surface roughness of the film. Therefore, the optimization of the sample preparation with regard to surface roughness is an important prerequisite for a successful reflectometry experiment. While examining certain types of thin films, such as lipid bilayers or photovoltaic films, it is often advantageous to prepare the film on top of a solid support which contains a buried layer of permalloy (81% Ni/ 19% Fe), a soft magnetic alloy. Due to the different interactions of oppositely polarized neutrons with the magnetic layer, two distinct reflectivity curves can be collected from an isotopically identical sample when performing a polarization-sensitive neutron scattering experiment. This magnetic reference layer technique increases the spatial resolution of the measurement and, in some cases, allows for a direct inversion of the reflectivity data into the scattering length density profile along the surface normal, from which the structural profile is derived. The permalloy film is typically deposited onto a silicon wafer using magnetron sputtering in a clean room environment. In order to minimize the surface roughness of the film, various parameters of the sputtering process have been optimized. This investigation examined the effect of wafer cleaning methods, sputtering power, substrate temperature, and radio frequency (RF) vs. direct current (DC) sputtering on the surface roughness. X-ray reflectometry and Atomic Force Microscopy scans were conducted to determine the surface roughness of the various samples.

Le Moyne College

Gathering Benchmark Data for the Examples of FiPy
Andrew Acquaviva

Measuring computational efficiency, including CPU and memory usage and performance time, is an important part of the development process in scientific computing. This presentation will describe our efforts to generate and automate efficiency measurements and display them on the web as part of the FiPy development process. FiPy is a well-established python tool for numerically solving partial differential equations. It is developed using modern software development techniques; specifically, it includes automated unit tests that are launched and displayed each time a developer commits to the code repository. However, FiPy development had not previously included an efficiency suite or any automated process for measuring and displaying efficiency data. Our work addresses this by both auto-generating benchmark cases from existing FiPy examples and by hooking a benchmarking tool known as Codespeed into the existing automated unit test framework. Codespeed both displays the data in a variety of easily digestible graph and table formats and also maintains an historic database of efficiency data. Historic data is vital for developers in order for them to discover where previous changes to the code may have made significant benefits or caused deterioration in the code's performance. Our efforts have cultivated the efficiency benchmark suite; coupled with the Codespeed repository, we have synthesized a system by

which the FiPy developers are now being provided feedback for further tweaks and improvements in the implementation.

Lebanon Valley College

Analysis and Model of Multi-Sensor-Fusion Data
Ian Younker

NIST works to develop the standards, tools, and methods necessary to help the manufacturing industry make more complex and customizable parts faster. Before these standards, tools and methods can be developed the manufacturing process must be better understood. For example, how long can a tool cut a specific material before it needs to be replaced because it is worn and affecting the cutting accuracy? What are the forces and heat that is present at the tool/material interface? The Analysis and Modeling of Multi-Sensor-Fusion Data is a project working to help answer these questions. It involves a suite of sensors – used to simultaneously measure temperature, acoustic/ultrasonic pressure, acceleration, and strain – for measurements of machining processes. Together these sensors should be sensitive to various machining phenomena, such as chip segmentation, chip breakage, tool vibration, tool chatter, and tool wear. Cutting experiments were performed on an automated turning center in the NIST Shops. Fifty-two cutting trials, with varying cutting parameters, on three different materials were conducted. Over 1.4 GB worth of sensor data was collected. To analyze all the data different techniques were carried out in the laboratory and by programming original MATLAB processing code. These codes included fast Fourier transformations (FFTs), sensor coherence and temperature modeling. Chips from the cutting experiments were also measured under a microscope, and the results were used to confirm sensor measurements. Explanations of the analysis processes, and results and conclusions from the data analysis will be presented.

Lehigh University

Characterization of Carbon Nanotubes in Composite Baseball Bats
Christopher Marvel

Carbon nanotubes are cylinders of carbon atoms with diameters as small as 1 nm and tens of nm in length and they have a higher strength-to-weight ratio than steel. CNTs are considered advantageous because of their superior mechanical properties compared to other fibrous materials and many of today's materials are enhanced by incorporating CNTs into their structures. One use of CNTs is to impregnate CNTs in carbon-fiber-reinforced polymers for improved strength and toughness of the polymer matrix. This type of CNT enhanced material is commonly used in many sporting goods. However, a widespread use of CNTs in consumer products raises some concern about their eventual environmental and health impacts. For example, recent studies have shown that CNTs can have similar health effects as asbestos in some situations.[1]

In this study, two commercially available CNT enhanced composite baseball bats (from two different companies) are evaluated. Our main goal was to develop sample preparation and analysis procedures for various microscopy studies to detect and characterize CNTs in the samples. Samples from the bats were first investigated via light optical microscopy to determine their overall structures. Scanning electron microscopy (SEM) with energy dispersive x-ray spectroscopy (EDS) was then utilized to collect elemental maps as well as higher magnification images. Elemental maps were used to identify the CNT enhanced composite layer within the bat material. Raman spectroscopy was conducted on this region to confirm if CNTs are present. A focused ion beam (FIB) SEM was then used to generate a 3D image stack of the CNT enhanced composite layer as well as produce a thin film transmission electron microscopy (TEM) sample for high resolution imaging. Ultimately, this project focuses on developing proper sample

preparation procedures as well as characterizing CNTs regarding their location, size, and concentration. Our evaluation to date shows that any accidental release of CNTs from these bats during normal use are not likely, since the CNT enhanced composite layer is confined to the inside of the bat and CNTs are embedded within the polymer matrix.

[1] J. Muller, F. Huaux, N. Moreau, P. Misson, J. Heilier, M. Delos, M. Arras, A. Fonseca, J. B. Nagy, D. Lison, Respiratory toxicity of multi-wall carbon nanotubes, *Toxicology and Applied Pharmacology*, Volume 207, Issue 3, 15 September 2005, Pages 221-231

Loyola University of Maryland

Roles of Atomic Force Microscopy and Nanoidentation in Building Metrological Foundations for Nanomechanical Property Testing

Kyle Slusarski

As advances in technology increase the scope of the observable world, nano-scale applications have come to the forefront of materials science research. One of the more prevalent topics in materials science is that of material property testing, which is used to determine properties such as hardness and Young's modulus. In light of these acknowledgements, there is a pressing need to establish reference materials and standards for determining these properties at micrometer and nanometer length scales.

This talk will discuss the roles of two methods for deriving such properties in building a metrological foundation for nanomechanical property testing; namely, atomic force microscopy (AFM) and nanoindentation. The techniques and their utilities are discussed in detail, followed by a presentation of the tentative standards and reference materials involved. Single crystal Ni specimens with known crystallographic orientation were scanned using a non-contact cantilever tip to determine surface topography before and after indentation. A gold fiducial pattern deposited on the surface via photolithography provides the points of reference necessary to produce indentations in the scanned regions. Nanoindentation was done using a standard Berkovich tip of known geometry and carried out at progressively smaller loads to investigate "pop-in" effects, which are caused by dislocation behavior in sub-surface regions of the material. Surface images generated from AFM scans and force-displacement curves generated during nanoindentation are also presented.

Miami University of Ohio

Imitating Ocean Reflectance Measurements with Diffuse Reflectance Standards

Alexis Denton

Diffuse Reflectance Standards provide reference standards for measurements of ocean surface reflectance. The standards, which are not Lambertian (the surface-reflected radiance seen from all angles is not constant), are characterized by the Bidirectional reflectance distribution function (BRDF). The BRDF describes how light is reflected at a surface, and is given by the ratio of surface-reflected radiance along direction, ωo to irradiance incident on the surface from direction, ωi. In remote sensing, surface-reflected radiance is an important factor in determining remote-sensing reflectance (the ratio of water-leaving radiance to incident sky irradiance) which has implications for understanding the health of the oceans. Water-leaving radiance, which is not directly measurable, is approximated by subtracting an estimated value of surface-reflected radiance from the total radiance of the water (volume and surface reflected radiance). Recent ocean-color validation experiments in Long Island have operated under major assumptions about measurement protocol and the properties of the standards. These assumptions are: the radiometers used are not sensitive to polarization of light by water, the diffuse reflectance standards are perfectly lambertian with BRDFs equal to ρ/π (where ρ is the reflectivity of the standards), and the non-

uniformity of the spectral sky radiance does not affect the measurements. To provide a better understanding as to why these assumptions are problematic to accuracy, the sensitivity to varying viewing/positioning angles and sky conditions was studied using a solar-illuminated standard and a Spectral Evolution Instrument (SEI). A solar tracker was built to move the standards to be normal to the incident sunlight and measure at a 45 degree angle in the plane of the sun, and also to reproduce the procedural methods of the Long Island experiments in which the standards were horizontal and the view angle was 90 degrees to the sun plane. The difference in these two measurement methods will be discussed, and the assumptions of the Long Island experiments will be challenged. The reflectance of the standards was also determined as a reference in support of and to compare to ocean-color validation experiments. Ultimately, limits on accuracy will be set for these types of measurements, by the uncertainty limits determined from the research conducted here at NIST.

A Charge-Based Capacitance Measurement Implementation on Printed Circuit Board

Derek Gooley

In order to effectively model the behavior of nanoscale devices, we must first be able to accurately characterize those devices by observation. Specifically, knowledge of the internal capacitances of nanoelectronic devices is important to programmatically predict their operating behavior within larger structures. Unfortunately, the parasitic capacitances created by the test structure itself make the measurement and characterization of such small devices challenging. The charge-based capacitance measurement method provides a way of compensating much of the parasitic capacitances of the test structure. Modifications to the CBCM circuit allow for high-resolution measurements of potentially sub-femtofarad values.

We present an implementation of a CBCM circuit on printed circuit board using discrete transistor components. A structure was added to the circuit to allow a reverse voltage bias to be applied to the device under test. A varactor diode was added to the reference branch of the CBCM circuit to allow for precise adjustments of the total capacitance of the reference branch. The PCB was constructed to be mounted onto an atomic force microscope probe package to allow it to interface directly with the AFM probe tip for nanoscale device measurements and to minimize the path length between the test structure and the DUT. Variations in parasitic capacitances between the reference and measurements branches due to asymmetric circuit layouts were considered and an effort was made to make the circuit paths symmetrical.

The implemented circuit was used to measure known capacitances on a previously developed test structure and demonstrates the performance of the CBCM method on a PCB. Usage of the bias circuit and varactor diode to more effectively compensate for parasitic capacitances is shown. Increased resolution is implied for an integrated circuit implementation.

Fabrication and Characterization of a Nanoaperture Array by Helium Ion Microscope

Andrew Hachtel

The confinement of photons by deep-subwavelength size apertures has been a hot topic in the field of plasmonics. The technique allows one to not only defeat the diffraction limit, but also achieve transmission greater than 100 % through the utilization of the surface plasmon polariton phenomenon. Applications include: optimization of near-field optical devices including optical data storage, light localization, Raman spectroscopy, and spatial/spectral multiplexing. Work has been done in the field utilizing focused Gallium ion beam milling; we report on the use of a Helium Ion Microscope to achieve finer resolution than that of the Gallium ion beam. We discuss the revitalization of a nanopatterning system, preparation of several suitable samples, the utilization of a Helium Ion Microscope to fabricate a periodic nanoaperture array in gold, and the optical characterization of the periodic array.

Simulation of Scanning Electron Microscope to Better Understand Errors in Cross-Correlation Image Correction Technique

Jeffrey Kleykamp

Scanning electron microscopes (SEMs) are an important tool to see beyond the optical diffraction limit. Often "fast scan" images suffer from poor signal to noise ratios while "slow scan" images result in strong distortions of the images. Averaging techniques allow for multiple "fast scan" images to be compiled into a single better image. These techniques, however, can also produce distortions due to vibrations in the sample that move each image slightly. Using cross-correlation it is possible to move the image to correct for the movement due to vibration in post processing. By using simulation, we are able to preform repeatable measurements. We characterize the error in the cross-correlation techniques deterministically using a number of changing variables such as noise, contrast, image size, blur and gold particle density. We find that error largely remains sub-pixel and the ability to correct remains strong.

Motion Characterization and Endurance Metrology of Microrobots

Douglas McNally

Presently the motion of microrobots is not fully understood and a novel approach that exploits the existing operating environment for these devices may provide some new insight to this problem. An overview of MicroElectroMechanical Systems (MEMS) technology is presented along with its relevance in a modern context. This subset of such technology, microrobotics, is introduced. The fundaments of this field including fabrication, locomotion, and end-user operation are overviewed and a new method of characterizing out of plane motion of untethered scratch drive actuators is the primary topic discussed.

The microrobots used herein are fabricated using a proprietary multi-user process which implements techniques such as chemical vapor deposition, lithography, and chemical etching and ultimately leads to microrobots made of polysilicon. Locomotion is achieved by placing the microrobots (specifically scratch drives in this purview) on a substrate consisting of interdigitated electrodes and a layer of a dielectric material. When current flows through these electrodes, capacitive coupling between the substrate and the microrobots takes place and there is a resulting attractive force causing flexure of the microrobots when it is sufficiently strong. Operation of these devices currently requires manual spatial initialization with microprobes and the driving is accomplished by generating a very specific electrical waveform to appear on the electrodes. This waveform is constrained by several characteristics of the system – primarily the strength of the attractive force needed to cause the aforementioned flexure – and can be tuned to change some parameters such as speed. Custom software is used for the waveform generation and manipulation.

The system as described can be approximated as a parallel plate capacitor. Under this approximation the current flowing in the system will change as the separation distance between the “plates” changes because of a change in capacitance and capacitive reactance therein. The new method of understanding the orthogonal out of plane motion of scratch drives relies on this concept. The current flowing in the system is measured in a highly precise way with an improvised current sensing circuit to the levels of 1 ppm. This current reading is then correlated with the separation distance between the “plates” of the capacitor – namely whether or not the microrobot is flexed and to what degree. Understanding these properties may well lead to improved designs and therefore lower failure rates and more stable and consistent operation.

Middlebury College

Nanoscale Electrochromic Patterning with a Lithium Focused Ion Beam
Joseph Allen

This project aims to create nanoscale optical patterns in tungsten oxide. Tungsten oxide, an optically transparent material, displays a dramatic increase in optical absorption when intercalated with lithium ions. This property enables the creation of electrochromic materials that are currently used to manufacture windows with adjustable opacity, known as "smart windows." Creating sub-optical-wavelength patterns could be useful in designing nanoplasmonic optical systems. A lithium focused ion beam (FIB) based on a magneto-optical trap ion source (MOTIS) recently developed at NIST allows lithium to be implanted directly into a sample to create absorptive patterns in the tungsten oxide film. I will describe our progress in creating and characterizing these patterned films.

Montana State University

Software Development for Probabilistic Modeling and Uncertainty Quantification
Katelyn Weber

Uncertainty quantification (UQ) is a best practice for computational models. UQ involves both uncertainty and sensitivity analyses, and is key for both model validation and improving predictive power. UQ is advanced by the development of computational software tools that improve computational ease and accuracy, promote the standard usage of transparent and verified codes, and greatly reduce unnecessary programming repetition.

The primary focus of this project was the implementation of an object-oriented model of univariate random variables in computational software. Using the numerical computing software package MATLAB, an extensible class framework was developed to coherently model both parameterized and empirically-defined random variable (RV) distributions. RV objects instantiated from any of the framework's classes have methods to calculate the probability density function (PDF), cumulative density function (CDF), and inverse cumulative density function, as well as for computing moments and generating random samples. Three CDF interpolation schemes for empirically derived RVs were implemented: discrete (piecewise constant), piecewise linear, and piecewise Hermite cubic (which has greater smoothness while preserving CDF monotonicity). The classes for empirically derived RVs are designed for usage scenarios where an RV's CDF is accurately known at sufficiently many points, but its type is unknown or nonparametric. The empirically defined RV classes were tested using NIST's eFITS tool.

To facilitate Monte Carlo simulation, the RV class contains two methods for inverse transform sampling that can generate random samples regardless of the underlying distribution: simple random sampling or Latin hypercube sampling (LHS). LHS was shown to greatly improve Monte Carlo simulation performance. Monte Carlo simulations typically generate thousands of random samples of a model's output, and these samples can be used directly to construct an object from any of the empirically defined RV classes, thus greatly facilitating the propagation of distributions in multistage simulations. To boost efficiency, the class can resample raw Monte Carlo data so that the CDF interpolation occurs over fewer points.

Montgomery College

Creating Stable Dispersions of Titanium Dioxide Nanoparticles in Environmental Matrices

Sarah Russell

Nanoparticles have unique physicochemical properties which have propelled their incorporation in a wide variety of mass consumer products. As nanoparticles penetrate consumer markets, it is imperative to elucidate their biological and environmental risks. Yet, available studies on nanomaterial risks have yielded highly inconsistent results, partly due to a lack of standardized testing protocols.

The goal of this project is to evaluate dispersion procedures for TiO2 nanoparticles in relevant environmental matrices. In particular, we study the effect of environmentally relevant parameters, such as ionic strength, natural organic matter content and pH on the stability of the particles in aqueous suspensions. Dispersion stability is assessed by use of two particle sizing techniques: Laser Diffraction and Dynamic Light scattering. Through testing, it was realized that higher ionic strengths caused agglomeration of the titanium dioxide nanoparticles, while natural organic matter could stabilize the nanoparticles under certain conditions.

Results of this work offer a preliminary insight into the different variables that affect nanoparticle stability in environmental systems, and their potential for transport and exposure, and ensuing human and ecological risks.

Mount Saint Mary's University

Calibration of NIST VaporJet and Preliminary Evaluation of Explosive Trace Detectors

Melissa Halter

Trace detection of explosives is an area of global importance in connection with issues of national security. As a result, explosive trace detectors (ETDs) are widely deployed to detect threats. Calibration of these systems is vital to insure accurate and reliable performance. NIST is working with the Department of Homeland Security (DHS) to develop methods for calibration of trace explosive vapor sampling ETD's. A custom built inkjet based vapor calibrator, the NIST Vapor Jet, is proposed as a method to generate a known concentration of trace explosive vapor with good reproducibility. However, independent quantification of the vapor produced by the system is required. In this study we quantify the amount of trinitrotoluene (TNT) printed from the VaporJet.

To quantify the printed material, the VaporJet was modified to expel trace amounts of TNT into tubes containing adsorbent resin. TNT was then extracted from the tube by flowing 5 mL of acetone over the resin, then collecting and evaporating the acetone and reconstituting the TNT in methanol/water. Various liquid extraction conditions were explored to establish a method for the most efficient extraction. The collected extractions were analyzed and quantified using high performance liquid chromatography (HPLC) with UV-Vis detection. Standard calibration curves were developed for TNT in water and acetonitrile. Following that, an isocratic separation on an E1 Dionex C18 column was used to separate TNT from any contaminate from the extraction process. Preliminary results show that TNT printed from a water solution in the VaporJet can be recovered and quantified using this method. The data collected will help validate the performance of the VaporJet.

Muhlenberg College

Characterizing the Morphology of the Bulk-Heterojunction of Organic Photovoltaics
Matthew Fitzsimons

Organic photovoltaics have the potential to play an important role as a renewable energy source of the future, and current high-efficiency devices are based on a bulk-heterojunction architecture. The active layer in such a device is typically 100 nm to 200 nm in thickness and consists of an interpenetrating network of an organic acceptor and an organic donor material. The three-dimensional nanoscale morphology of this network is thought to play a significant role in the resulting device performance, and is strongly influenced by the processing parameters chosen. The relationship between these variables and the resulting morphology is non-trivial, and robust characterization may provide insights into creating more efficient devices. In the present study, we have utilized energy-filtered transmission electron microscopy (EF-TEM) to characterize the morphology of the most common bulk-heterojunction system based on poly-3 hexylthiophene (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM). In particular, we have investigated the morphological changes imparted by thermal annealing treatments and the presence of solvent additives during film processing. Cross-sections for TEM analysis were prepared using focused ion beam milling and sample liftout, and the direct imaging of the vertical morphology profile was compared to that indicated by three-dimensional electron tomography. Examining films prepared under a wide array of processing conditions could provide insight into the effects of these parameters on morphology and, in turn, on the resulting device efficiency.

North Carolina State University

Slow Crack Growth Resistance at the Micron Scale in High Density Polyethylene
Andrew Hewitt

Bimodal High Density Polyehtylene (HDPE) has been used successfully in the natural gas and water industry for the past 50 years. HDPE has many advantages over metal pipe such as ease of assembly, chemical and corrosion resistance, and predicted lifetime of 100 years. The main long term failure mechanism for HDPE pipe is slow crack growth (SCG) that occurs after decades of use. The measurement of SCG resistance and predicting HDPE lifetime is critical for resin producers, pipe producers, and users. One consequence of successful innovation in HDPE resin formulation is the long test times (> 15,000 hrs) required to measure SCG resistance. This challenge is even greater when extending these measurements to HDPE fusion joints. HDPE joints are formed by thermally fusing two pipe faces together under heat and pressure. HDPE melting during the fusion process changes the microstructure which has implications for the long term performance of the joint. The HDPE industry has been developing new test methods that can accelerate test times without significantly altering failure mechanisms and are applicable to both pipe and fusion joints.

One promising method utilizes the strain hardening parameter to rank the SCG resistance of different bimodal resin formulations. The slope of the tensile test curve over its natural draw ratio, referred to as strain hardening, can be used as a measure of the resistance to slow crack growth. While this technique does not provide quantitative lifetime prediction, it successfully ranks SCG in a matter of hours rather than weeks. Nanoindentation is a surface measurement technique that can measure elastic and plastic properties at micrometer length scales. This technique was used to measure the viscoelastic/plastic properties of three commercial HDPE resins with different melt flow indices. The materials were subjected to two different thermal processing treatments. This talk will explore whether measurements of

plasticity conducted using a nanoindenter are relevant to SCG mechanisms of failure observed in HDPE pipe.

Optimization of Cell Growth in Minimal Media
Nathan Jones

Neutron scattering measurements could benefit from deuterated (labeled) protein systems. To achieve this, we must know how to produce proteins efficiently. My research primarily involved optimization of cell growth and protein expression in various media. E. Coli bacterium with DNA plasmids were used to grow and express the Human Growth Hormone protein. To optimize the system, cells were grown under various conditions. Growth curves were measured using spectra photometry to determine the peak cell growth and best time to start the protein expression process. The primary growth media was Lysogeny Broth (LB). Unfortunately, later applications of the protein rendered LB problematic. Minimal growth media (M9) is used for labeling purposes but allows very little cell growth since only the basics for cell growth are provided. Once the media had been optimized for cell growth, protein must be purified from the cell and optimized to achieve greatest yield. My work will help the final goal of deuterating protein for neutron scattering.

Pennsylvania State University

Quest for Precision: The Performance Evaluation and Compensation of a Meso-Scale Machining Center
Mark Rubeo

Standardized performance testing and evaluation of numerically controlled machine tools has become increasingly important as the demand for more precise machine tools escalates. Characterizing machine tool performance provides suppliers/manufacturers of machine tools with a means of confidently stating the accuracy and repeatability of their product while simultaneously allowing users to verify those claims. Additionally, users can gain an enhanced understanding of their own machining capabilities. A production facility that accurately recognizes their manufacturing abilities will operate more efficiently and generate more revenue.

Machine tool performance evaluation is based on measurements of the errors that contribute to the relative position displacement between the tooltip and the workpiece. In general, the primary source for these errors is geometric imperfection stemming from the manufacturing of the machine tool. Machine tools may employ linear axes, rotary axes, or a combination of both. Linear axes may exhibit up to six motion errors that correspond to the six degrees of freedom. The six error motions include three linear translation errors and three angular errors in the X, Y, and Z coordinate directions. Primary focus is on the XY linear translation errors of a unique 3-axis meso-scale machining center which uses a Heidenhain PP281 gridplate encoder for positioning. The machining center was designed and constructed at NIST Gaithersburg in 2005.

A displacement measuring interferometer (DMI) is utilized to assess the linear positioning accuracy and repeatability in accordance with ISO 230-2:2006. Measurements are conducted at multiple locations throughout the work volume to evaluate the performance of the gridplate encoder. To obtain measurements with a high degree of certainty, the sources of error must be identified and minimized. Pre- and post- measurement uncertainty analyses were conducted as dictated by the standards set by ISO 230-9:2005(E). Also, to avoid the complications of realigning the DMI to the axis of travel for each measurement, a measurement fixture was designed using Solidworks 2011 and applied during the experiment. Software compensation derived from the aforementioned measurements was implemented in order to improve the machine's positioning accuracy.

This presentation will illustrate the theory, procedure, and results of the performance evaluation and compensation of the machining center known as the "Heidenhain Machine."

Tissue Engineering Reference Scaffolds to Enable Inter-Lab Comparison of Cell Culture Measurements
Sai Sunkara

Tissue engineering is a field of science in which the ultimate goal is to make artificial organs that can be implanted in humans to replace damaged tissue. This requires cells, bioactive factors, and scaffolds. 3D scaffolds are crucial in this process as they provide the 3D template for cell attachment and differentiation. Cells are typically grown on flat 2D surfaces, but our organs are 3D, hence the requirement for scaffolds. There are certain features that scaffolds must have including degradability, biocompatibility, reproducibility, porosity, appropriate mechanical properties, and the ability to support cell adhesion, proliferation, and differentiation. However, there are minimal standards set in the field of tissue engineering. Thus, NIST has developed reference scaffolds to enable inter-lab comparison of cell culture measurements.

Previously, NIST released reference material scaffolds characterized for structure (porosity, strut diameter, strut spacing). However, scaffolds are most commonly used for biological testing. Thus, a second generation reference scaffold is being developed for cell culture testing. These scaffolds come in a set of 24 with which one can test cell adhesion and proliferation both qualitatively (staining) and quantitatively (DNA assay). The adhesion and proliferation of three cell types on the reference scaffolds has been characterized: osteoblasts (MC3T3-E1), fibroblasts (L-929), and stem cells (human bone marrow stromal cells). All cell types adhered and proliferated on the scaffolds in a repeatable fashion. Thus, the scaffolds can be used as a NIST reference material to enable inter-lab comparison of cell culture measurements.

Princeton University

An Evaluation of Local Shape Descriptors for 3D Shape Retrieval
Sarah Tang

As the usage of 3D models increases, so does the importance of developing accurate 3D shape retrieval algorithms. Most prominently, shape descriptors are used to describe the geometric and topological properties of objects and compared to determine two objects' similarity. They are split into two categories – global and local. As local descriptors are in general more invariant to rotation, translation, and scaling, and can additionally be applied to articulated models and partial matching problems, many have been proposed. However, these descriptors are often evaluated independently and on different datasets, making them difficult to compare. Using the SHREC 2011 Shape Retrieval Contest of Non-rigid 3D Watertight Meshes dataset, we systematically evaluate a collection of local shape descriptors. We choose to apply them to the bag-of-words paradigm, where each object is represented as a histogram counting occurrences of each word of a visual dictionary. In addition, the role of vocabulary size and number of sample points taken from each object in performance is assessed. Salient point detection methods are applied to determine if the number of sample points can be decreased without sacrificing accuracy. Finally, information from two local descriptors is combined in a number of ways and changes in performance are investigated.

Dataflow: A Web-Based Solution to Data Reduction
Andrew Tracer

The NIST Center for Neutron Research (NCNR) is a user facility, a laboratory whose neutron-scattering instruments are available for use by all qualified researchers through a competitive proposal process. The NCNR currently provides a suite of data reduction programs for its users, including the Data Analysis and Visualization Environment (DAVE), Relfpak, and the SANS Igor package. Data reduction software is designed to help newcomers with the difficult task of data reduction and to expedite the workflow of experienced researchers. Web-based data reduction offers a few advantages over standard, local data reduction packages: portability, ease of version control, collaborative interactions, and interaction with real time data.

Last summer, SURFer Joseph Redmon was able to make significant strides toward creating a web-based data reduction application. His application, WRed, was designed to perform data reduction for one particular instrument, the triple-axis spectrometer, and was met with approval and support from the NCNR community.

The Dataflow project is the next generation of WRed. Like WRed, Dataflow carries with it the advantages of a web-based application. Unlike WRed, however, Dataflow will provide data reduction capabilities out-of-the-box for four classes of NCNR instruments: Small Angle, Triple-Axis, Specular Reflectometer, and Off-Specular Reflectometer. More importantly, Dataflow was designed with expansion in mind; adding a new instrument to Dataflow is relatively painless.

My contributions to the Dataflow project include:

1. Setting up the overall Web Server and development environment.

2. Implementing Wiring Editor, a WireIt plugin. The Dataflow project abstracts data reduction procedures as data flowing through a pipeline of data reduction steps and uses WireIt, an open-source, Javascript library for creating wiring diagrams, to provide the user with a visual representation of a reduction procedure. The Wiring Editor plugin provides a graphical interface that allows the user to edit existing pipelines and to create new pipelines.

3. Creating the File Association Table. The File Association Table is an interface that allows users to load files quickly into a reduction pipeline.

Rensselaer Polytechnic Institute

Direct Browser Integration of 3D Graphics with X3D and X3DOM
Halley Coplin

With the advancement of web technologies, the sophistication of browsers and the Internet is growing at a rapid rate. However, while images, video, and games now permeate the web, these new uses are not currently capable of being interpreted directly by the browser and often require third party plug-ins such as Flash, Java, or Shockwave. Inconsistencies and compatibility issues arise with the introduction of third party software, thus reducing the user's experience. X3D, an XML based 3D graphics language, aims to change that. The daughter language, X3DOM, aims to integrate a fully functional X3D environment directly into webpages, or the DOM, without a plugin, and in conjunction with existing languages such as JavaScript. X3DOM, however, is still very new and its full range of functionality has not been extensively explored. Beginning to test its potential has been my job for the summer. The final goal of the

project is to make a fully interactive web environment that simulates and expands upon the RAVE experience here at NIST, with the focus on understanding the human body in terms of structure, movement, and more. This was done by first animating the RAVE human model using Blender, and then embedding it in a jQueryUI enhanced X3DOM environment. Current features on the site include organ selection, organ system selection, and various viewpoints of the body. Features currently in progress include selection of the organs directly in the environment with information overlay displays and tracking body movement by generating geometries in real time to show the path of motion of various body parts.

Residential Appliance Energy Research: Clothing Washers
Peter Willette

In today's society, 81% of residential power is consumed by appliances. Consumers need a method to compare the energy use of appliances they are considering purchasing. In conjunction with the Department of Energy (DOE), a standardized test procedure for these appliances has been created and implemented. Data produced from these procedures allows consumers to identify the differences in energy use between two similar appliances. It is NIST's job to assist DOE in updating the standard test procedure for some types of appliances, including Residential Clothes Washers (RCW). To assist DOE, NIST needs a test facility capable of meeting the requirements in the test standard. This was the task at hand for this summer.

This summer, a residential clothes washer test facility was constructed at NIST Gaithersburg campus (Building 226). This test facility is capable of performing the DOE test procedure, which includes obtaining temperature measurements of the input and output water flow and the ambient room temperature, the water pressure readings and water flow readings at the appliance inlet water supply. This data is collected via a LabView based data acquisition program. Most of the summer was spent becoming oriented with LabView, a visual programming interface designed to acquire and manipulate data. The second part of the summer was devoted to calibrating the instruments that collect the data.

Once this system was in place, extensive testing and troubleshooting was carried out. In particular the flow meters had many issues. Many of these issues were later traced back to be wiring, configuration or software communication issues, all of which have since been resolved.

The final step in this data acquisition process is to receive a round robin clothing washer that has been tested at several other sites. Data from this test site will be compared with the data obtained from the other test sites. This comparison will determine if the test procedure is accurate and reliable.

Rochester Institute of Technology

Understanding and Optimizing the Epitaxial Growth of Graphene on Silicon Carbide
Colin Jacob

Graphene is a single atomic layer of graphite. As such, it has very interesting electrical properties due to the carbon lattice structure and two-dimensional confinement of electrons. Graphene turns out to be a quite useful substance for resistance metrology via the quantum Hall effect (QHE). Epitaxial growth on silicon carbide (SiC) can produce monolayer graphene of large area, ideal for QHE standards. Pairs of SiC wafers are placed in a graphite furnace with silicon faces touching, and the furnace is then brought to 2000 °C. The process is carried out at atmospheric pressure in argon. The focus of this project is to optimize the graphene production process (create monolayers) and to gather as much information as possible about each furnace run. The furnace is controlled by a software suite iTools, and the data from the run are collected and analyzed via LabVIEW.

Saginaw Valley State University

Shape Evolution of Polymer Structures with Thin Residual Layers Prepared by Nanoimprint Lithography

Anthony Lucio

Nanoimprint lithography (NIL) is a patterning technique with numerous applications in nanotechnology. Here we measured the shape evolution of nanoimprinted polymer gratings during thermal annealing using a spectroscopic ellipsometer and analyze the data using a rigorous-coupled-wave analysis (RCWA). Previous work on the project successfully characterized the shape evolution of the NIL gratings and it was found that samples with ~10 nm residual layers decay more slowly. The work presented here focuses on polymer gratings of poly (t-butyl styrene) (PtBS), poly (methyl methacrylate) (PMMA) and polystyrene (PS). Highly entangled polymers were annealed above their glass transition temperatures (T_g) for 600 minutes to study the reflow characteristics. Our results indicate that the polymer samples with thin residual layers need to be annealed well above the T_g (up to T_g+25°C) in order for the reflow process to occur in a timely manner. All the samples increased in height before eventually decaying. Possible mechanisms for the slow reflow include: chemical grafting to the substrate, polymer crosslinking, or physical adsorption to the substrate. Our results suggest that physical adsorption of the polymer to the substrate is the likely mechanism for slow reflow in polymer samples with thin residual layers.

Saint Mary's College of Maryland

Effects of Film Processing Parameters on Organic Photovoltaic Device Performance

Lucas Carneiro

Organic solar cells are an exciting and promising technology because of their low cost, ease of manufacture and flexibility. Even though organic photovoltaics (OPVs) are not as efficient as their inorganic counter parts, their low cost and their recent rise in efficiency could make them a competitive, economically viable energy source. One particular advance in OPV technology has been the advent of the bulk heterojunction (BHJ) active layer, which is a thin film consisting of photon absorbing and electron accepting organic materials. Still, before companies can adopt this new technology, we must understand how processing parameters affect device performance.

During the summer we studied BHJs prepared by a film deposition technique called flow-coating. By keeping the vapor pressure constant for each solvent utilized, we were able to independently vary parameters such as speed of film deposition, concentration and solvent composition and determine their effects on both film thickness and BHJ morphology. Film thicknesses were measured via spectroscopic ellipsometry, and morphologies were measured via UV-Vis spectroscopy, grazing-incidence x-ray diffraction, and solid-state nuclear magnetic resonance (NMR) spectroscopy. The impact of film processing on OPV device efficiency was determined by fabricating devices with constant thicknesses (≈200 nm); variations in device efficiency were related to morphological changes in the BHJ active layer.

Analysis of a High Performance Flow of Suspensions

Gregory Herpel

The performance of a highly parallel computation depends on many factors, including the speed of the processors, memory access, the communications network that links the processors, as well as the number of levels and sizes of the available memory caches. In addition to these hardware characteristics, the specifics of the system to be simulated can also have a significant effect on the overall performance of the

computation. Support software, such as the compiler and software libraries can also make a significant difference in program performance. Identifying the best way to improve the performance of a computation is often not possible without extensive testing and analysis.

The simulator under study, which simulates the flow of dense suspensions such as cement and concrete, regularly runs on a range of machines such as small desk-side machines with four to eight processors, medium sized Linux compute clusters at NIST with approximately one thousand processors, and the supercomputer class machine "Intrepid", which is a 163,840 processor IBM Blue Gene/P at Argonne National Laboratory. The performance on each of these machine is different, making performance tuning that is portable across all of them nearly impossible. Our goal is to discover the most effective optimizations to pursue that will result in good performance on each of these machines.

This project first required instrumenting the simulator to time various phases of the simulation, focusing on the communications overhead within the simulator. During a simulation, this timing information is periodically logged to files, for a subset of the processors. Next, a set of post-processing programs were developed to extract this timing information from the log files and generate various graphs showing the breakdown of the simulation time. Finally, a suite of instrumented simulations were run, varying the number of processors as well as several of the basic simulation parameters.

The use of these tools will help identify potential areas for improvement in this simulator. As we will show, some "obvious" optimizations do not always help.

"Premature optimization is the root of all evil" – Donald Knuth

Saint Olaf College

Lateral Force Calibration Methods for Atomic Force Microscope
Sarice Barkley

The atomic force microscope (AFM) is commonly used to perform nanoscale friction measurements, or lateral force microscopy (LFM), but there are many different methods for calibrating these experiments. In this study, two existing lateral force calibration methods for AFM are compared with the goal of improving LFM methodology. The Hammerhead method, developed by Reitsma et al., takes advantage of the geometry of a specially fabricated T-shaped cantilever to calibrate the torsional signal by way of its relationship to the normal deflection signal. The diamagnetic lateral force calibrator (D-LFC) method, developed by Li et al., utilizes a pre-calibrated magnetic levitation spring system to directly convert the lateral signal in volts to force in Newtons. These two methods, although different in principle, produce consistent calibration results for the force-voltage conversion factor to within 10 %, validating both as accurate AFM calibration methods. Further tests on the D-LFC method show that a relatively stiff cantilever is capable of pushing the levitating graphite piece out of its equilibrium height, causing significant measurement inaccuracy. Additionally, a comparison between the constant height mode and constant force mode for the D-LFC method reveals a slight discrepancy in calibration results, where the latter is more consistent with the Hammerhead method.

Smith College

Atmospheric Abundances of Greenhouse Gases from Prehistoric to Current Times
Kathryn Aloisio

The pioneering work that Svante Arrhenius published in 1896 suggested that increases in atmospheric abundances of greenhouse gases (for example, carbon dioxide and methane) were bound to induce

increases in the global atmospheric temperature. This project focused on the statistical analysis of measurements of such abundances in samples of air from pre-historic to recent times.

The samples of pre-historic atmospheres are air bubbles entrapped in ice cores drilled in Greenland and in Antarctica, some reaching as far back as 700,000 years before present. These data are kept in the Paleoclimatology section of NOAA's National Climatic Data Center. The samples of recent air have been collected regularly for over forty years at several observatories, including Mauna Loa (Hawaii), and are maintained by NOAA's Earth System Research Laboratory.

With carbon dioxide (CO_2) being the second most abundant greenhouse gas and methane (CH_4) having a high global warming potential the analysis focused on their concentrations. Statistical methods were used to study the variability of these concentrations in ice cores from Antarctica and Greenland, in particular to gauge their similarities and synchronicity. By comparing locally polynomial regression models we found that Greenland had slightly higher CO_2 and CH_4 values but for the most part the records for the two hemispheres were similar.

After pasting together the data from ice cores with the data from the current atmospheric observatories, we observed that at no time during the most recent 700,000 years did atmospheric CO_2 concentration exceed about 300 parts per million by volume; however, over the most recent 200 years this concentration has increased to over 380 ppmv. (Arrhenius's theory predicted that a 2.5 to 3 fold increase in the concentration of CO_2 would translate into an increase of 8 to 9 degrees Celsius of the atmospheric temperature in the Arctic regions). Over the same period, methane increased from 400-800 parts per billion by volume to over 1900 ppbv.

I also visited the laboratory of NIST's Gas Metrology Group to learn how values are assigned to standard reference gas mixtures, and measured daily maxima and minima temperatures at NIST's research weather stations, together with scientists from the Temperature, Pressure and Flow Metrology Division.

State University of New York Albany

Improvements in Ultrasonic Calorimetry for Dosimetry
Magdalen Lovell

We are developing a new method of calorimetry which uses ultrasound to create a precise map of millikelvin temperature differences in water. Our equipment includes a circular array of 128 transducers, which send and receive sound pulses, finding the temperature differences by way of phase difference, since water changes in density with temperature and sound changes speed with density. We were able to make a clear image of a battery of resistors (serving as heaters) bent into the shape of a V.

The current data acquisition process can take around 4 seconds, enough time for the delicate millikelvin temperature distribution to change. Therefore, we are using pseudo-random noise correlation such as that used in cellular telephones to improve the efficiency of the process, allowing several transducers to send signals concurrently. We have conducted a proof-of-concept experiment using two speakers and a microphone. We were able to show that, using pseudo-random noise, we can determine the physical separation of the speakers. We can also pick out which speaker is where.

This technology can be used to calibrate the very fine ionizing radiation lasers now used in cancer treatment. It is ideal for dosimetry because it does not introduce foreign material into the area of measurement like the previous thermistor probe method, which measured temperature at a single point. It

also has potential applications in many areas of science and medicine, such as hadron therapy and the detection of very small vibrations.

State University of New York Binghamton

Scanning Kelvin Force Microscope Based on a Tuning Fork
Michael Carson

Presently, the Scanning Kelvin Force Microscope (SKFM) uses a cantilever and laser detection system in order to measure the charge on the surface of a material. But my project is working on achieving this ability through the implementation of a quartz tuning fork as the sensor. Due to the quartz tuning fork's piezoelectric property, it will oscillate on its own when a voltage with the resonant frequency is applied. The advantages to the quartz tuning fork setup are mainly the fact that it would yield a much higher resolution because of its large Q-factor, and it would eliminate the need for a lot of equipment; such as the cantilever, laser detection system, and external oscillator. Therefore, my project was to convert our Atomic Force Microscope that we currently have, into a Scanning Kelvin Force Microscope and to implement the quartz tuning fork design.

To start off, I had to design and construct a circuit that would convert the current signal, which was the tuning fork's response to our applied AC signal, into a voltage signal and then amplify it. With this setup we were able to run frequency responses to check the resonance of the tuning fork. Once we verified that everything worked, the next step was to modify the tuning forks. The leads (on the base of the tuning forks) measured the response of the tuning fork to the applied AC signal, but the SKFM needed to measure the charge of the surface we were testing. So, I had to attach an extremely small gold wire at the end of one prong of the tuning fork. This tip would measure the induced current between the tuning fork and the surface of the material that we were measuring when the tuning fork resonated. In order to keep the two prongs balanced so that they would resonate, I attached a Macor chip to the other prong. Once these steps were completed we were able to see a change in the resonant frequency peak when the tuning fork is lowered and close to the surface; and we were also be able to measure the induced current which would tell us the charge on the surface.

The final step is to design and build a feedback loop that will keep the driving signal at the resonant frequency of the tuning fork (in case there are any slight changes) for when we are measuring the surface charge. This will insure that the tuning fork is always resonating and we will get an accurate measurement.

Energy Consumption and Lifecycle Cost of Buildings in the United States
Brian Presser

In the modern world, few commodities are more important than energy. With fuel prices on the rise and the threat of global warming ever-present, the push for buildings to become more energy efficient has grown stronger than ever before. The energy efficiency of a building is a product of numerous interacting factors, including its materials and equipment. In addition, the location of the structure and the prevailing building codes can play a major role. The goal of my project is to study each of these factors by simulating their effect on different types of buildings. The results of these whole building energy simulations will be used to create a database of energy usage and lifecycle cost.

Currently, the database contains data from twelve different types of commercial buildings in 226 locations across the United States. These simulations were run for the 1999, 2001, 2004, and 2007 editions of American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) 90.1, a commercial building energy standard. In addition, a low energy case (LEC) was simulated to show the

impact of adapting requirements that are stricter than the most current edition. My task this summer was to use the commercial building simulation results as a framework to create similar residential counterparts. Also, I was asked to create files that simulate how tree shading affects the energy efficiency of a house. In total, over one million unique files were created for this stage of my project. My talk will discuss my approach to creating these files, as well as the impact that the energy database will have on national building practices.

Electrical Characterization of Flexible Solution-Processed Oxide Memristors
Walter Zheng

In 1971, Leon Chua postulated the existence of the fourth passive circuit element, dubbed the "memristor," which related flux and charge [1]. Memristors can serve as non-volatile memory due to their ability to switch between an ON and an OFF resistance state. TiO_2-based memristors were fabricated on flexible polyethylene terephthalate (PET) substrates through hydrolysis of a spun-cast sol-gel precursor and thermally-evaporated Al contacts [2-3]. Sol-gel hydrolysis occurred either by allowing samples to dry in air overnight or by drying in air for 1 hour followed by annealing for 10 minutes at 150°C on a hot plate. The devices fabricated were either "large area" (2 mm × 2 mm) or "small area" (100 um × 100 um) memristors and had various thickness of TiO_2 (≈4 nm, 8 nm, 10 nm, 17 nm, 33 nm, and 45 nm). In addition to TiO_2, solution-processed HfO_2 and $HfSiO_4$ films were also used to investigate if memristors could be fabricated using these films.

Current-voltage (I-V) measurements were performed to analyze the switching capabilities of these memristors. On average, the large area memristors switched to the ON state at ≈4 V. In attempt to switch the memristors to the OFF state negative voltages of up to -10 V were applied, but most remained in the ON state. The small area memristors required a larger voltage to switch to the ON state but, like the large area memristors, most could not be switched to the OFF state. Due to a limited sample set, the voltage bias at which the memristor switched was relatively consistent between the various thicknesses. Current-time (I-t) measurements were performed using a constant voltage bias to investigate if these memristors exhibited the same increase or decrease in resistance over time as traditional sputter-deposited TiO_2 memristors [4]. Additionally, programs to automate the I-V and I-t measurements were written using LabView.

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[2] N. Gergel-Hackett et al., IEEE Electron Device Lett. **30**, 706 (2009).
[3] J.L. Tedesco et al., ECS Trans. **35**, 111 (2011).
[4] M.D. Pickett et al., J. Appl. Phys. **106**, 074508 (2009).

Towson University

Constructing a Magnetic Field Probe for Use Regarding the NIST-4 Watt Balance
Alexander Siregar

NIST-4, the next generation Watt Balance at NIST, will realize the kilogram based on a fundamental constant, Planck's constant, *h*. An essential feature of a Watt Balance is a strong, but uniform, magnetic field (in this case approximately 0.5 T), which will be generated by a permanent magnet. The magnet system has been designed and will be constructed soon. The magnet system has cylindrical symmetry and features a 3 cm wide gap at a mean radius of 21.5 cm. The magnetic flux density inside the gap is inverse proportional to the radius. In order to verify and characterize its magnetic field, a custom magnetic field probe is needed. The probe has to measure the magnetic flux density as a function of position in the gap.

The probe consists of a cylindrical probe head that rotates at about 300 rotations per minute about its axis. The probe head contains a wire coil and a differential capacitor that is coaxial with the coil. As the probe head rotates, a voltage is produced in the coil which is proportional to the magnetic flux density. The differential capacitance is modulated at the rotation frequency. The modulation amplitude is proportional to the position of the probe inside the grounded magnet. By finding the point of smallest amplitude, the probe may be centered in the 3 cm wide gap, and the magnetic field can be measured consistently at different locations in the gap.

The performance of the probe is evaluated using a test magnet that has similar gap width and field strength as the NIST-4 magnet. In the presentation, the design, construction, and performance of the magnetic field probe will be discussed.

LabVIEW Integration in a Mass Calibration Process
Joshua Tyler

NIST offers training in advanced mass calibration to State Weights and Measures laboratories and industry. This training uses automated mass calibration software that was originally developed in C++ in the early 1990's. Automated mass calibration software allows the acquisition of data without introducing further errors into the mass calibration process. The current software is not designed for (*will not work on)* the latest operating systems.

This project involved writing LabVIEW programs (Virtual Instruments, VIs) that (i) automate data collection from balances and environmental sensors (ii) input to a data file for data reduction in mass calibrations, and (iii) generate a calibration report. The LabVIEW software improves the functionality of the existing software and operates on modern computer architectures. Additionally, we considered and implemented a more user-friendly design. The LabVIEW interface still need to go through a software verification and validation process before it can be distributed to other mass laboratories. I will discuss the replacement of the current software with a LabVIEW interface, difficulties that were overcome during the project, and provide a brief demonstration of the interface.

Tulane University

The Metrology of Shaping and Detecting X-Rays
Elliott Ortmann

Metrology is defined as the scientific study of measurement. Although one could easily make rather low-accuracy measurements of ordinary objects with a common measuring device, such as a meter stick or a tape measure, in order to obtain accurate and precise measurements on submicron (and oftentimes sub-nanometer) scales other measurement techniques must be devised. X-ray characterization is one such technique utilized by the X-ray Metrology Project in the Ceramics Division to make measurements on such small scales. Through the use of x-ray reflectometry and x-ray diffraction, one can measure with high accuracy the atomic spacing of the lattice structure that makes up many materials. Measurements of this type are of fundamental importance in the production of Standard Reference Materials (SRMs), which in turn are of fundamental importance in the study of materials. This presentation will focus on various experimental and analytical techniques that can be used to control and shape the x-ray beam that ultimately strikes the material sample to be studied, as well as how one goes about detecting x-rays. Specifically, multiple configurations of the parallel beam diffractometer used by the Structure Determination Methods Group will be discussed, including their advantages and disadvantages for metrology and what these different configurations can tell us about our x-ray beam. Also, unusual behavior by a new detector for use with the group's divergent beam diffractometer will be discussed as well as simple ways in which the effects of this systematic bias can be minimized in the collection of data.

University of California Los Angeles

Development of Sustainability Measurement Tools and Methods for Manufacturing Enterprises

Jessica Lopez

Sustainability is the ability of an organization to continue development and maintain economic benefits with minimal negative impact on the environment and society. The need for sustainability in manufacturing has recently come to the forefront due to growing environmental concerns, government regulations, limits to resource availability, and the importance of ethical responsibility. The measurement of environmental and societal impacts in the development process provides necessary data to track the progress of an organization and allow management to make appropriate decisions. Sustainability measurement, thus, becomes a necessary activity for tracking and analyzing an organization's performance in achieving their sustainability goals.

The focus of this project is to further develop NIST's Sustainable Manufacturing Indicator Repository (SMIR) to provide manufacturers with tools to facilitate a systematic sustainability assessment process. The development of these software tools is to enable users to define goals, identify sustainability metrics, specify measurement methods, and generate measurement reports. Specifically, users will be able to breakdown a high-level sustainability goal to measurable subgoals, easily select indicators from a repository to satisfy subgoals, allow users to enter measurement data, calculate the results, and generate forms to show sustainability progress. Software modules include user interfaces to support user interactions, a database to store user data and measured results for analysis, sustainability report forms generation, and plotting charts for analysis. Finally, test cases will be created and used to test the developed software. This talk includes a discussion on our approach, a summary our progress thus far, and future steps of the project.

University of Colorado Boulder

The Effects of Scaling and Scanning Order on Image Signatures Based on Space-Filling Curves

Stetson Zirkelbach

Image retrieval has been an open research problem for years, however a technique proposed for use in robotics could be applied to medical images as an efficient way to identify and retrieve similar images. This method scans the image using a space filling curve and then uses a wavelet decomposition to generate a signature which preserves spatial information. This signature and can then be used in a variety of retrieval-based applications such as the retrieval of structurally similar images and the time compression of wireless capsule endoscopy videos by removing unnecessary similar frames.

The focus of this research was to explore the effects of certain design choices associated with the signatures with an eye towards improving computational efficiency. The main areas of investigation were how different space filling curves affect the signature and how resizing the images affected image retrieval. The analysis was performed on frames from wireless capsule endoscopic videos, and shows that further study is warranted because the image signatures show potential for retrieving similar frames and reducing the number of frames requiring examination by gastroenterologists.

University of Delaware

Standard for Lead and Cadmium Content in Polyvinyl Chloride
Caroline Bibb

Polyvinyl chloride (PVC) plastic has been a growing concern for product safety for many years due to its use in household applications and its presence in children's products. In the past, compounds of lead and cadmium were used for their performance properties as ingredients in this plastic. Both of these elements are toxic with continuous exposure, especially during childhood development. The National Institute of Standards and Technology, in conjunction with the US Consumer Product Safety Commission, is developing a standard reference material (SRM) for the detection and quantification of these harmful elements in PVC. Standard reference materials verify the accuracy of methods used to test quality of products. For this SRM, elemental analyses of lead and cadmium will be performed using X-ray fluorescence spectrometry (XRF) for which calibration standards must be prepared. In order to create PVC samples in a disk form useful in XRF instruments, the disks must be sufficiently homogeneous, able to survive irradiation for long enough, and have known lead and cadmium values traceable to other NIST SRMs or to the mole through pure compounds. To prepare these samples, different amounts of spectrometric lead and cadmium solution SRMs were added to PVC powder and dried off before being melt pressed into disks suitable for measurement by the XRF instrument. Micro XRF maps, which show the elemental composition of a sample at chosen points, were made to demonstrate the homogeneity of the melt pressed disks. The test method developed will use wavelength-dispersive XRF as one of several independent methods to quantify lead and cadmium in the new SRM for PVC. The disks made and pressed according to the specifications above were used successfully to calibrate the spectrometer. The calibration curve and other measurement performance parameters will be statistically analyzed considering the uncertainty of the spectrometric solutions, repeatability, and the fit of the equation found from the calibration curve. These results will be validated using other PVC reference materials and alternative methods of combining the lead and cadmium with PVC by comparing these readings with the calibration curve.

Research Contributions to Enhance the Sustainability Standards Portal
Anna D'Alessio

The adoption of sustainability standards as best practices can improve the sustainability performance of products (e.g., usage, recycling, and end-of-life), processes (e.g., manufacturing, supply chain, and production), and services. These standards vary in scope, application domain, and implementation strategies and it is a challenge for stakeholders to identify, select and implement applicable standards. The Sustainability Standards Portal (SSP) developed at NIST is an effort to inform various stakeholders about different sustainability standards (voluntary and mandatory) through the intersection of information abstraction and modeling perspectives. The SSP provides a mechanism for stakeholders to familiarize themselves with sustainability standards through stakeholder analyses while also providing a methodology for detailed technical analyses based on the Zachman framework. It has been demonstrated that these analyses can be used to identify both gaps and overlaps between these standards.

The work presented here adds more information to the existing analyses and prototypes a formal model (using ontology) for representing the results. As part of this work, a set of ten critical sustainability standards were selected and summarized using the templates provided by the SSP. This information supplemented the existing stakeholder analysis content of the SSP while also serving as the basis for more detailed technical analyses. In these Zachman-based analyses the scope of each of the ten standards was determined and then captured as a list of key terms associated with each standard. The analysis results of three of the ten analyzed sustainability standards used in prototyping a formal representation of their

scope and subsequently identified gaps and overlaps. Three simple ontologies (a simple taxonomy) were developed to represent the three selected standards and then harmonized as a single ontology. The result of this work is a simple prototype where different sustainability standards are formally compared and their gaps and overlaps defined. This presentation will also discuss the educational experience, the exposure to new ideas and concepts, and the interest in research gained during this internship.

University of Illinois

Laser Diode Interferometry
Gautham Ragunathan

In regulating dynamic MEMS devices, sensor instrumentation is needed to monitor the displacement of their moving parts. Especially in nanomanipulators, which make use of various actuators, these sensors need to be able to detect displacement changes when xyz translation/rotation takes place. Interferometry is a methodology used to determine displacement with nanometer sensitivity, using a laser diode optical source (i.e., in our case a 1550 nm wavelength laser).

The interferometer system uses a laser wave output reflected off a reference point and compares with a reflection off of the target, some displacement from the reference. The relative change in intensity also provides information regarding the phase, which in turn can be calculated to provide information about the displacement. To increase sensitivity and also to obtain more data, what is similar to a heterodyne detection system is used, where a modulated wave source is used instead of a DC current driven laser diode source. By using a modulating current to drive our laser diode, more sampling points can be obtained and thus more precision can be attained in our measurements.

An oscillator, which creates a sinusoidal voltage, which is controlled and converted to a current through a controller are two of the most vital parts of the circuit. From there, this current is transmitted into the laser diode, which in turn creates the modulated optical beam. The oscillator and laser diode controller were originally built through the use of larger equipment (i.e., function generator, laser diode controller module). Our focus was to use circuit level, integrated circuits (IC) replacements of these parts to reduce the size and cost of this sensor controller and reduce it to a single circuit board size.

University of Maryland Baltimore County

The Role of Metrology in X-Ray Diffraction
David Harvey

For nearly a century, X-ray diffraction has been employed by crystallographers to determine the atomic structures of crystalline materials. X-ray diffraction is theoretically governed by Bragg's Law, but in actuality, this law makes important assumptions about the geometry of the experiment that must be accounted for if precise and accurate measurements are to be made with this technique. Specifically, in its traditional scalar form, Bragg's Law requires that the X-rays incident upon the crystal be coplanar with the lattice planes of that crystal; deviations from this condition will result in measurements that do not precisely follow Bragg's Law. These deviations are typically due to the misalignment of the X-ray source, detector, or the crystal being studied. Misalignments arise from several sources, including machining and assembly errors as well as physical phenomena such as thermal expansion and elastic deformation of materials under gravitational loads. Where feasible, experimental data were collected to study how these phenomena affected the positioning of the instruments used in the diffraction experiments. In situations in which experiments were either not expedient or risked damaging the instruments, an FEA software package was employed to simulate these effects. This study examines the effect of these phenomena using both the experimentally collected data and FEA simulation software.

Residential Appliance Energy Research
Christopher Iglehart

Consumer appliances account for a significant portion of home energy use. NIST supports the Department of Energy's appliance program by developing testing and rating procedures for residential appliances. Manufacturers use these procedures to determine values such as estimated yearly electricity use and operating cost. These values are clearly presented on the yellow EnergyGuide labels found on many new appliances. The EnergyGuide labels enable consumers to easily compare the efficiency of all available appliances. The development of new appliance technologies in recent years has created the need to revise current test procedures for dishwashers, clothes washers, and clothes dryers.

This summer, two new residential appliance test facilities are being constructed at NIST for dishwashers and clothes washers. The test facilities will include data acquisition equipment and representative appliance models. This enables NIST engineers to analyze and verify proposed test procedure modifications before they are published. A future goal is to implement automation of the test facility.

Over the past 11 weeks, I concentrated on constructing the dishwasher lab. My advisor and I worked together to construct the facility. My first task was to complete the plumbing. Next, we researched, acquired, calibrated, and installed all necessary sensors and instrumentation. These include water flow meters, pressure transducers, thermocouples, humidity sensors, digital power meters, and data acquisition equipment. I wired the various sensors to the data acquisition equipment and wrote a LabVIEW program to automatically take data during a test. This facility has the ability to measure water temperature, water flow, water pressure, room temperature, room humidity, and energy consumption. In addition, this program also has the ability to detect which cycle the dishwasher is currently running (such as filling, heating, washing, and draining) and control solenoid water valves. For added protection, a water leak detection system will be installed. In the event of a leak, water valves are automatically shut off, an alarm goes off, and several phone numbers are dialed to alert specific people.

Developing a Root-Based Semantic Vocabulary
Laura Anzaldi

There is a lack of cohesive vocabulary among those in the medical, chemical and biological fields. This discrepancy in dialect makes the process of combining and sharing data via computers difficult. Computers cannot easily differentiate between synonyms or variations in spelling; to a computer a different set of vocabulary words is a completely different language. The instantiation of a root-based vocabulary, inspired by languages such as Latin and Sanskrit, will streamline communication among researchers. Such a vocabulary can be easily expanded and its words intuitively defined. A common set of roots will serve as a unifying denominator underlying data from different sources. With scientific information aligned by root words, computers can be used to logically organize, store and search through data.

In order to form a new root-based system, first current vocabulary schemas needed to be considered. Biologists selected a representative collection of over 90 ontologies from which to collect data. The ontologies were converted from OBO/OWL format into XML so that they could be more easily manipulated. Each term was extracted from the ontologies and uploaded to a central database. The frequency and context (in the form of parent-child relationships) of each term were also recorded in the database. This information will aid in the analysis of determining which terms will serve most naturally as roots. The database of over 1,100,000 terms can be explored using a webpage, Bioroot Search, developed using Perl CGI. This webpage displays frequency and contextual information about terms in response to a query. A second webpage, Bioroot Editor, allows biologists to annotate and classify terms, assign roots and communicate with other researchers. Root words are easily concatenated, easy to say

and useable in a variety of contexts. A root-based vocabulary will facilitate cohesive information among scientific companies and organizations.

Bioroot Search: http://xpdb.nist.gov/bioroot/bioroot.pl
Bioroot Editor: http://xpdb.nist.gov/bioroot/bioEditor.pl

Putting a Spin on Solid Sampling via Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)

Naomi Bier

Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) is a fast-expanding solid sampling technique used in many fields to measure major, minor, and trace elements, as well as isotope ratios in solid samples. The laser, focused at the surface of the sample, produces an aerosol which is transported to an ICPMS for ions detection. Precise and accurate quantitative analyses by LA-ICP-MS are limited by the need for matrix-matched calibration standards due to a phenomenon known as elemental fractionation (the aerosol has a different composition than the sample). Fernandez et al. addressed this issue in their work presenting a new methodology for fast, accurate and precise quantification of trace elements in powdered samples combining isotopic dilution mass spectrometry (IDMS) and femtosecond-LA-ICPMS. Their work demonstrated a fast scanning beam device to perform quasi-simultaneous ablation of both a natural abundance soil sample and an isotopically enriched solid spike. By ablating the two materials in a short time (15 to 150 milliseconds) the aerosol transported to the ICP-MS from the ablation cell consisted of particles from both the soil sample of interest and the isotopically enriched-spike solid, removing the need to make a matrix matched spike for each sample individually. The method cut down sample preparation time as well as cost as compared to other ID-ICPMS techniques. However, the lasers commonly used in the elemental analysis field are equipped with a stationary nanosecond laser beam. In this sense, our work describes the efforts to adapt the accomplishments of Fernandez et al. to accommodate a classic nanosecond laser ablation system, The proposed solution involved the design and implementation of an ablation chamber that would suitably house a micromotor, which will rotate the sample of interest and the isotopically spiked pellet during ablation, in place of a moving laser beam. Standard addition was used in place of isotopic dilution for preliminary studies of the new design since it allows for studying of the mixing of the two aerosols at a lower expense. Home-made glasses of SRM 2710a (Montana I Soil) and multi-elemental solutions were fused, cut and polished for these studies. The design of the new ablation cell will be presented as well as preliminary results obtained on NIST SRM 2710a using standard addition.

Nanofluidics of Polymer Chains Under Confinement

Lilian Johnson

Advances in nanofabrication techniques have made the construction of nanofluidic devices possible. These are flow channels with at least one characteristic dimension below 100 nm. Nanofluidic devices differ from conventional fluidic designs because the material to be handled is confined – that is, the length scale of the molecules being sampled is of the same order of magnitude as the device. The use of such nanofluidic devices to manipulate and transport individual biomolecules, typically, single strands of DNA, has become increasingly important in biophysical metrology, but a better understanding of the polymer physics and flow dynamics under confined conditions is needed.

One such device under study at NIST is a nanofluidic staircase which consists of an array of nanoslits of increasing depth arranged in steps [1]. The staircase generates slit-like confinement, or confinement in one characteristic dimension. Experimental observations show that a DNA molecule will diffuse down the nanostaircase from the top step, under high confinement, to regions of lower confinement, in an effectively one-dimensional path. This mass transport is due to an entropy gradient that moves the

biomolecule towards regions of greater entropy. Thus, the device functions as a Brownian motor, using thermal energy to transport the molecule without the use of external forces.

The molecular dynamics simulation program LAMMPS [2] was used to simulate the behavior of individual DNA molecules in the nanostaircase for confinement regimes which were greater than the polymer Kuhn length, but less than the polymer radius of gyration. To create a suitable computer analogue to the λ-phage DNA used experimentally, the number of beads, chain stiffness, and interactions between the walls and molecule were varied. Linear chains were observed in bulk to characterize their diffusive motion, radius of gyration, and Kuhn length. When an appropriate ratio of polymer contour length to radius of gyration was achieved, the chain was analyzed for its behavior in the nanostaircase. The model will be evaluated for its ability to correspond to experimental data and to elucidate the behavior of the polymer in various levels of confinement.

[1] Stavis, S. M., Strychalski, E. A., & Gaitan, M. (2009). Nanofluidic structures with complex three-dimensional surfaces. *Nanotechnology*, *20*(16), 165302.
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Interdiffusion Studies of Organic Solar Cell Components

Mary Kelly

Solar power in the form of photovoltaic cells is a promising form of alternative energy, and solution processed organic photovoltaic cells (OPVs) offer a low cost route to broader applications of this technology. Unfortunately, OPVs have not reached the efficiencies and stabilities of their semiconductor counterparts. Engineering OPVs with higher efficiencies requires a better understanding of the physics that determine the performance of the active layer in an OPV.

The Bulk Heterojunction (BHJ) is a fundamental motif in the structure of high performing OPVS. A BHJ consists of a nanoscale (10-20nm) interpenetrated network of a light harvesting polymer and an electron transporting fullerene. The network is formed dynamically during film drying and typically represents a meta-stable state. Changes in the morphology with subsequent thermal processing can either improve or degrade the device. Real time, in situ studies of the nanoscale behavior are beyond current techniques. We are attempting to study both the kinetics and steady-state behavior of polymer/fullerene systems by initially preparing a macroscopic, idealized interface (a bilayer) and subsequently allowing the system to knit. It is hoped that this will provide insight into both the stability of nanostructure interfaces and the kinetics of their formation.

Specifically, this study focuses on two high performance polymers, P3HT and PCDTBT, which differ in both glass transition temperature and degree of crystallinity. These are paired with two candidate fullerenes, PCBM and bisPCBM, which differ in size. We use variable angle spectroscopic ellipsometry to monitor the knitting of the two layers as a function of temperature.

Several trends have emerged from the study. First, it is clear that larger bisPCBM exhibits less, or slower, knitting than PCBM. It is also clear that more fullerene diffuses into the less crystalline PCDTBT than into semi-crystalline P3HT. Secondly, in our studies of PCDTBT we noted that the characteristic temperature at which the knitting begins is, in the case of bisPCBM, the glass transition temperature of the polymer. However, in studying PCBM, the knitting began at a lower temperature, 110°C. Additional studies investigating the role of the polymer's glass transition temperature in thermal knitting will be pursued.

Fabrication of Controlled Diameers of Nanofiber Scaffolds and Study of Stem Cell Response

Neha Kumar

Biophysical cues, such as nanotopography, heighten cellular activity and could enhance cell response to biochemical signaling, and thus help to determine cell fate, i.e., differentiation and proliferation. This information can ultimately lead to tissue development. Electrospinning is a simple technique that is being used to prepare scaffolds with different nanotopography mimicking the extracellular matrix (ECM). However, preparation of the fiber with narrow size distributions using this technique is challenging. In this study we have optimized the process of fabrication of nanofiber scaffolds with controlled fiber diameters using electrospinning. A series of polystyrene (PS) based nanofiber scaffolds, with characteristic curvatures of 100 to 4000 (± 10%) nm diameters, were prepared. Different diameters of fibers were achieved by varying the concentration of PS (w/w) in PS-dimethylformamide (DMF) solutions and controlling the parameters involved in the electrospinning process. Seven different concentrations of PS solutions (e.g., 10, 12, 14, 17.5, 20, 25 and 30 % (w/w)) were used to obtain the required fiber curvatures, or diameters. Stem cell (MC3T3) response, i.e., cell proliferation, cell differentiation and cell morphology, to the nanotopography was studied. Polymer coated tissue culture plates (absence of nanotopography) were used as control materials in this study.

An Improved Ultrasonic Measurement of Radiation Dosage

Daniel Litwak

Through the use of ultrasonic tomography the temperature profile of a water phantom can be determined, since the propagation of sound is temperature-dependent. From this the energy deposition of a radiation beam can be retrieved. To accomplish this, a circular array of transducers emit and receive ultrasound within a water phantom, and this data is filtered and analyzed to extrapolate the temperature profile. The circular array is an improvement for radiation dosimetry because it does not disturb the temperature measurement area with extraneous material and it reproduces a surface of the temperature distributions. This is dissimilar to previous methods which introduced a thermistor probe into the environment, reading out the temperature at a point. However, current hardware is limited by its data throughput, and thus a full scan of this phantom takes upwards of 4 seconds. As measurements are on the scale of milli- and eventually micro-Kelvin changes in temperature, the time it takes to complete a full scan is long enough for the delicate temperature profile of the phantom to change. A faster method for data acquisition is necessary and is thought to be achieved through maximal length sequences and orthogonal signals, such as those used in cell phone communications. The cross-correlation of emitted and received signals will allow the entire phantom to be imaged at the same time without loss in temperature resolution.

To further understand cross-correlation, a mic-speaker setup was used to distinguish millisecond time delays and to measure the speed-of-sound in air through a Labview interface. Additionally, a pseudorandom noise generator circuit was constructed and tested at baseband frequency, which is useful as it can be run at audio levels through speakers and ultrasonic levels to test the response of the ultrasonic transducers. This produces maximal length sequences, which maintain a low autocorrelation and are ideal for parallel data acquisition from the transducer array.

Glass Shard Dynamics in Fire Visualization Simulation

Nadezhda Serov

An important area of research within NIST is the effects of fire on various structures. There is a utility that has been developed to visualize a burning room in 3D with several components. This visualization uses various parallel processes and data to model the burning of furniture, structural beams, etc. One

component involved in the visualization is a glass window. During a fire in the room, the glass window shatters and the shards fall to the floor.

Last year, two students developed a program to model the pattern of glass breakage and to animate it using the Bullet Physics Engine. However, the animation does not look realistic, as shards fly in strange directions.

The goal of this year's project was to make the visualization more realistic. In order to do that, the parameters of the animation were analyzed and adjusted. The parameters included the mass, centroids, inertia tensors, and initial velocity of each shard. In addition, the linear and angular damping in the animation was considered.

Verification and Validation of the Fire Dynamics Simulator
Michael Van Order

The Fire Dynamics Simulator (FDS) is a computational fluid dynamics model of fire. The software numerically solves a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow, with an emphasis on smoke and heat transport from fires. Verification and validation are important processes to test and improve the model. Verification ensures that the model equations are solved accurately, whereas validation confirms that the physical model is an adequate representation of reality. An example of model verification is to compare calculated versus exact solutions of the radiation heat transfer equation in ideal geometries. A sample of validation is to simulate liquid fuel fires and compare burning rates with experimental data. The sensitivity of the results in this validation case are greatly dependent on the model inputs, in particular the absorption coefficient of the liquid fuels. Using the absorption spectra of these liquid fuels, we numerically integrate the spectral absorption coefficient and blackbody emission spectrum over relevant wavelengths to obtain an effective absorption coefficient for each hydrocarbon fuel. Obtaining these absorption coefficients are essential in yielding the best results and highest accuracy that FDS is currently capable of modeling. Depending on the agreement with experimental data, further investigation into the model may be required.

University of Maryland College Park

Testing of Automated Impactor for In Situ Monitoring of Machine Tool Dynamics
Reuben Abraham

In a competitive world market, increased machining efficiency and quality is needed to ensure the success of U.S. manufacturers. Consequently, manufacturers are constantly working towards increasing machining performance, whether or not better performance is to maximize the material removal rate or the precision of the cut. In either case, the determination of the tool point dynamics before machining of a part is needed for process optimization, e.g., to avoid the machining instability known as chatter. However, analysis to pre-determine the machining stability is time-consuming and still has a significant level of uncertainty. This is why an automated impactor was created at NIST some years ago: The impactor allows repeatable tool tip impacts for efficient and reliable monitoring of the tool point dynamics.

In this talk, we will present a detailed study of the impactor device, improvements made to the device, and its use for the determination of tool point dynamics. Various tests were performed to investigate the repeatability of impactor actuation and to understand the errors in data acquisition due to fiber optic sensor vibration. A summary of the procedures developed for calibration of the impactor sensors will also be presented. After calibration, the impactor was used in on a 5-axis machining center to gather force and displacement data for various tools. For each tool, multiple impacts were performed to study

the ability to reliably measure the tool tip dynamics. The acquired data was used in a commercial software package called CutPro to estimate the stability boundaries (depth of cut versus spindle speed), and the predicted stability lobes were compared to experimental ones collected during machining of Al 6061-T6. The results showed that the impactor allows for repeatable tool tip impacts for efficient and reliable monitoring of the tool point dynamics, even as the machine warms up during machining operations.

Characterizing Dispersion and Degradation of Nanoparticle-Filled Polymer Coatings
Catherine Ashley

Nanoparticle filled polymeric coatings are used in a variety of applications in the construction, building, automotive, and aerospace industries to increase the life cycle performance of coated products. Differences in the nanoparticle dispersion of these coatings affect their durability when exposed to weathering conditions over time. To determine the correlation between degradation due to weathering and particle dispersion, nano-TiO2 filled polymer films of different dispersions were exposed to simulated extreme weathering conditions of high intensity UV radiation, high temperature, and high humidity over a period of four weeks. Physical changes in surface morphology and chemical changes in degradation kinetics of the polymer samples were measured and analyzed using laser scanning confocal microscopy and infrared spectroscopy. Generally, samples with poor particle dispersion exhibited the most severe degradation while samples with good particle dispersion showed less severe degradation. It was determined that particle dispersion and other characteristics such as polymer/nanoparticle type and particle photoreactivity are significant factors that affect degradation in coatings exposed to extreme weathering conditions. The results of this experiment will contribute to ongoing research to provide the fundamental science for the improvement of nanoparticle filled polymeric coatings.

Enzyme Digestion and Mass Spectral Characterization of Glycoproteins
Jennifer Au

Glycosylation, the enzymatic addition of carbohydrates to a protein, is one of the most abundant post-translational modifications found in nature. There is variability in the number, location, and identity of the glycans attached. As a result, a glycoprotein consists of a number of glycoforms with different combinations of glycans, potentially resulting in different stability, toxicity, and activity. This is especially important in clinical diagnostics, where specific glycoforms may act as biomarkers for diseases, and in the biopharmaceutical industry, where product consistency and safety are vital.

Glycoprotein analysis involves a number of mass spectrometry-based techniques, each of which provides various aspects of characterization. One approach involves the enzymatic release of glycans from the protein, labeling with 2-aminobenzamide, and analysis using LC-fluorescence-MS/MS. Recombinant Immunoglobulin G3 were studied using this method, allowing analysis of glycosylation profiles. A second approach was also explored that utilizes pronase and aminopeptidase, mixtures of proteases capable of cleaving any peptide bond. A typical digest gives glycopeptides for glycosylation site identification via solid phase extraction and MALDI-TOF MS, as well as glycan characterization using graphitized carbon LC-MS/MS. Microwave-assisted digestion was assessed for its ability to digest the protein completely, leaving only the amino acid asparagine attached to a glycan. Complete digestion conditions were optimized for Ribonuclease B. This sample treatment serves as the first step in a workflow that will make absolute quantification of glycans possible for the first time.

String Searching on Container Files
Matteo Bellistri

There is a critical need in the law enforcement community to ensure the reliability of computer forensic tools. Among the many features that computer forensic tools offer, string searching is of particular interest. Forensic string search tools are used by forensic examiners of digital evidence to search digital media for evidence relative to a legal issue in both civil and criminal investigations. The court is interested in the validity of any results derived from such tools. Computer Forensic tools are extensively tested with differently structured data sets to ensure consistency, accuracy, repeatable and objective test results. The goal of the CFTT (Computer Forensic Tool Testing) project is to establish a methodology for testing forensic tools by creation of functional specifications, test procedures, test criteria, test sets, and test hardware. The results provide the information necessary for toolmakers to improve tools and for users to make informed choices about acquiring and using computer forensics tools.

In order to exercise the string searching capabilities of the computer forensic tools, we developed test data to determine the accuracy with which the tool searches for known strings located within common types of container files. The container files tested are zip files, tar files and other commonly used container files. The known strings include both unique and common content across all test files.

Nafion and Platinum Degradation Studies with Thin-Film Fuel Cell Models
Pavan Bhargava

Fuel cells have the potential to become a significant source of clean energy, but to become more economical, improvements to both efficiency and longevity are required. In an effort to increase their durability, we have investigated the source of degradation in fuel cell test structures by studying layered thin-films that mimic the nanoscale structure at the PEM-catalyst interface. Test structures are fabricated with varying parameters, such as platinum thickness and Nafion annealing temperature, and then subjected to different environmental conditions to determine the extent of degradation. My goal this summer has been to optimize the test structure for future degradation experiments and gain initial insights into fuel cell degradation on these optimized test structures.

Previous test structures were created by sputtering platinum on top of a silicon substrate, spin coating Nafion, and annealing to promote its adhesion. Several problems arose with this structure. A layer of PtSi forms, which complicates Neutron Reflectometry analysis of the layer structure and can evolve over time or under conditioning, adding additional uncertainties to the measurements. The initial test structure was annealed at 210C to ensure Nafion adhesion during electrochemical processing. Such a high temperature could cause interactions that compromise the structure. This processing caused significant degradation of the test structure relative to its initial structure, measured one year prior.

Here, we discuss experiments performed at the NCNR to optimize the test structure and investigate degradation at electrode/membrane interfaces. X-ray Reflectometry has confirmed consistent quality with more efficient substrate preparation methods. Pt-Nafion layers annealed at varying temperatures are inspected to determine the lowest temperature required to properly adhere Nafion to the Pt. Finally, electrochemical and X-ray Reflectometry measurements are performed on Pt-Nafion layers deposited on silicon and sputtered Cr layers to explore the Cr substrate as a stable and less-ambiguous test structure for future Pt-Nafion degradation studies.

Extraction of Series Resistance from Advanced CMOS Devices
Serghei Drozdov

The rapidly increasing speed of microprocessors is largely dependent on the downscaling of transistor dimensions. However, as these transistors get smaller, new issues arise. One of the most serious issues facing transistor scaling is series resistance. Unfortunately, the established methods used to measure series resistance become unreliable in these highly-scaled transistors. In this work, an alternative series resistance extraction technique, which is less susceptible to transistor scaling, is examined.

The established series resistance extraction methods are prone to error due to several assumptions which become unreliable in highly-scaled transistors. The new method discussed in this work attempts to limit these assumptions and improve the measurement accuracy. In addition to a careful analysis of this new method, a slightly more accurate extraction method is also developed and analyzed with moderate success. These changes have been made to the original equation to have more consistent results.

These alternative series resistance extraction methods were applied to a range of transistors from the 40 nm technology node. Careful parametric variations were employed to identify the strengths and weaknesses of this new series resistance extraction technique.

Sustainability Performance Analysis of a Water Bottling Facility
Daniel Ettehadieh

According to the National Association of Manufacturers, the industrial sector accounts for 31% of all the energy consumed in the United States (NAM, 2009). Manufacturing alone accounts for 65% of the industrial sector's energy consumption. With manufacturers looking to diversify their energy supplies and improve their energy efficiency due to an increasing energy price tag and concerns of climate change, a model for sustainable manufacturing among industries has become imminent. A framework for determining a model that systematically takes into account the sustainability performance would have to not only include the environmental impacts of the production operations, but must account for the building facility which houses the manufacturing equipment. With the building sector accounting for 40% of the United States' primary energy consumption; as well as, 40% of the total carbon dioxide emissions, 12% of the water consumption, and 68% of the electricity consumption various environmental issues come into play when considering the building facility (Net-Zero Energy, 2008). The objective of this research is to systematically address the sustainability performance of manufacturing processes in tandem with the building facilities based on a model of a real-life water bottling facility. Measuring the combined impact of the manufacturing processes together with the building facility will provide manufacturer's the ability to accurately measure their performance in meeting sustainability objectives. These sustainability objectives deal with building services such as lighting, HVAC (Heating, Ventilation, and Air Conditioning) systems, and water consumption along with manufacturing operations such as machine utilization, transport systems (forklift, conveyor), and other plant floor processes. In addition to extending sustainability in manufacturing, this research demonstrates that modeling and simulating the production processes integrated alongside the facility processes will assist companies in achieving maximum production efficiency.

Reducing the Area of Magnetic Tunnel Junctions Using a Focused Ion Beam
Marissa Galfond

Magnetic tunnel junctions (MTJs), devices composed of two ferromagnetic wires separated by a thin insulating layer, can be used as hard drive read sensors and for magnetic random access memory (MRAM). The two ferromagnetic wires are perpendicular to one another, thus forming a nominally

square MTJ with a constant resistance x area (RA) product. Due to signal noise, the measured resistance of the MTJ has an error relative to the device resistance. As the device resistance increases, the relative error decreases. By decreasing the area of the device, we can increase the resistance and, therefore, decrease the relative error. In this talk, I discuss the feasibility of using a focused ion beam (FIB) to decrease the device area. Additionally, I compare optical and scanning electron microscopy techniques in determining device areas.

Fast, Versatile Quenching in a Single Photon Avalanche Diodes for Quantum Key Distribution

Alexander Golden

Quantum Key Distribution (QKD) systems are currently seen as the future of communication encryption. They do not rely on simple computational complexity to provide their security, but on the physical laws of quantum mechanics. One of the main hurdles in the implementation of QKD systems in industry are the speed limitations in the Single Photon Avalanche Diode (SPAD) circuits. To push the transmission speeds of this technology to more competitive levels, it has been necessary to develop control circuits capable of detecting single photon events at very high speeds, with high precision. Additionally, it is desirable to keep a design from becoming over-specified and locked in to a single type of SPAD. These two constraints required a new type of design, which consists of two main ideas. First, by the combination of high-speed comparator circuits and state-of-the-art telecommunications transistor designs, which allow very fast response times. Second, a novel quench/reset circuit design enables very high detection rates.

Develop an Analytical Reverse Blocking Model for Si and SiC Diodes and Incorporate the Model into the Diode Model Parameter Extraction Software Using LabWindows/CVI

Musa Ibrahim

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. In order for circuit designers to perform a system level simulation, compact models for these devices are needed in circuit and system simulation tools. The goal of this project is to develop an analytical reverse blocking model for Si and SiC PiN diodes and incorporate the model into the Diode Model Parameter Extraction Tools (DIMPACT) software using LabWindows/CVI. This software is used to extract the data necessary to establish a library of Si and SiC PiN diode models and to provide a method for quantitatively comparing between different types of devices and establishing performance metrics for device development.

The reverse leakage program developed in this work consists of a graphical user interface (GUI) which allows the user to load the reverse leakage measurement data for performing model parameters extraction. These model parameters include breakdown voltage (BV), current at breakdown voltage (I_{BV}), space-charge life time, and their temperature coefficients. The model parameters extracted using this program will be used in Saber model for validation. The program has demonstrated using a 10 kV SiC PiN and a 4.5 kV Si PiN diodes.

Solutions in Perception Challenge

Tommy Ji

Over the years, great strides have been made in robotics technology. However, there are still limitations in robot capabilities specifically those that are more organic in nature. Perception, touch, and grasping are

just a few examples of tasks that are simple for a person to perform, but very difficult for an artificial intelligence to imitate.

To address these problems in current robotics technology, the robot development company Willow Garage has been conducting research on improving robotics technology and recently developed the Solutions in Perception Challenge competition. The competition involves having teams from different universities around the world program a robot to be able to detect and identify 100 different items that are commonly found in drug stores and supermarkets. The purpose of the competition is to promote innovation in the field of robotics and the importance of perception technology in robotics research.

While the first Solutions in Perception Challenge showed success, there were some problems with the format of competition. One problem that is most relevant to my work is the test rig that was used for the competition. For the competition, a test rig was used as a platform to put the different items on to be identified while being able to determine the locations of the items based on a coordinate system used for the test rig. The major problems for the test rig were, it lacked modularity, depending on the programming algorithms used by a team, the setup could be very predictable, there was no way to provide training rigs for the contestants to use before the competition. My role was to redesign the test rig so as to have increased modularity, find cheap alternatives to producing the rig so it can be built by each university beforehand to train with and make it that the setup could not become easily predictable by the contestants' programming.

Structural and Electrical Characterization of Metal-Molecule-Silicon Junctions Produced by Flip Chip Lamination

Benjamin Jones

As the semiconductor industry approaches the physical limitations of conventional Complementary Metal-oxide-semiconductor (CMOS) transistors, new materials are being explored as possible candidates for the next generation of electronic devices. Organic molecules have been suggested as a new material for nanoelectronic devices because they are a versatile material which can be used to fabricate devices such as photovoltaics, chemical and biological sensors, or transistors. Molecules can also self-assemble on devices to make fabrication much faster and more efficient. The integration of organic molecules with silicon is particularly interesting as modern electronics is primarily silicon based, enabling the use of a wide fabrication and knowledge platform to incorporate new materials and functionality.

The fabrication of metal-molecule-silicon devices has been performed in many different geometries and techniques and each presents specific complications. Flip-chip lamination (FCL) is a novel process incorporating nanotransfer printing and molecular self-assembly that was used to create metal-molecule-silicon junctions. A set of bifunctional molecules were used for devices that were fabricated using FCL and characterized. Structural characterization of the molecular layers was performed by Polarized Backside-Reflection Absorption Infrared Spectroscopy (pb-RAIRS). Electrical characterization was performed by taking IV measurements to study the effects of molecular length, functionality, device size, temperature, and silicon doping on the devices' electronic properties.

Planar Arrays of Core/Shell Nanowires for Light Generation and Detection

Kun Li

Planar ZnO/CdS core/shell nanowire (NW) arrays are synthesized via a multi-step process and their physical, optical, and electrical properties are characterized before and after deposition of the CdS outer layer. To create the arrays, Au is first deposited on a-plane sapphire by photolithography and thermal evaporation in vacuum. The Au is patterned in lines and fiducial marks, allowing for control over the location and direction of NW growth and alignment of additional layers to create a semiconductor

heterostructure device. Planar ZnO NWs are then grown epitaxially on sapphire by the vapor-liquid-solid method, using the Au patterns as catalysts for growth. The planar configuration permits selective coating of the NWs with a CdS shell by combining lithography techniques with a successive ionic layer adsorption and reaction (SILAR) wet chemical method. The CdS layer has controllable thickness proportionate to the number of SILAR cycles performed, and its ability to tune the optical emission of ZnO NWs from green to UV by varying this thickness is shown. Atomic force microscope, scanning electron microscope, cathodoluminescence, energy dispersive x-ray spectroscopy, and transmission electron microscope are used to characterize the ZnO/CdS heterostructures. The NW arrays are then used to create a charge transport device, with contacts on the core/shell NWs and an overlaid Pt electrode. Light generation and detection by planar ZnO/CdS NWs is shown.

Safety of Humans Near Powered Industrial Vehicles
Li Peng Liang

Powered Industrial Vehicles such as forklifts are widely used in many industries. The National Institute of Standards and Technology's Intelligent System Division has been researching advanced 3D imaging sensors and their use towards improving both automated and manned forklift safety. An operator's visibility from powered industrial vehicles is required to meet certain criteria specified by standards. Standards ANSI B 56. 5, ANSI 56.11.6 and ISO/DIS 13564-1 require measurement and evaluation of Visibility from powered industrial vehicles.

Our project evaluated the visibility of a forklift by following the above ANSI and ISO/DIS standards and then developed recommendations for better test methods. Visibility is evaluated by casting shadows of the forklift onto a screen and observing the dark and illuminated areas on the screen being moved along specific test paths around the forklift.

We will then investigate the patterns and locations of the shadows so as to integrate advanced sensors onto forklifts to prevent accidents. A light source array of 13 55w halogen lamps was fabricated to provide light from the various operator eye positions onto a screen. The Seat Index Point (SIP) is a reference point to locate the various positions of light source array. Following Standard ISO5353, we fabricated the SIP device and located the light source array according to the SIP. Our team also applied 100N horizontal force and 400N vertical force at the SIP device to simulate an average weight operator sitting in the forklift. Besides the mechanical set-up, we also fabricated electrical circuits for the halogen lamps and selected the proper power supply. Eleven visibility tests were then performed by casting shadows in different directions onto the screen moved along the standard test paths. Besides the required tests according to the standards, we also conducted tentative tests to develop recommendations for test methods. For example, we studied the patterns of shadows of a pallet of boxes, on standard test pieces and on a mannequin.

XMPP Services for Smart Transducers
Rachel Liao

Sensors are widely used to obtain information about our environments and utilized in many manufacturing applications. With the advancement of microprocessor technology, sensors are equipped with more capabilities, such as self-describing, processing, and network communication – they become so-called "smart sensors." However, to gain the optimal benefits from these smart sensors, the efficient interactions between them and their users for secure information exchanges are vital. It is becoming necessary to have a set of common communication standards for smart sensors that everybody can follow. The IEEE 1451 standards provide such family of smart transducer (sensor or actuator) interface standards so that interoperable and secure communications between smart transducers and their users can be facilitated.

For my project I am investigating a new approach for providing a network interface for smart transducers running on wired or wireless IP (Internet Protocol)-based networks. This approach will provide the ability to easily and securely interface a large number of smart sensors onto a large number of networks. This will also help establish communication interface interoperability between sensors and existing networks that then enables equipment "plug and play" capability.

To accomplish this, I am developing and implementing a method for transporting IEEE 1451 messages over a network using the Extensible Messaging and Presence Protocol (XMPP). We decided to use XMPP because it is an Internet Engineering Task Force (IETF) open standard, easily extensible, and it utilizes eXtensible Markup Language (XML) data format.

In the span of this summer, I hope to be able to establish a secure session initiation and communication between the smart sensors and the users through XMPP. By using characteristic identification information from the smart sensors' Transducer Electronic Data Sheet (TEDS), I will be able to verify valid sensor connections as well as reject invalid sensor connections. Once a connection is established, I will, through a web-based client interface, be able to request information from the smart sensors and receive a converted and workable response. At the end of my project, I hope to have integrated XMPP services with the IEEE 1451 smart sensor networks.

Stability of Terpene Gas Mixtures in Aluminum Cylinders

Janice Lin

Ozone formation in the lower level stratosphere leads to photochemical smog. This process is fueled by oxidizers in the air such as hydrocarbons, which are released from car emissions and biomass burning, and terpenes, which are released from plants. To develop effective control methods to regulate the amount of ozone in the lower level, atmospheric chemists need accurate concentration measurements of the chemicals in the air. Therefore, gravimetric gas cylinder standards containing stable mixtures of gases in a matrix gas are increasingly becoming a necessity for atmospheric chemistry. Gas metrologists develop standards, which serve as points of reference, for this purpose. Standard Reference Materials (SRMs) that have been tested for stability and composition can provide a universal ratio to which laboratories around the world can relate their measurement records. National Metrology Institutes are collaborating to develop terpene gas standards to assist the World Metrological Organizations Global Atmospheric Watch Program for volatile organic compounds.

The Gas Metrology Group at NIST previously developed several stable standards of hydrocarbon mixtures in aluminum cylinders that have been treated by a U.S. specialty gas company to passivate the internal surface. Some but not all terpenes prepared in these treated aluminum cylinders have shown degradation since small orifices in the cylinder wall coating have been found to expose aluminum oxides to the terpenes. A suitable cylinder has yet to be found to develop a stable mixture of terpenes. We prepared low concentration mixtures of terpenes, including two important terpenes α-pinene and ß-pinene, in a European specialty gas company passivated aluminum cylinder. One to four terpenes were introduced in a cylinder, mirroring the concentration levels to that of the atmosphere. Benzene, which has shown years of stability in the aluminum cylinders, was used as an internal standard. Using gas chromatography, the mixtures were analyzed for stability over time. Data show that α-pinene degrades at a higher rate in the U.S. cylinder than in the European cylinder; however, the rate of degradation of ß-pinene is consistent in both cylinders. Other terpenes show no consistent results. Another type of gas cylinder made of stainless steel, using water to act as the inner coating, has yet to be tested. Once a stable mixture of terpenes is developed, atmospheric chemists can use the concentration trends to more accurately gauge the levels of terpenes in the air.

Method Development for Characterizing TiO_2 Nanoparticle Surfaces by Mass Spectromery

James McCarthy

Titanium dioxide (TiO_2) is a commercially widespread material, present in everything from paints, to cosmetics, to solar energy devices. Nanoparticulate TiO_2 has received particular attention for its photocatalytic properties and its incorporation into sunscreen products. As with all nanoscale materials, TiO_2 nanoparticles are of health-related and environmental concern due to their small size. With such small size, the nanoparticles have large surface area-to-volume ratios that enhance their reactivity relative to bulk, or even microparticle TiO_2. Since this reactivity is largely dependent on surface properties, developing methods to study the surface chemical composition of these particles is essential in order to understand and predict nanoparticle behavior in different environments.

This research examined TiO_2 nanoparticles with secondary ion mass spectrometry (SIMS), a surface analysis technique which generates a mass spectrum from ions desorbed from a solid surface. A variety of measurements were used to quantify TiO_2 nanoparticles in solution so that dilutions could be made to account for initial concentration differences. Various solvent compositions were used for the dilutions in order to study the effects of the surrounding environment on surface chemistry. Methods were subsequently developed to prepare nanoparticle samples using a precision inkjet printer system in order to ensure a consistent deposition and aggregation of material. Inkjet-printed samples were analyzed using a time-of-flight SIMS instrument as well an environmental scanning electron microscope (ESEM), which reveals the morphology of the deposited aggregates. A MATLAB code was developed to identify and integrate peaks of interest, and ratios between areas of different peaks allowed for surface changes to be monitored as a function of particle size or depth of analysis into the aggregates. The effects of particle size on surface properties were studied for a range of particle diameters. Depth-profiling investigations of nanoparticle aggregates were conducted to understand surface/bulk differentiation for nanoparticles of different sizes as well. It is believed that the methods developed in this research will guide future investigations in sample preparation and spectral acquisition for studies of nanoparticle surface chemistry, enabling a better understanding of nanoparticle reactivity and behavior.

Feature and Task-Based Evaluation of Robot-Generated Maps

Mark Mifsud

Simultaneous Localization and Mapping (SLAM) is a major focus in the field of mobile robotics. A robot uses SLAM is to localize itself within an environment while simultaneously creating the map of that environment. This is done by using data from internal sensors, such as odometry or encoder data, to estimate a path, and then using external sensors, such as a laser range finder or camera, to correct this path and map the environment.

One problem with the advancement of SLAM is the lack of a standardized map evaluation methodology. The primary evaluation procedure is visual inspection, which is neither quantitative nor consistent. Some quantitative techniques exist, but they evaluate maps using different criteria which are not consistent. These quantitative evaluation methods generally work by comparing the location of features in the ground truth map with those in the robot-generated map. An alternative to this process, which could lead to more consistent results, is a task-based evaluation. A task-based evaluation would compare the paths for a robot-generated map and its ground truth. An evaluation of this nature would ensure the robot map allows the robot to perform the job at hand, and therefore serves as a true mark of the robot-generated map's quality.

The purpose of this research is to compare various feature-based map evaluation methods with a task-based map evaluation procedure. This was done by using two feature-based map evaluation toolkits, as well as a task-based evaluator, to rate the quality of various robot-generated maps with respect to the ground truth map. Map evaluation analysis was done using various MATLAB programs, resulting in a final ranking of the maps for each toolkit.

Validation of the Fire Dynamics Simulator
Taylor Myers

The Fire Dynamics Simulator (FDS) is a computational fluid dynamics program that simulates the complex phenomena of fire. In order to ensure the accuracy and applicability of FDS's modeling in different fire scenarios, validation must be performed. Validation entails determining if the model is a viable representation of the real world, i.e. that the physics and assumptions we are applying are correct. To perform this validation, model results must be compared with real world experimental data.

A large number of cases representative of common and not so common fire scenarios have been constructed. Data from individual instruments is compared as well as more overarching comparisons of large scale trends. This data is then analyzed with respect to experimental uncertainty in an attempt to quantify just how well FDS is capable of predicting fire behavior. The FDS Validation Guide that is assembled from the ever increasing number of test cases is an invaluable tool for the growing FDS user base. These tests are used to establish a parameter space table, which identifies ranges for various parameters where FDS has been demonstrated to be accurate. With the guide experts and non-experts alike are able to assess the efficacy of using FDS as a model in their particular situation, as well as demonstrate the accuracy of their predictions without resorting to costly physical experiments.

Cloud Interoperability: Migrate (Fully-Stopped) VMs from One Cloud-Provider to Another
Brady O'Connell

The Cloud Computing model has emerged as an enabling technology for providers to deliver software solutions, lower costs and improve efficiency as they service their customers. However, as more cloud providers appear in the market, interoperability of services between clouds becomes of fundamental importance. Currently, if a cloud consumer wishes to switch cloud providers or employ multiple providers, difficulties in ensuring a smooth transition exist in the migration of virtual machines (VMs) and client data from one provider to another.

One solution is to generate a configuration file that provides a complete specification of the virtual machine under consideration for migration. This is a crucial step to migrate fully stopped virtual machines. The configuration file should include the full list of required virtual disks plus the required virtual hardware configuration, including CPU, memory, networking, and storage. DMTF developed the Open Virtualization Format (OVF) Specification, which describes an extensible format for the packaging and distribution of software to be run in virtual machines. Many providers are adopting OVF as a standard and are building around it, so that it can now be used as a middle ground to transition between proprietary VM configuration files.

As part of the SAJACC project, a cloud interoperability use case was implemented in JAVA to demonstrate the feasibility of migrating VMs between providers to determine future cloud interoperability requirements for cloud computing standards. To accomplish this, the program takes advantage of OVF and other public interfaces and tools from VMWare, Amazon Web Services, Citrix XenServer, and

VirtualBox to convert each provider's unique VM configuration formats to OVF in order to import into another provider's service.

Long-Term Durability of Polymeric Materials for Photovoltaic Applications: Chemical and Physical Degradation of PMMA During UV Exposure

Lee Phuong

The emergence of photovoltaic (PV) technology has shown tremendous promise in recent years. However, the success of PV will ultimately hinge on its cost and long-term reliability. Concentrating photovoltaic technology (CPV) becomes economically advantageous when the cost is reduced using optical components that are relative inexpensive. Many CPV systems use Fresnel lenses made of poly (methyl methacrylate) (PMMA) to obtain a high optical flux density. Oftentimes, manufacturers like to replace glass frontsheets with polymers such as PMMA. However, polymeric materials are susceptible to typical PV environmental conditions including ultraviolet (UV) irradiation, humidity, and temperature. This research aims to investigate the long-term durability of PMMA using the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) at different relative humidities and ultraviolet irradiances. These results are compared to samples subject to outdoor weathering so that a correlation can be made and we can predict the service life of PMMA in PV applications. The chemical and optical properties are analyzed through Fourier transform infrared (FTIR) and ultraviolet-visible (UV-VIS) spectroscopies while the surface morphology and the microstructures were studied using Atomic Force Microscopy.

Diffusion Coefficient Calculation of Phospholipids on Membrane Bi-Layer Enclosing Protocells via Matlab

Aman Rahman

Fluorescent Recovery After Photobleaching (FRAP) was utilized to measure the diffusivity of labeled lipids in membrane bilayer on protocell surfaces to better understand viral interactions. Protocells used in the experiments were 10 μm in diameter with porosities of 5 nm, 10 nm, 50 nm and 100 nm. Fluorescently labeled lipids in the membrane were visible with ultra-violet illumination under a microscope. A small membrane area was bleached using a diode laser. Images were taken during fluorescent recovery over time. Matlab was used to process the images in order to quantify the diffusion coefficient. Protocells are biomimetic cellular particles; the ones used in this experiment contained receptors to attach to G-proteins on paramyxoviruses. This family of viruses has been known to cause fatal inflammations in the human brain. Both human to human and animal to human transmission have been identified. Previous research has shown the inactivation of viral infectivity with protocell exposure. Those experiments measured viral inactivation with different membrane compositions and at different temperatures; these measurements provide data on the membrane diffusivity to explore possible mechanisms.

Human Response Processes for Emergency Communication

Carolyn Sandler

At present, many buildings and building campuses in the United States are installing mass notification or emergency communication systems to improve communication from the building or emergency officials to the public. The National Fire Alarm and Signaling Code (NFPA 72), 2010 edition, provides requirements for the application, performance and installation of emergency communication (or mass notification) technology. However, NFPA 72 provides little guidance on how to use these systems for effective emergency communication. Little guidance is given on the *specifics* of the message, including message content and length, speaking rate, frequency of delivery, and other important aspects of emergency notification.

In the United States, there is little guidance or requirements outside of the building codes for message providers on the content and dissemination strategies for emergency messages. The people providing the messages in a disaster may not have the necessary tools, techniques, guidance, and training required to provide information to the public when a disaster is imminent or unfolding. There is also a lack of standardized messages for specific emergency and technology combinations for message providers to use when a given emergency occurs. Therefore, the purpose of this project is to provide guidance on message creation and dissemination for a full range of building emergencies likely to occur in the United States, with a specific focus on visual emergency communication.

For my project, I worked on a literature review about how people process and respond to emergency communication. Before people perform an action, they go through a five stage process in order to make a decision: Perception, paying attention to the message, comprehension, warning belief and personalization of risk. Visual signage and emergency communication must properly affect those five stages to instruct people how to properly behave in an emergency. I looked at information in various fields including sociology, fire protection engineering, and human factors and ergonomics to understand how to improve emergency communication processes. This research will directly influence current codes and standards, including NFPA 72. Using this review, we hope to improve communication for building occupants in emergencies.

Integrated Factory Operation and Building Science Simulation
Jeffrey Sze

There are many opportunities to reduce energy costs within a manufacturing facility. To achieve an energy efficient manufacturing system, manufacturing planners need to understand, measure, and analyze the combined impact of process energy from manufacturing operations, equipment, and facility energy from building services such as HVAC (Heating, Ventilation, and Air Conditioning), lighting. A case study based on the NIST's fabrication facility and machine tool is explored.

To analyze and optimize the setting of a facility, an energy model is required. The software that is being used, Energyplus with SketchUp plug-in has a reputation for accurate building simulation. The creation of the energy model then will allow parametric studies in HVAC system, infiltration, insulation, fenestration and etc. The method of integrating factory operation into building science is by estimating the peak energy load with an asummption of complete conversion from electrical energy into heat, then incorporating a working schedule into the energy usage and combining with energy modeling.

The next stage in further lowering energy cost is to investigate in renewable energy source, which solar thermal water heating technique is chosen to be studied. These systems are known for high initial cost and relatively unstable energy input, however they are usually more practical in some applications. Therefore the calculation of payback period using simulation software will best demonstrate their potential in replacing convention systems in specific areas like electric water heater in this case.

Concrete Rheometer Automation
Andrew Trettel

Concrete rheology is the study of the flow and deformation of concrete. Fresh concrete is a non-Newtonian fluid that typically behaves as a Bingham plastic, a fluid with a yield stress and plastic viscosity. One of NIST's commercial concrete rheometers (a device that measures rheology) comes with inadequate software for measuring rheological properties, so NIST needed new, user-friendly software that collects more data than before, displays and analyzes the data in real-time, can be modified easily in the future, and allows for different test protocols (for example, a speed sweep test to determine the plastic viscosity and approximate yield stress, and a constant speed test to determine, by stress growth, the yield

stress). The new software greatly expanded the rheometer's capabilities. The challenge was that the rheometer's source code and documentation were written in C++, while the new software needed to be written in LabView. This mismatch created timing issues for sending commands to the rheometer, created conversion issues for interpreting the rheometer's unusual format for floating point numbers, and created programming issues for porting the documentation's lower-level C++ commands into the final product's higher-level LabView commands. After the software was complete, documentation was written to allow researchers to use the software now and update it later.

Firelab Development: A Sandbox for Improving the Fire Dynamics Simulator
Benjamin Trettel

The Fire Dynamics Simulator (FDS) is a computational fluid dynamics (CFD) code that solves fire-driven flow problems in fire protection engineering. Planned improvements to FDS require major changes to the code architecture and are hard to implement. Consequently, a simpler CFD code (Firelab) was developed as a sandbox to test new algorithms before implementing them in FDS.

Firelab solves the 2D Navier-Stokes equations (which govern fluid motion) in a periodic domain. Firelab's calculation was compared against the exact solution for this test case to check the accuracy of the calculation. FDS and Firelab are both second-order accurate in space, but FDS is second-order accurate in time and Firelab is third-order accurate in time. In addition, three forms of the transport terms of the Navier-Stokes equations were compared numerically to check for further gains in speed or accuracy.

FDS's Lagrangian particle transport method also was improved. FDS can introduce water or fuel droplets into the simulation. Drag laws and momentum conservation govern the motion of these particles. FDS uses an exact solution for the motion of the droplets under drag for stability. This solution does not include gravity and no solution in 3D that includes gravity can be written in terms of elementary functions. FDS used an approximation of gravity's effects prior to this work. FDS's convergence properties were assessed with exact solutions to simplified cases. A major error was found in the particle positions and velocities with gravity. This error was corrected and consequently FDS became first-order accurate in the terminal velocity. A second-order approximation was derived, implemented in FDS, and verified against exact and approximate solutions.

Evaluating Searches Over Large Indices of Brief Documents
Mark Villarrubia

It is difficult to determine what qualifies a search as a "good" search, as such values are qualitative and subjective. It is possible, however, to state a list of qualities which a good search will have. Searches can be objectively rated based on, among other things, the number of false positives and false negatives, as well as each positive hit's proximity to the first index of the first page. Certain other traits can be specified as undesirable; for example, responses in languages other than the query language or reposts of older hits can reasonably be specified as invalid.

This project focuses on evaluating a variety of searches over a search space composed of microblog entries, in this case Twitter. Individual documents, or Tweets, are sharply limited in their size, ranging up to a maximum 140 characters.This limitation disrupts the traditional algorithms which rely heavily on word count and proximity, and on an idealized average document significantly larger than a mere one-hundred and forty characters. This project attempts to experimentally find an appropriate search, by building multiple searches and having human assessors rate their performance based on the proximity to the top of positive hits over 50 searches. These searches include filtered, front-heavy, and word-count

based searches, which are compared against the "out-of-box" Lucene search and against each other to find an optimal search for this environment.

Improving Velocity Measurement in NIST-3 Electronic Kilogram Apparatus
Sean Weerakkody

The kilogram, one of seven SI Base Units, is the only unit of measurement defined by a physical artifact as opposed to unchanging properties of nature. With the mass of the international prototype of the kilogram drifting at an estimated 50ug/100 years, it has become a key goal of metrology to obtain a definition for the kilogram in terms of fundamental constants. The NIST-3 Watt Balance is a step towards this ultimate goal, providing high accuracy measurements of Planck's Constant. An accurate measurement of Planck's Constant would allow us to redefine the kilogram in terms of the meter, second, volt, and ohm. The Watt Balance consists of two stages, a force stage where the magnetic force on an induction coil is balanced by the gravitational force of a mass standard (mg= IBL) and a velocity stage where the same coil moving through the same magnetic field at a constant velocity by Faraday's Law generates a voltage (V= BLv). Solving, we get mgv = IV, a balance of electrical and mechanical power. By making of use of Josephson Voltage standards and Hall Resistance standards, the NIST-3 has been able to measure Planck's Constant to within an uncertainty of 36 ppb (2005). The ultimate goal of my project is to improve uncertainties in velocity measurements during the second stage of the Watt Balance experiment in hopes of attaining a better uncertainty for Planck's Constant.

Three laser interferometers measure the position of the induction coil. As a result of Doppler shifts, there is a 6kHz difference between our 2MHz reference and three measurement signals in velocity mode. By counting the difference in the number of pulses generated by the reference and measurement signals we can determine the absolute position of the coil. To determine position, I helped write Labview programs to control a scaler/counter and a high resolution event timer. The event timer, or fractional counter, in addition to counting pulses, provides a time stamp with picosecond resolution enabling us to determine position to within a fraction of a picometer. Due to data transfer and memory demands, a pulse generator enables the timer for at most 50 times a second at continuous 158 uS intervals, preventing us from knowing the absolute position. The scaler or integer counter, provides a single count per trigger and when combined with the event timer provides an absolute count and position for the induction coil. The counter however does not have a time stamp and as a result determining relative delays in triggering the event timer and scaler is a crucial challenge in implementing a new and precise means of velocity measurement in the Electronic Kilogram Experiment.

Web-Based User Interface for Sustainability Modeling and Optimization
David Westbrook

A growing number of manufacturing industries are initiating efforts to address sustainability issues. Energy efficient manufacturing and low carbon manufacturing are gaining particular attention. Peak Electric Demands are a significant component in the cost of electricity and large sums of money can be saved if the energy is used more efficiently. High-speed milling can significantly reduce the large environmental burden associated with conventional milling and its carbon emissions. The analyses of different options are important to decision makers as it allows them to make decisions to avoid unnecessary high cost of energy. A decision guidance database allows for the optimization of the manufacturing process and energy allocation. A web-based user interface can then conveniently provide decision makers the analysis results and the appropriate decision recommendations.

The web-based user interface is implemented using Tomcat, HyperText Markup Language (HTML), Java Server Pages (JSP), and Java Database Connectivity (JDBC). Tomcat is used to execute the interface, which can be accessed from anywhere at any time. By using JSP to embed Java programming with

HTML, the web server will be able to dynamically respond to user requests and display the content. A layout has been developed to provide regular users of the system the opportunity to easily view data in terms of the input, computations, and optimizations of the manufacturing process. The four possible users for the system are vendor, customer, decision maker, and developer. A mechanism has been designed to allow these specific users to change the view to meet their particular interests. After verification of identity, the user can gain access to their particular functions.

Recommendation for the purchase of machining centers that lead to minimum emissions can be obtained. Suggestion of the number of local generators in order to control the peak demand and minimize the energy cost can be provided. The specified web-based user interface can be easily extended and used for more manufacturing processes in the future.

Stacked Electrode Back Contact Thin Film Heterojunction Solar Cells
Matthew Widstrom

A growing emphasis is being placed on clean and renewable energy as the increasing energy demands of the global community raises environmental concern over carbon-based fuels. A promising alternative to these carbon-based fuels are photovoltaic (PV) devices that harness energy from the sun. Three dimensionally (3D) structured PV devices seek to improve the overall thin-film device efficiency over that of planar devices through improved light management and charge carrier collection.

We report on a stacked contact geometry consisting of a traditional planar back contact and a three-dimensional embedded front contact, upon which the p-type absorber (CdTe as well as SnSe) is placed. The embedded front contact consists of an interdigitated electrode comb placed on an underlying oxide comb to electrically separate the electrodes from the underlying planar n-type semiconductor (Si), beneath which the planar back contact electrode is positioned. The absorber contacts the underlying n-type silicon to form the p-n junction while remaining isolated from the second electrode. This geometry places both electrodes behind the absorber, eliminating the need for a conductive oxide and allowing all incident light to reach the absorber.

Fabrication and Characterization of Carbohydrate-Functionalized Surfactant Vesicles
Jiemin Wu

The use of monoclonal antibodies (mAbs) for the production of therapeutic drugs is increasing throughout the biopharmaceutical industry. One of the major factors that contributes to the efficacy of mAbs is glycosylation, a post-translational process whereby oligosaccharide chains, or glycans, bind to specific sites on the mAbs. Achieving consistent glycosylation patterns in mAbs is vital since glycan structure heavily governs the biochemical properties of the mAbs such as bioactivity and stability. In order to properly monitor the quality and consistency of mAb production, methods to characterize the glycan structures that potentially bind to mAbs must be thoroughly investigated and developed.

The objective of the project was to prepare and characterize catanionic surfactant vesicles modified with a specific carbohydrate. Vesicles were fabricated by combining cationic and anionic surfactant molecules with a specific glycoconjugate *n-dodecyl-β-d-maltose* in three different concentrations. These vesicles are composed of a charged bilayer of hydrophobic tails and hydrophilic head group regions that assumed a spherical conformation due to thermodynamic stability. Size exclusion chromatography was performed to purify the modified vesicles which were then characterized using dynamic light scattering to determine the polydispersity index and vesicle size. Colorimetric tests and UV-vis spectroscopy were implemented to assess the amount of glyconjugate that incorporated onto the vesicle surfaces during formation. Results showed that the vesicles were relatively monodisperse and were successfully functionalized with the *n-dodecyl-β-d-maltose* glycoconjugates. Preliminary work was also performed to investigate the binding of

the functionalized vesicles with lectins, proteins with highly specific carbohydrate-binding functionalities, in solution. The vesicles will be utilized to develop a glycan array platform which will serve as an invaluable tool to understand the specific interactions between lectins and glycans. The characterized lectins will potentially be used to quantify the various glycan structures of mAbs.

University of Michigan – Ann Arbor

Automation and Control of Variables in a Cryogenic Environment
Navneet Gill

About two-thirds of all the experiments performed at the NIST Center for Neutron Research (NCNR) use cold neutrons with wavelengths longer than 4 Angstroms. The NIST reactor has a liquid hydrogen cold neutron source which is used to maximize the output of cold neutron flux for neutron scattering experiments that are performed in the guide hall. Reactors normally have a Maxwell-Boltzmann neutron distribution so there are not many neutrons lower than the thermal range of 25 meV and 1.8 Angstroms. These neutrons are well suited for many condensed matter experiments but cold neutrons are superior probes for materials with interatomic spacing on the order of 100 Angstroms (polymers, nanotubes, biological membranes, etc). Placing a cryogenically cooled moderator called a cold source in the reflector of the reactor causes a shift to lower neutron energies and hence produces the longer wavelengths needed to study materials with larger interatomic spacing.

The main goal of the project was to successfully configure and program a programmable logic controller (PLC) system to control vacuum and temperature measurements in a cryogenic environment. A PLC processor was installed and a functional ladder logic program was created for vacuum and temperature data acquisition at the BT-9 cold neutron source at the NIST reactor. Sensors generated electrical signals that were sent to an input module. The signal was then processed by the control unit and an output was sent allowing any required actions to be performed. Silicon diodes were used for temperature measurement in order to understand the level of neutron thermalization. Pirani gauges made reasonably low vacuum measurements. The neutron cold source requires a vacuum layer around the liquid hydrogen to guarantee there was no transfer of heat through molecular motion.

A three dimensional computer aided design (CAD) was also created to model the hydrogen and vacuum systems. These models were used to create displays which contained both a pictorial view and numerical data about the relevant systems. The displays had some functionality which allowed operators to control things such as the open/close position of a valve.

Degradation of Polyesters Used in Blast Resistant Glasses and Protective Glazing Systems
Amy Langhorst

The series of tornados that recently terrorized Alabama and the mid-west have exposed the dangers of residential glass in high wind natural disaster situations. One way to reduce this risk is by replacing ordinary residential windows with blast resistant glasses. However, there has been little exploration of the effectiveness of the polymers used in these systems after many years of exposure to the sun. To determine the post-weathering performance of these protective glazing systems, two different polyester specimens were exposed to ultraviolet radiation and one of four different temperature and relative humidity (RH) conditions—30˚C & 0% RH; 30˚C & 75% RH; 55˚C & 0% RH; 55˚C & 75% RH. Mechanical tensile testing as well as attenuated-total-reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and ultraviolet-visible (UV-Vis) spectroscopy were used to determine the extent to which each condition degraded the polymers. The rate of photodegradation increased with higher temperature and higher humidity. Samples exposed to higher temperature and humidity conditions generated a greater concentration of oxidation species and experienced more yellowing for a given exposure time than lower

temperature and humidity conditions. Also, tensile testing showed that the elongation to break and the strain energy density decreased with exposure time for all samples.

Fourier Methods to Describe the Shape of Biological Cells
Lo-Hua Yuan

Cell morphology both controls and responds to a myriad of biological processes, from differentiation to locomotion. For this reason, measurements of cell size and cell shape provide valuable quantitative information for cell biology. While traditional size and shape parameters like area, perimeter, roundness, and aspect ratio are commonly employed in practice, they do not capture all the important aspects of size and shape. The complex Fourier transform method, on the other hand, can be used to comprehensively describe any 2-dimensional cell shape in terms of a finite set of coefficients. In fact, a fairly small set of coefficients often suffices to define a very close approximation to the boundary of the cell. These descriptors can be calculated for any closed curve, not only for so-called "star-shaped" curves; in addition, they do not depend on landmarks or chain codes, and are invariant to scaling, rotation, and translation in cell boundary. A package of functions for the R environment for statistical analysis was developed that facilitates 2D object shape analysis using Fourier methods.

I used these Fourier methods to compare two populations of human bone marrow stromal cells (hBMSC). One population was cultured on biocompatible poly-(ε-caprolactone) (PCL) nanofiber scaffolds; the other, on flat spun coat PCL surfaces. It has been shown that hBMSC morphology directs cell fate: cells cultured on nanofiber scaffolds differentiate into osteoblasts, while cells cultured on flat surfaces do not undergo osteogenesis. To compare the morphology of the two hBMSC populations, I first used the image processing software ImageJ to extract xy-coordinates of points on each cell's boundary. Then I applied the complex Fourier transform method to obtain Fourier descriptors for the cells. I investigated the use of AIC, R^2, and Mallows C_p as criteria for choosing an appropriate model order. Finally, I performed statistical tests and confirmed a significant difference in the spread and kurtosis of the Fourier spectrographs for the two hBMSC populations.

University of New Hampshire

Measuring Thermal Properties of Materials at High Heating Rates Using a Nanocalorimetr
Khanh Nguyen

Nanocalorimeter measurements are based on microfabricated silicon chips with a 50nm thick platinum heating strip that is deposited onto a 100 nm thick silicon nitride membrane with a 3 nm titanium adhesion layer in between. The chips provide a typical heating rate of 10^5K/s and a maximum temperature of 1023K. Based on these working ranges, the nanocalorimeter is an ideal platform for testing thermal properties of materials that operate at high heating rates and temperatures.

This work discusses the design, fabrication and evaluation of a new circuit board and LabView virtual instrument to perform these measurements. The circuit board can be used with one chip or two chips in a differential measurement mode. An experiment consists of an arbitrary waveform, created in the virtual instrument, being applied to the chip from a digital-to-analog output card and boosted with a unity gain buffer amplifier.

I have demonstrated measurements on two unusual materials using this apparatus. The first is to measure the high-rate thermal properties of concrete from a NASA launchpad. The nanocalorimeter can only perform measurements on small sized samples, consequently, experiments were first performed with a macro scaled Netzsch STA 449 calorimeter to make sure that concrete cores and finely ground concrete powder gave similar results. The second application was to measure the thermal behavior of trace

quantities of explosives while simultaneously recording high speed video of the experiment to understand how the sample decomposed during a measurement.

University of New Haven

Quantitative Measurement of Enzyme Activity Loss on Biofunctionalized Gold Nanoparticles
Danielle Gorka

Biofunctionalized gold nanoparticles (AuNP) are being investigated as a next-generation drug carrier used to target cancer cells due to the unique properties of nanoparticles. Before biofunctionalized nanoparticles can be used as effective drug carriers, a method needs to be determined to ensure the efficacy and quality of the attached therapeutic enzymes. Ultraviolet-Visible Spectroscopy (UV-Vis) can be used to quantify the activity retention or loss of enzymes on the biofunctionalized nanoparticle when the enzymes catalyze the formation of absorbing molecules. Atomic force microscopy (AFM) can be used to determine the number of attached enzymes through the use of gold immunolabeling which is a similar method traditionally used with transmission electron microscopy (TEM) samples. This causes the formation of a raspberry like structure, which can be imaged and counted, here by AFM.

In this work, horseradish peroxidase (HRP), a well studied enzyme, was functionalized to a gold nanoparticle via peptide coupling chemistry. UV-Vis was used to perform enzyme kinetic measurements to show the activity of the HRP both by itself and functionalized to a AuNP, thereby determining the loss in enzyme activity due to attachment to the AuNP. AFM was used to determine the actual number of enzymes that became attached to the AuNP by counting the number of small antibody-AuNPs that self assembled onto the larger enzyme-AuNPs. These enzyme attachment yields were compared to those calculated from the enzyme kinetic loss experiments.

Formation and Characterization of Monolayer Nanoparticle Clusters
Nicole Reardon

Gold nanomaterials have unique physiochemical properties compared to their bulk counterparts with applications in catalysis, optical devices and as drug delivery platforms. An important step in understanding specific size-property relationships is synthetic procedures to produce aimed, isolated products. Understanding the reduction, nucleation and growth mechanisms, which includes information of the chemical species, should provide tunable control of syntheses. This study uses gold nanoclusters as a model system for examining the chemistry of reduction and nucleation of gold-ligand complexes. Two different distributions of gold complexes with two different phosphine ligands are used to examine the relationship of the initial gold-ligand complexes and cluster growth. Reduction of a gold precursor, chloro(triphenylphosphine) Gold(I), or equimolar concentrations of equilibrated $AuClPPh_3$ and L_3=1,3 bis(diphenylphosphino)pentane, in two different solvent systems is examined. The syntheses are initiated by the addition of either two different boron containing reducing agents that have different reduction rates, sodium borohydride($NaBH_4$, fast) or borane-tert-butyl amine(BTBC, slow), that allow differentiation between reduction-nucleation processes and solution phase processing. The gold nanocluster evolution was monitored using UV-Vis spectrometry, electrospray ionization mass spectrometry (ESI-MS) and dynamic light scattering (DLS). A colorimetric assay was employed to temporally investigate the evolution of the total distribution of both ionic and neutral clusters into two different cluster size bins, because all reported gold clusters, Au_x, $x \leq 13$, have distinct transitions in the UV-vis spectrum. The colorimetric assay provides information about the total concentration and evolution of all clusters; therefore, appearance of specific clusters can be identified through reduction-nucleation processes or through subsequent solution phase growth and etching processes known as size-selective processing.

University of Puerto Rico

Precisely Measuring Currents on the Nano-Ampere to Femto-Ampere Range Using an Automated Current-to-Voltage Converter

Aida Colón-Berrios

Metrology is the science of measurements. Calibration is the process of comparing measurements of an unknown to a standard of known accuracy and precision. In the Quantum Electrical Metrology Division, Metrology of the Ohm project, at the NIST (National Institute of Standards and Technology), we develop high resistance standards and measurement techniques to calibrate resistances in the range of 10 MΩ (Mega-Ohms) to 100 TΩ (Tera-Ohms) and develop new methods for calibration of not only resistances but also small currents traceable to the international system of units (SI) through high resistance standards.

The calibration of small currents, mostly in the range of nano-Amperes (10^{-9}) to femto-Amperes (10^{-15}), is very complex. When measuring a current there is a possibility of leakage currents which would be very noticeable in the operational range for calibrations. Since it is easier to measure voltage, a current-to-voltage converter system was built in which twelve different but known voltages were inputs. Applying Ohm's Law, voltages were divided by the source resistance, and the source current was obtained. Then the output voltage was measured to verify the precision of the system. Initially the system was running manually and it took approximately 2 to 3 hours to take three measurements per voltage; now the system is automated and can take two hundred measurements per voltage in a time span of 10 hours. The automation of the measurement system was accomplished using Microsoft's Visual Basic 5.0 to control the programmable DC voltage source and the output voltage detector (nano-voltmeter). The application of this system will establish a new and more precise method to measure and calibrate very small currents. The system uses high resistance standards for the generation and measurement of the small currents. These measurement techniques have application in providing SI traceability from the quantum Hall resistance for the calibration of aerosol electrometers, measurement of photodiode currents, measurement of ionizing radiation currents, and other small currents.

Credential Revocation Service

Eliezer Ferŕa

There are many types of credentials, all with varying form factors, which makes implementing a uniform credential revocation procedure difficult. A web service with different types of verification and/or revocation of credentials may be a good start for a uniform credential revocation procedure. My project consisted of developing a web service that takes care of the four main aspects of credentials: validation, status, risk factor, and revocation. Validation is performed through an expiration date check, and if passed, the status is checked. The status of a credential can be revoked, suspended, or active. Once the status is reported, a risk factor is given to that credential of high, medium, or low, which indicates the likelihood that the credential has been compromised. Should any of these checks fail, the service will also provide a 3-level revocation of the account, credential, and procedure.

Develop an Additional Computer-Controlled Thermal Cycling Station In Order to Support Reliability Analysis for High-Power, High-Temperature, Power Semiconductor Devices and Modules

Joseph Marcano Estévez

Silicon-Carbide (SiC) material and device fabrication technology has led to the development of new high-voltage, high-frequency (HV-HF) power devices. SiC devices are suitable for high-temperature

applications because they are wide bandgap semiconductors, but in order to be reliable, the packages for these high power devices must also withstand the high temperatures that they face during normal and sometimes extreme operational environments. In order to do the package material analysis for high-power and high-temperature devices we need to develop a software-controlled thermal cycling station. The software used is LabWindows/CVI. The user interface permits the flexible definition of testing parameters such as variable data acquisition rates, customizable cycle transition's duration and the independently controlled heating and cooling rates of the test. The cycle's heating is provided applying power using a controlled power supply and heating elements, while two independent mass flow controllers provide the cycle's cooling control, which can be a combination of air and water flows depending on the package's temperature, which we monitor using a thermocouple. The user interface provides visual feedback by continuously showing the hotplate temperature and the thermal cycling measurements at the same time. The package in which the devices are going to be tested are inside an insulated enclosure and the testing temperatures are within the range of 25°(C) to 200°(C).

Temperature Control System for Pulse-Heated Kolsky Bar
Alexander Ortiz-Lozada

The Kolsky Bar, also know a Split-Hopkinson pressure bar, is capable of performing materials properties tests, such as stress versus strain, at strain-rates far exceeding typical tests done on mechanical testing devices. The Pulse-Heated Kolsky Bar is an experimental setup unique to NIST that allows the testing sample to be on very high heating rates, exceeding a temperature of 800 °C in as fast as milliseconds. These test conditions approach to those in high speed machining process. These measurements play an important role for the improvement of manufacturing methods. The sample is heated by controlling an electrical current through the sample, and the temperature is monitored using a pyrometer. Proper execution of a test requires precise control of the heating process and an appropriate signal to trigger the beginning of the sample deformation.

NIST's Science Based Manufacturing Group has the need for an updated program to control the heating of the Pulse-Heated Kolsky Bar. The task of the project is to implement an improved control algorithm in Microsoft's Visual Basic 6.0 and National Instrument's Measurement Studio that monitors the temperature of the sample, controls that temperature by adjusting the current, and outputs a trigger signal when the sample's temperature reaches the desired level. The results of the tests of this system can yield valuable insights that may lead to improve cutting processes of materials, or better blast resistant structures that can significantly reduce development cost.

The Study of Person Matching Algorithms for Healthcare
José Osorio

Considering that healthcare records for a patient can be distributed across various setting such as doctor offices and hospitals which maybe in different states, we want to extend our testing to consider how a PIX/PDQ implementation handles person matching algorithms. When searching for a specific individual record, what level of confidence exists that the patient identifier truly matches the individual of interest. My research will help to determinate how to measure the actual performance of a specific patient matching algorithm. To accomplish this, I am working with an existing implementation. The goal will be to isolate the code that implements the matching algorithms and improve it to resolve the problem stipulated before.

Building the Graphic User Interface for the "Model-Based Testing Project"
Angel Rosado Rosado

Theorem Proving is the most well-developed subfield of automated reasoning (AR). The study in AR helps produce software that allows computers to reason completely, or nearly completely, automatically. The Model-Based Testing Project creates a Reasoner and uses its power for reasoning with complex ontologies. My job this summer was to create a Graphical User Interface for the Theorem Prover for demos and debugging using Netbeans Platform Project with Maven Plugins as the base.

I developed the second version of the Graphic User Interface (GUI) for an automatic deduction system called PrIKL. Also, I created a parser that allows the conversion of files from existing test cases to be able to use them with the Prover.

In the presentation I will give a quick brief of what is a Theorem Prover and how it can be used. Also, I will be talking about the power of the Netbeans Platform, explain how I learned to use the Model-View-Controller (MVC) and work with modules and how I applied that in my GUI.

University of Texas Dallas

Effects of Dental Monomers and Initiators on Metabolic Activity and Biomass of Oral Biofilms

Courtney Keeler

Polymeric dental materials are increasingly being used to treat tooth decay, which the Center for Disease Control reports affects over 40% of children (ages 5 to 17) and most adults. However, most polymeric composites must ultimately be replaced due to secondary caries (recurrent decay). One factor contributing to secondary caries is bacterial biofilms such as *Streptococcus mutans*, a commonly studied oral bacterium that contributes significantly to tooth decay. Recent studies at NIST have shown that these biofilms are affected by chemicals that leach out of polymeric materials over time in the mouth. These leachables are known to include unincorporated monomers and initiators, but the specific components and resulting effects are not known. The objective of this study was to quantify the effects of individual monomers and initiators on biofilm metabolic activity and biomass.

Concentrated solutions of triethyleneglycol dimethacrylate (TEGDMA), camphorquinone (CQ), ethyl 4-N,N-dimethylaminobenzoate (4E), and bisphenol A glycerolate dimethacrylate (BisGMA) were prepared. *S. mutans* biofilms were grown for 4 h or 24 h in the presence of a dilution series of each chemical. The 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) and crystal violet (CV) assays were used to quantify biofilm metabolic activity and overall biomass, respectively. The final pH of the growth medium was measured to characterize changes in acid production of the biofilms.

Results from the MTT assay, CV assay, and pH measurements were interpreted together to allow for a broad assessment of intact *S. mutans* biofilms over time. TEGDMA, CQ, and BisGMA altered biofilm growth at the highest concentrations tested. Additional experiments are needed to determine if the changes in metabolic activity are indicative of cell death or altered biofilm growth rates.

In conclusion, several monomers and initiators used to prepare dental polymers affect oral biofilm growth. These chemicals are known to leach from polymeric composites and thus may affect biofilm growth and potentially the development of secondary caries *in vivo*. By measuring the effects of individual components on *S. mutans* biofilms, the bioactive chemicals can be identified and the development of novel polymeric dental materials to control biofilm growth can be improved.

University of the Sciences Philadelphia

Modeling of the Transparency and Conductivity of Carbon Nanotube Networks

Amanda Huon

Carbon Nanotubes (CNTs) are electrically conductive nanomaterials with a diameter of about 1 nm and a length of several micrometers. Therefore, CNTs can conduct electricity over long distances, while being virtually invisible at optical wavelengths in the range of 400 nm to 800 nm. Networks of interconnected tubes can be arranged into conducting films with a high transparency that is unobtainable by any other conventional conductors such as indium-tin-oxide or thin metal films. Understanding the fundamental relation that governs transparency and conductivity of such networks is of primary importance from both scientific and practical view points. Throughout recent literature, the transparency equation [1] describing the electromagnetic properties of thin continuous metallic films has been applied with various modifications to CNT films.

We have simulated these semi-empirical equations and found that they fail to describe the experimental transparency and conductivity of CNT films, particularly near the percolation transition, where the films are most transparent [2]. Our goal is to discover a correlation between the optical and electrical properties of the CNT thin films within the framework of the percolation theory that better quantifies these properties in the broad range of conductivity and transparency. We will justify our model with measurements of the conductivity and transparency of CNT films across the concentration range of the percolation transition.

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University of Virginia

Characterization of Magnetic Nanoparticles for Biomedical Applications

Eric Olson

A number of applications within the biomedical field have been developed recently with critical roles for magnetic nanoparticles, including magnetic resonance imaging, hyperthermia, and magnetic particle imaging (MPI). Understanding the physical and magnetic characteristics of these nanoparticles, as well as how the particles interact with each other, is essential in determining their directed use and efficacy in hyperthermia applications and MPI. Examples of these properties include the saturation magnetization (maximum magnetization) and the effective anisotropy (K_{eff}), which impacts the response of the nanoparticle to a changing magnetic field. In this system iron oxide nanoparticles are used, with a crystallite size of approx. 7.5nm (as determined by x-ray diffraction) and are dispersed in H_2O. The nanoparticles were characterized at 300K in the range of +/- 7 T and at sample dilutions of 1:1, 1:10, 1:100, 1:1000, and 1:10,000 to determine magnetic properties. The corresponding magnetic moment per particle and number of particles per volume were estimated using the Langevin Paramagnetism model, and deviations from the model were determined. The moment per particle was relatively constant ($5.9*10^{-20}$ J/T) within a sample as a function of dilution, except for the lower limit of 1:10,000 ($3.71*10^{-20}$ J/T). The deviations from the model were most prominent at 1:1 concentrations, but had disappeared by 1:10,000 dilutions. From this we can estimate the anisotropy field ($\mu_0 H_A$) to have a maximum of 0.15 T. Thus, at 1:1 dilution, the K_{eff} was $3.16*10^{-5}$ J/g; at 1:100, $K_{eff} = 3.29*10^{-7}$ J/g; and at 1:10,000, K_{eff} was (within the error of the measurement) 0 J/g. This decrease in K_{eff} over dilutions directly correlates with a decrease in the interactions between nanoparticles; resulting in effective superparamagnetic behavior in

the dilute limit of 1:10,000. This information will be correlated with measurements under an alternating magnetic field to determine parameter regions of interest for biomedical applications.

Virginia Polytechnic Institute and State University

Automation of the Microscope
Mikala Michalski

High content screening is very important for cell study. In order to understand protein expression in cells and how it affects their morphology and behavior, a lot of biologically relevant data needs to be acquired and analyzed. Currently, in order to acquire cell images it is required to capture them manually from a sample using a microscope. Once acquired, all images are then sent into a separate program in order for the analysis to take place. This process is proven to be time consuming and requires a great deal of effort. One major advancement in this area of study is the automation of microscopes to establish communication between microscopes and image analysis software. Once automated, the transitional step between acquiring and analyzing images is eliminated.

Creating communication between the microscope and image analysis software allows us to capture images while simultaneously performing all the required calculations for the analysis of the cells. The biggest challenge to this connection is the creation of a feedback loop from image analysis to the microscope. This missing link is important to enable information obtained during analysis to be sent back to the microscope as commands for further acquisition. The most beneficial data sent through this feedback loop are the coordinates of the centroids of each cell. With this information, the microscope is able to use these data values as the center for its field of view. This ensures that the center of the cell is in view when the user revisits a cell of particular interest.

The current study to achieve automation is performed on a plate with dead cells that are fixed and stained for sub-cellular analysis. The future objective is to eventually establish a much higher degree of communication to allow real-time cell tracking and analysis for important biological event detection.

Structure and Dynamics of Peripheral Membrane Proteins
Arielle Strong

Biological membranes are vital structures that ensure the survival of a cell. Membranes are supplemented by many proteins that bind or insert into the lipid bilayer in order to carry out their function. We focused on two membrane protein systems i) regulation of mitochondrial function by tubulin through binding and modification of the membrane environment and ii) molecular simulations of the HIV-1 matrix (MA) protein which plays a role in viral assembly. To understand these complex biological phenomena and the forces that govern protein binding to biological membranes, both computational and experimental techniques are required.

Experimental protein binding involved depositing a solution of diphytanoyl-glycero-phosphocholine (DPhyPC) lipid onto a gold surface covered in a tethering compound. After the membrane had formed, tubulin was introduced to the lipid bilayer. Binding to the membrane was measured using surface plasmon resonance (SPR). The initial experiments suggest that when adding tubulin there is a slow increase in surface binding that stabilizes over time. However the resulting data was affected by many different variables including membrane integrity, tethering molecule density and protein oligomerization. After controlling for other factors we found that the inability to inhibit tubulin's native tendency to polymerize during our experiment was the greatest source of variability.

The HIV-1 MA protein is the primary membrane-targeting domain of the viral assembly protein Gag. MA uses multiple biochemical interactions to regulate lipid association. Previous experimental investigations suggested electrostatic interactions with charged membranes influence the binding orientation of the protein on the membrane surface. A comparison of a neutral POPC and charged POPC:POPS molecular dynamics simulation showed markedly different motions of the protein on the lipid bilayer. We further looked at the re-organization of the charged lipid species in the context of the protein-membrane binding interface. Simulations provided insights into molecular mechanisms of protein interaction unattainable by experimental techniques.

Washington University St. Louis

Standardizing Building Codes for Unpredictable Winds
Cyril Draffin

When constructing a building in the US, the design team needs to make sure the newly constructed building will be able to last, even in adverse conditions. There are a variety of potentially hazardous conditions that the building needs to withstand, including floods, snow, and earthquakes, most of which are well documented. Wind is another story. Standardized wind conditions are hard to gather as there are a number of different kinds of storms which cause different wind patterns. On top of normal storms there are also hurricanes and tornadoes which are often unpredictable and localized, so the chance that a tornado will pass directly over a weather station is slim. Nevertheless there needs to be building codes which describe how much wind or pressure a building must be able to withstand.

The American Society of Civil Engineers (ASCE), among other bodies, writes these building codes; however the codes often do not fully describe wind conditions. Here at NIST we are trying to come up with better ways of gathering this wind data and analyzing it so that ASCE can improve the precision and quality of their building codes. Before the data can be analyzed, it needs to be collected, sorted and standardized. In the US there is in fact a standardized anemometer, and standardized measurement procedure. However, as many airports and other weather stations, have not always used the same standardization technique, all measurements must be adjusted accordingly. As mentioned earlier, the type of wind is also important, so using a combination of historical records we can often categorize winds as thunderstorm, tropical storm, or fair weather. Once years of data from different sources are brought together and standardized we can start to make statistically significant conclusions about what wind speeds, and what kinds of storms can be expected all around the US. All of this data will then lead to more precise and accurate building codes, which can help ensure buildings are constructed safely, and without unnecessary costs.

Weber State University

Investigation of Turmeric by Liquid Chromatography
Caleb Porter

Turmeric is a perennial plant which is primarily grown in Southeast Asia. The rhizome of the plant is harvested and used as a textile dye, a natural food coloring, a spice, and as a traditional medicine/dietary supplement. A number of positive health benefits have been attributed to turmeric, including use as an anti-inflammatory, to counteract Alzheimer's disease, and as an antiseptic agent. The compounds unique to turmeric that may be responsible for these health benefits are curcuminoids, which are yellow in acidic solution and orange in basic solution. Because turmeric is a highly valued commodity, products have been found to be economically adulterated with compounds such as Sudan dyes, which are added to enhance the color and value of the crop. The focus of this work was to develop methods to evaluate turmeric products based on their curcuminoid content as well as to screen products for economic

adulteration.

In this study, one liquid chromatography (LC) method was developed to detect economic adulterants in commercial turmeric products. A second LC method was optimized for measurement of curcuminoids. LC method development explored various stationary phases, mobile phase compositions, and isocratic versus gradient elution techniques. The extraction of curcuminoids from turmeric powders was optimized through the investigation of numerous solvents, temperatures, and extraction techniques. Using the optimum extraction approach and LC method, a number of commercial products were screened for Sudan dyes and evaluated for their curcuminoid content. In the future, these methods will be used for the certification of a suite of turmeric-containing Standard Reference Materials (SRMs), enabling independent laboratories to evaluate the quality of turmeric samples.

Radiative Absorption and Freezing Characteristics of Black Carbon Immersed in Aqueous Aerosols
Nicholas Smith

Black carbon (formed from combustion processes) constitutes the main absorbing aerosol particle in the atmosphere. Sulfate aerosols (originating, for example, from ocean spray, volcanic emissions, and the decomposition of organic matter on land and in water) coat atmospheric black carbon and change its ice nucleating effectiveness, as well as influence its optical properties. Because of the large uncertainty in the optical properties of atmospheric aerosols in general, detailed measurements of absorption for these aerosols can provide useful property data for input into global climate change models. Furthermore, recent studies in the literature have focused on better understanding the freezing parameters of ice nuclei with representative coatings. However, these studies have mostly used cloud chambers that confine an ensemble of ice crystals with a large distribution of sizes and compositions. In this investigation, an experimental apparatus has been designed and fabricated to study the absorption and freezing parameters of individual droplets consisting of black carbon ice nuclei internally mixed in an aqueous solution of either sulfuric acid or ammonium sulfate. The apparatus is engineered to enclose an ultrasonic acoustic levitator directly inside a copper cylindrical chamber. Ambient conditions can be controlled in this chamber, such as temperature, humidity, and pressure. Temperatures between -40 ^{o}C and -80 ^{o}C (well below that of homogeneous freezing of water droplets) can be achieved within the chamber, and a protocol was formulated to control and determine the humidity. The chamber has been sealed and tested to a pressure less than 100 Torr (lower than that of the upper troposphere) with a levitated particle remaining in place. A mist of droplets is introduced into the chamber using a vibrating syringe, where one or more of these droplets can be captured for further analyses. An existing laser-heating technique [Nazarian, A. and Presser, C. 2008] is to be modified to measure the absorption of the levitated ice crystals.

Nazarian, A., and Presser, C. (2008). Thermal and chemical kinetic characterization of multiphase and multicomponent substances by laser heating. International Journal of Heat and Mass Transfer, 51(5-6):1365-1378.

Western Kentucky University

A Pallet Planner
Derrick Johnson

The Distributer's Three-Dimensional Pallet-Packing Problem may be stated as follows: Given a fixed rectangular area, and fixed maximum stacking height, "What is the optimal method of stacking N boxes within the rectangle, in order to guarantee maximum volume utilization?" Exact solutions to this NP-Hard

problem are prohibitively expensive in terms of computational resources. Thus, approximate solutions have applications in industry.

The goal of this SURF project was to take an existing algorithm written by Erhan Baltacioglu, and make it more practical for the purposes of a broader NIST project (PerfSim). Towards this end, the following considerations may be made: restrictions on box orientations, maximum weight on top of boxes, and keeping "families" of boxes together on the same pallet.

This SURF project accomplished several such goals. The input and output formats were parsed into XML data files, based on templates called "XML Schema". Having these universal templates facilitates automation of the pallet-planning process. Next, several transformations performed by the algorithm were reversed, so that the original pallet layout is preserved. The third completed task of this SURF project was incorporating Stock-Keeping Unit (SKU) identifiers into the process. This allows the distributer to ensure against discrepancies between what is ordered, and what is shipped.

Western New England College

X-Ray Photoelectron Spectroscopy Used to Map Compositional Variations In Combinatorial Thin Film Libraries
Julie Jackson

X-ray photoelectron spectroscopy (XPS) is a materials surface analysis technique. Its importance in materials science lies in the fact that all solid materials interact with their surroundings through their surfaces. The physical and chemical composition of these surfaces determines the nature of these interactions. The surface chemistry of a material is of particular importance because it affects corrosion rates, catalytic activity, adhesive properties, wettability, contact potential, and failure mechanisms of a material. XPS has the ability to provide both quantitative elemental and chemical state information for the great majority of elements on the periodic table, on virtually any vacuum compatible surface.

XPS works by exciting the surface of the material with X-rays or UV radiation, causing core level photoelectrons to be ejected from the surface of the material. The ejected photoelectrons are then analyzed by an electron spectrometer and the data is presented as a plot of intensity verses electron energy. This data can then be used to identify elements and their bonding environment. XPS can be used to characterize a variety of organic and inorganic materials.

The objective of this project was to assemble and calibrate the Kratos X-ray photoelectron spectrometer, and then utilize it to map compositional variations on combinatorial thin film libraries. The XPS was used to take spectra at many (x, y) points on a Bi_2Te_3 - Sb_2Te_3 combinatorial thin film library, to interrogate the compositional variation by measuring the relative areas under the emitted photoelectron peaks that are representative of each element present. The results and findings of this series of experiments will be reported in detail in my presentation.

Whitman College

The Effects of Helium Upscattering on the Neutron Lifetime
Nathan Abrams

A free neutron is known to decay into a proton, electron, and an electron antineutrino. The current accepted lifetime for the unstable neutron is 881.5 ± 1.5 s. However, the two most recent ultracold neutron bottle experiments produced neutron lifetimes varying by 6.5 standard deviations, indicating unknown systematics with measurements. Accurately knowing the neutron lifetime affects both the

Standard Model of particle physics and our understanding of the Big Bang. The experimental setup is centered upon a quadrupole and two solenoids which form a magnetic trap that contain ultracold neutrons via their magnetic moment. The trap contains ultrapure helium-4 at temperatures around 250 mK. When a neutron beta decays, the electron travels through the liquid helium, ionizing and exciting the helium into meta-stable He_2 states. As the helium returns to the ground state, extreme ultraviolet photons are emitted. After converting the extreme ultraviolet photons to blue photons, the photons are transported to two photomultiplier tubes which detect the decay events. The decay events map out an exponential decay whose lifetime is the mean neutron lifetime. Given that the purpose of this experiment is to accurately determine the value of a lifetime that already has debate over its value, identifying and quantifying the numerous systematic effects becomes essential. Several such effects include helium purity, cosmic muon background events, marginally trapped neutrons, majorana transitions, and helium upscattering. Helium upscattering occurs when energy from helium is transferred to the neutron through the absorption of a phonon, which gives the neutron enough energy to escape the magnetic trap. This early exit gives the appearance of a more rapid decay, resulting in a lower neutron lifetime. The upscattering has a temperature dependence that goes as T^7. The specific goal of my project is to determine the systematic effect of the helium upscattering on the neutron lifetime. The presentation will explain why the neutron lifetime matters, outline how the experiment works, address helium upscattering and other systematic effects, and describe the process of determining the value of the systematic effect for helium upscattering.

Williams College

Setting Up a Four-Wave Mixing Experiment in Cesium
David Kealhofer

Four-wave mixing in a rubidium vapor has previously been studied at NIST. Christina Knapp and I assembled a four-wave mixing experiment for use with a cesium vapor cell. The process has four steps: 1) the atoms in the vapor are excited by a strong 'pump' beam, 2) a weak 'probe' beam returns the atoms to a lower energy, 3) the atoms are excited again by the pump and 4) the atom returns to the ground state, emitting a photon at the 'conjugate' frequency. The production of the four waves in question--two pump beams, a weak probe beam and its conjugate--requires two lasers. One serves as the two pump beams, another serves as the probe, and the process produces the conjugate. We performed the experiment with two frequency-locked grating-tuned diode lasers. The two lasers' frequencies are slightly detuned from two hyperfine components of the D1 894 nm transition in cesium, and it is necessary to be able to fine-tune the frequency of the lasers on the GHz scale, both to find the appropriate transitions and to combat drifting in the cavity length due to temperature changes and mechanical instability. The power of these lasers (on the order of 100 mW) is sufficient to produce the probe beam, but insufficient to produce the pump. To increase the power at one of the two frequencies, we constructed a tapered amplifier (TA), which can amplify 10-30 mW of optical power to around 1.5 W. We will present various data characterizing the behavior of the TA and gain in the four-wave mixing process.

Optical Squeezing and Laser Locking
Christina Knapp

In quantum mechanics there exist restrictions on the minimum uncertainty of pairs of variables. Just as the Heisenberg uncertainty principle relates the precision to which we can know the momentum and position of a particle there exists a similar relation in optics between the amplitude and phase of a light beam. A squeezed state refers to a state of a particle or wave in which the uncertainty of one variable is decreased in exchange for an increase in the uncertainty of another. In optical squeezing we observe a decrease in the noise level of the light intensity and an increase in the noise level of the phase or vice versa. This ability to manipulate the noise properties presents exciting opportunities for greater precision measurements.

Previous experiments at NIST have demonstrated optical squeezing through four-wave mixing in Rubidium vapor. Our project hopes to demonstrate squeezing in a similar manner with Cesium vapor. This requires two beams of light tuned to the D1 line of Cs (894 nm), but separated by the 9.2 GHz hyperfine splitting of Cs with a few MHz uncertainty. We generate the light beams with grating tuned diode lasers and employ two separate locking circuits to keep the lasers from drifting off the atomic transitions.

We use a microwave interferometer lock to maintain a constant frequency separation between the two lasers. To do this we send both beams of light into a high frequency photodiode which detects the 9 GHz beat frequency. The photodiode feeds a signal into a microwave interferometer, which then sends an electronic signal into a Proportional-Integral-Differential (PID) control. If the beat-note begins to drift, the PID control feeds a signal into one of the lasers to tune the beat-note back to 9 GHz.

We also employ a Dichroic-Atomic-Vapor Laser Lock (DAVLL) to keep one laser's frequency stable relative to a component of the D1 line. The DAVLL relies on the frequency dependent rotation of polarization that results when a laser beam goes through a Cs vapor cell placed in a magnetic field.

Worcester Polytechnic Institute

Evaluation of the Consolidated Model of Fire Growth and Smoke Transport (CFAST)

Andrew Nelson

Computational models of fire growth allow predictions to be made for the design of structures and understanding the effects of fire on these structures. Understanding these effects allows for better safety planning in order to reduce and prevent the loss of property and life. Evaluation of these models is necessary to determine their usefulness and accuracy and is accomplished through verification and validation. Verification is the process of comparing the model to theoretical predictions, while validation is the process of comparing the model to real fires and experiments. Various input parameters were altered, while keeping other input parameters constant, to observe the impact that a change in each parameter has on the model output. These model outputs were compared to the theoretical formula for hot gas layer temperature developed by McCaffrey, Quintiere, and Harkleroad. One parameter that has a particularly strong influence on this formula is the thermal conductivity of the structure materials. Computational models were also created to represent real fire experiments, and these results were compared to the data collected during the experiments.

2011

SURF STUDENTS

BY UNIVERSITY

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UNIVERSITY	STUDENT	TITLE OF TALK	OU
Agnes Scott College	Franzel, Christine	The Effect of Tethering on the Glass Transition Temperature in Thin Polymer Films	MML/NCNR Matls Science
Appalachian State University	Villanova, John	Surface Topography Analyses for Images of Firing Pin Impressions Acquired via Confocal Microscopy	PML
Arizona State University	Alena Matusevich	Organic Photovoltaic Devices: Band Gap Engineering	PML (ARRA)
Arizona State University	Bowman, William	Ionic Conductivity in Gadolinium and Praseodymium Doped and Co-Doped Cerias for Solid Oxide Fuel Cell Electrolytes	CNST (ARRA)
Arizona State University	Patel, Varun	Oxidatively Induced DNA Damage Analysis of Shrimp Exposed to Conditions Resembling Those of the Deepwater Horizon Oil Spill	MML/NCNR Chemistry (ARRA)
Brigham Young University	Gurney, Lisa	Mitigation of Set Time Delays in High-Volume Fly Ash Cement Pastes Through Fine Limestone Additions	EL (ARRA)
Carnegie Mellon University	Baldwin, Christopher	Tight-Binding Analysis of Twisted Graphene Bilayers	CNST
Carnegie Mellon University	Swisher, Matthew	Interferometer for the Measurement of a MEMS Device in a SEM	CNST
Carnegie Mellon University	Zakrzewski, Brian	Photoinduced Magnetizaiton in Prussian Blue Analogue Tri-Layer Films	MML/NCNR Matls Science (ARRA)
City College of New York	Afzal, Annas	Characterization of the Effect of Thermal Cycling on the Signal Integrity of Interconnect Structures Used in 3D Integrated Circuits	PML (ARRA)
City College of New York	Fon, Kaly	Massive Parallel Long-Term Reliability	PML
City College of New York	Markland, Errol	Web Application Development on Computer Security Metadata	ITL
College of William and Mary	Lowery, Ethan	Constructing a Crygenic Dipper for Tunneling Magnetoresistance Measurements of Cross-Wired Devices	PML
College of William and Mary	Zora, Kyle	Probing the Validity of Theoretical Models for Predicting Vibrational Spectra of Alanine and Its Polypeptides	PML
Colorado School of Mines	Johnson, Joshua	Reactor Software Upgrades and Analysis of Test Stand Behavior	MML/NCNR Matls Science
Colorado School of Mines	Robbins, Bryce	Persistent Currents in a Rotating Toroidal BEC	PML
Colorado School of Mines	Stortz, Tristan	Optical Femtocalorimeter	MML/NCNR Matls Science (ARRA)
Colorado School of Mines	Thurston, Bryce	Frequency Conversion through Four-Wave Mixing Bragg Scattering	CNST (ARRA)
Colorado School of Mines	Villars, Brenden	Spatial Uniformity of a Three-Element Optical Trap Detector	PML
Columbia University	Orthwein, Jonathan	Chipped-Pule Terahertz Spectroscopy	PML

UNIVERSITY	STUDENT	TITLE OF TALK	OU
		for Broadband Trace Gas Sensing	
Converse College	Casil, Julianne	pH Dependent Kinetics of Ion Channel Formation of *Bacillus Anthracis* Protective Antigen 63 (PA63)	PML (ARRA)
Cornell University	Choi, Christopher	Layer by Layer Self Assembly on Soft Foams: Reduced Foam Flammability Using Nanoparticle Filled Coatings	EL (ARRA)
Cornell University	Lu, Daniel	FHS-LAB: A GUI for Simulating Structural Behavior Subjected to Fire	EL
Cornell University	Ma, Jun	Electron Spin Resonance	PML (ARRA)
Davidson College	Pagnonis, Demetrios	Dealloyed $Pt_{100-x-y}Co_xNi_y$ Catalysts for Oxygen Reduction Reaction	MML/NCNR Matls Science
DePauw University	Baker, Catherine	Circuit Synthesis for Cryptographic Applications	ITL (ARRA)
Duke University	Rohlfing, Anne	Shelf Life Study of Silver Nanoparticles	MML/NCNR Chemistry
Eastern Kentucky University	Hegwood, Jerrod	Verification and Modeling of Results from Nuclear Power Plant Control Room Fire Tests	EL
Eastern Kentucky University	Lenhof, Timothy	Modeling Smoke in Room-Scale Fires	EL
Fayetteville State University	Gunn, Reid	Microscopic Analysis of Synthesized Mixed-Phase Atmospheric Particles	MML/NCNR Chemistry (ARRA)
George Washington University	Bagchi, Shelly	Transformative Applications: Using Android-Powered Smartphones to Enhance Soldier Operations	EL
George Washington University	Cano, Michelle	Software Improvement of Visualization Tools for Video Analytic Evaluations	ITL
George Washington University	Cunningham, Hailey	Hemoglobin Saturation as Expressed by its Absorbance Curve	PML
Georgia Southern University	Benton, Brandon	Prototyping Method for Bragg-Type Atom Interferometers	PML
Hamilton College	Adelman, J. Elliott	Analysis of aCORN Data	PML
Harvard College	Boling, Robert	Determining Switching Mechanisms and Switching Field Distributions in Bit-Patterned Media	MML/NCNR Matls Science (ARRA)
Harvey Mudd College	Brent, Taylor	USARSim: A High-Fidelity Simulation of Robotics	EL
Harvey Mudd College	Sio, Hong	Band Alignment Study Using Internal Photoemission: Applications to Metal-Gate / High-k Dielectric / Semiconductor Interfaces	PML (ARRA)
Hood College	Haines, Andrea	Improving Electronic Health Record (HER) Usability, Research, and the Communication Effort	ITL
Hood College	Hill, Jennifer	Creation of an Evaluation Interface for Human Assessments of Machine Translations	ITL
Hood College	Jacobson, Nathan	Access Control Policy Tool (ACPT)	ITL (ARRA)
Jackson State University	Shelton, Melanie	Measuring the Efficacy of Ligand	MML/NCNR

UNIVERSITY	STUDENT	TITLE OF TALK	OU
		Displacement on Gold Nanoparticles – Applications in Nanomedicine	Matls Science (ARRA)
James Madison University	Crawshaw, Fay	Tether Lipid Molecules for High Precision Metrology of Integral Proteins	MML/NCNR Matls Science
James Madison University	Vess, Eric	Novel Methods for Remote Sensing Based on DIAL	PML
Johns Hopkins University	Joress, Howard	A Statistical Approach to EDS Peak Identification: A Proof of Concept	MML/NCNR Chemistry
Juniata College	Ginley, Theresa	Optimizing the Sputtering Parameters for Permalloy Thin Films to Minimize Surface Roughness	MML/NCNR Matls Science
Le Moyne College	Acquaviva, Andrew	Gathering Benchmark Data for the Examples of FiPy	MML/NCNR Matls Science
Lebanon Valley College	Younker, Ian	Analysis and Model of Multi-Sensor-Fusion Data	EL
Lehigh University	Marvel, Christopher	Characterization of Carbon Nanotubes in Composite Baseball Bats	MML/NCNR Chemistry
Loyola University of Maryland	Slusarski, Kyle	Roles of Atomic Force Microscopy and Nanoidentation in Building Metrological Foundations for Nanomechanical Property Testing	MML/NCNR Matls Science
Miami University of Ohio	Denton, Alexis	Imitating Ocean Reflectance Measurements with Diffuse Reflectance Standards	PML
Miami University of Ohio	Gooley, Derek	A Charge-Based Capacitance Measurement Implementation on Printed Circuit Board	PML (ARRA)
Miami University of Ohio	Hachtel, Andrew	Fabrication and Characterization of a Nanoaperture Array by Helium Ion Microscope	PML
Miami University of Ohio	Kleykamp, Jeffrey	Simulation of Scanning Electron Microscope to Better Understand Errors in Cross-Correlation Image Correction Technique	PML
Miami University of Ohio	McNally, Douglas	Motion Characterization and Endurance Metrology Microrobots	PML (ARRA)
Middlebury College	Allen, Joseph	Nanoscale Electrochromic Patterning with a Lithium Focused Ion Beam	CNST
Montana State University	Weber, Katelyn	Software Development for Probabilistic Modeling and Uncertainty Quantification	EL (ARRA)
Montgomery College	Russell, Sarah	Creating Stable Dispersions of Titanium Dioxide Nanoparticles in Environmental Matrices	MML/NCNR Matls Science
Mount Saint Mary's University	Halter, Melissa	Calibration of NIST VaporJet and Preliminary Evaluation of Explosive Trace Detectors	MML/NCNR Chemistry
Muhlenberg College	Fitzsimons, Matthew	Characterizing the Morphology of the Bulk-Heterojunction of Organic Photovoltaics	MML/NCNR Chemistry
North Carolina State University	Hewitt, Andrew	Slow Crack Growth Resistance at the Micron Scale in High Density Polyethylene	EL
North Carolina State	Jones, Nathan	Optimization of Cell Growth in Minimal	MML/NCNR

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University		Media	Matls Science (ARRA)
Pennsylvania State University	Rubeo, Mark	Quest for Precision: The Performance Evaluation and Compensation of a Meso-Scale Machining Center	EL
Pennsylvania State University	Sunkara, Sai	Tissue Engineering Reference Scaffolds to Enable Inter-Lab Comparison of Cell Culture Measurements	MML/NCNR Matls Science
Princeton University	Tang, Sarah	An Evaluation of Local Shape Descriptors for 3D Shape Retrieval	ITL
Princeton University	Tracer, Andrew	Dataflow: A Web-Based Solution to Data Reduction	MML/NCNR Matls Science
Rensselaer Polytechnic Institute	Coplin, Halley	Direct Browser Integration of 3D Graphics with X3D and X3DOM	ITL
Rensselaer Polytechnic Institute	Willette, Peter	Residential Appliance Energy Research: Clothing Washers	EL
Rochester Institute of Technology	Jacob, Colin	Understanding and Optimizing the Epitaxial Growth of Graphene on Silicon Carbide	PML
Saginaw Valley State University	Lucio, Anthony	Shape Evolution of Polymer Structures with Thin Residual Layers Prepared by Nanoimprint Lithography	PML
Saint Mary's College of Maryland	Carneiro, Lucas	Effects of Film Processing Parameters on Organic Photovoltaic Device Performance	MML/NCNR Matls Science
Saint Olaf College	Barkley, Sarice	Lateral Force Calibration Methods for Atomic Force Microscope	CNST
Smith College	Aloisio, Kathryn	Atmospheric Abundances of Greenhouse Gases from Prehistoric to Current Times	ITL (ARRA)
St. Mary's College of Maryland	Herpel, Gregory	Analysis of a High Performance Flow of Suspensions	ITL
State University of New York Albany	Lovell, Magdalen	Improvements in Ultrasonic Calorimetry for Dosimetry	PML
State University of New York Binghamton	Carson, Michael	Scanning Kelvin Force Microscope Based on a Tuning Fork	PML
State University of New York Binghamton	Presser, Brian	Energy Consumption and Lifecycle Cost of Buildings in the United States	EL
State University of New York Binghamton	Zheng, Walter	Electrical Characterization of Flexible Solution-Processed Oxide Memristors	PML (ARRA)
Towson University	Siregar, Alexander	Constructing a Magnetic Field Probe for Use Regarding the NIST-4 Watt Balance	PML (ARRA)
Towson University	Tyler, Joshua	LabVIEW Integration in a Mass Calibration Process	PML
Tulane University	Ortmann, Elliott	The Metrology of Shaping and Detecting X-Rays	MML/NCNR Matls Science (ARRA)
University of California Los Angeles	Lopez, Jessica	Development of Sustainabiity Measurement Tools and Methods for Manufacturing Enterprises	EL
University of Colorado Boulder	Zirkelbach, Stetson	The Effects of Scaling and Scanning Order on Image Signatures Based on Space-Filling Curves	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Delaware	Bibb, Caroline	Standard for Lead and Cadmium Content in Polyvinyl Chloride	MML/NCNR Chemistry
University of Delaware	D'Alessio, Anna	Research Contributions to Enhance the Sustainability Standards Portal	EL
University of Illinois	Ragunathan, Gautham	Laser Diode Interferometry	EL
University of Maryland Baltimore County	Harvey, David	The Role of Metrology in X-Ray Diffraction	MML/NCNR Matls Science
University of Maryland Baltimore County	Iglehart, Christopher	Residential Appliance Energy Research	EL
University of Maryland Baltimore County	Anzaldi, Laura	Developing a Root-Based Semantic Vocabulary	MML/NCNR Chemistry (ARRA)
University of Maryland Baltimore County	Bier, Naomi	Putting a *Spin* on Solid Sampling via Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)	MML/NCNR Chemistry
University of Maryland Baltimore County	Johnson, Lilian	Nanofluidics of Polymer Chains Under Confinement	MML/NCNR Matls Science
University of Maryland Baltimore County	Kelly, Mary	Interdiffusion Studies of Organic Solar Cell Components	MML/NCNR Chemistry
University of Maryland Baltimore County	Kumar, Neha	Fabrication of Controlled Diameters of Nanofiber Scaffolds and Study of Stem Cell Response	MML/NCNR Matls Science
University of Maryland Baltimore County	Litwak, Daniel	An Improved Ultrasonic Measurement of Radiation Dosage	PML
University of Maryland Baltimore County	Serova, Nadezhda	Glass Shard Dynamics in Fire Visualization Simulation	ITL
University of Maryland Baltimore County	Van Order, Michael	Verification and Validation of the Fire Dynamics Simulator	EL
University of Maryland College Park	Abraham, Reuben	Testing of Automated Impactor for In-Situ Monitoring of Machine Tool Dynamics	EL
University of Maryland College Park	Ashley, Catherine	Characterizing Dispersion and Degradation of Nanoparticle-Filled Polymer Coatings	EL
University of Maryland College Park	Au, Jennifer	Enzyme Digestion and Mass Spectral Characterization of Glycoproteins	MML/NCNR Chemistry
University of Maryland College Park	Bellistri, Matteo	String Searching on Container Files	ITL
University of Maryland College Park	Bhargava, Pavan	Nafion and Platinum Degradation Studies with Thin-Film Fuel Cell Models	MML/NCNR Matls Science
University of Maryland College Park	Drozdov, Serghei	Extraction of Series Resistance from Advanced CMOS Devices	PML
University of Maryland College Park	Ettehadieh, Daniel	Sustainability Performance Analysis of a Water Bottling Facility	EL
University of Maryland College Park	Galfond, Marissa	Reducing the Area of Magnetic Tunnel Junctions Using a Focused Ion Beam	PML
University of Maryland College Park	Golden, Alexander	Fast, Versatile Quenching in a Single Photon Avalanche Diodes for Quantum Key Distribution	PML
University of Maryland College Park	Ibrahim, Musa	Develop an Analytical Reverse Blocking Model for Si and SiC Diodes and	PML (ARRA)

UNIVERSITY	STUDENT	TITLE OF TALK	OU
		Incorporate the Model into the Diode Model Parameter Extraction Software using LabWindows/CVI	
University of Maryland College Park	Ji, Tommy	Solutions in Perception Challenge	EL
University of Maryland College Park	Jones, Benjamin	Structural and Electrical Characterization of Metal-Molecule-Silicon Junctions Produced by Flip Chip Lamination	PML
University of Maryland College Park	Li, Kun	Planar Arrays of Core/Shell Nanowires for Light Generation and Detection	MML/NCNR Chemistry
University of Maryland College Park	Liang, Li Peng	Safety of Humans Near Powered Industrial Vehicles	EL
University of Maryland College Park	Liao, Rachel	XMPP Services for Smart Transducers	EL
University of Maryland College Park	Lin, Janice	Stability of Terpene Gas Mixtures in Aluminum Cylinders	MML/NCNR Chemistry
University of Maryland College Park	McCarthy, James	Method Development for Characterizing TiO_2 Nanoparticle Surfaces by Mass Spectrometry	MML/NCNR Chemistry (ARRA)
University of Maryland College Park	Mifsud, Mark	Feature and Task-Based Evaluation of Robot-Generated Maps	EL
University of Maryland College Park	Myers, Taylor	Validation of the Fire Dynamics Simulator	EL
University of Maryland College Park	O'Connell, Brady	Cloud Interoperability: Migrate (Fully-Stopped) VMs from One Cloud-Provider to Another	ITL
University of Maryland College Park	Phuong, Lee	Long-Term Durability of Polymeric Materials for Photovoltaic Applications: Chemical and Physical Degradation of PMMA During UV Exposure	EL
University of Maryland College Park	Rahman, Aman	Diffusion Coefficient Calculation of Phospholipids on Membrane Bi-Layer Enclosing Protocells via Matlab	MML/NCNR Matls Science
University of Maryland College Park	Sandler, Carolyn	Human Response Processes for Emergency Communication	EL
University of Maryland College Park	Sze, Jeffrey	Integrated Factory Operation and Building Science Simulation	EL
University of Maryland College Park	Trettel, Andrew	Concrete Rheometer Automation	EL
University of Maryland College Park	Trettel, Benjamin	Firelab Development: A Sandbox for Improving the Fire Dynamics Simulator	EL
University of Maryland College Park	Villarrubia, Mark	Evaluating Searches Over Large Indices of Brief Documents	ITL
University of Maryland College Park	Weerakkody, Sean	Improving Velocity Measurement in NIST-3 Electronic Kilogram Apparatus	PML
University of Maryland College Park	Westbrook, David	Web-Based User Interface for Sustainability Modeling and Optimization	EL
University of Maryland College Park	Widstrom, Matthew	Stacked Electrode Back Contact Thin Film Heterojunction Solar Cells	MML/NCNR Matls Science
University of Maryland College Park	Wu, Jiemin	Fabrication and Characterization of Carbohydrate-Functionalized Surfactant Vesicles	MML/NCNR Chemistry (ARRA)

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Michigan	Gill, Navneet	Automation and Control of Variables in a Cryogenic Environment	MML/NCNR Matls Science
University of Michigan	Langhorst, Amy	Degradation of Polyesters Used in Blast Resistant Glasses and Protective Glazing Systems	EL
University of Michigan	Yuan, Lo-Hua	Fourier Methods to Describe the Shape of Biological Cells	ITL
University of New Hampshire	Nguyen, Khanh	Measuring Thermal Properties of Materials at High Heating Rates Using a Nanocalorimeter	MML/NCNR Matls Science
University of New Haven	Gorka, Danielle	Quantitative Measurement of Enzyme Activity Loss on Biofunctionalized Gold Nanoparticles	MML/NCNR Matls Science
University of New Haven	Reardon, Nicole	Formation and Characterization of Monolayer Nanoparticle Clusters	MML/NCNR Chemistry
University of Puerto Rico	Colon-Berrios, Aida	Precisely Measuring Currents on the Nano-Ampere to Femto-Ampere Range Using an Automated Current-to-Voltage Converter	PML
University of Puerto Rico	Ferra Otero, Eliezer	Credential Revocation Service	ITL (ARRA)
University of Puerto Rico	Marcano Estevez, Joseph	Develop an Additional Computer-Controlled Thermal Cycling Station in Order to Support Reliability Analysis for High-Power, High-Temperature, Power Semiconductor Devices and Modules	PML (ARRA)
University of Puerto Rico	Ortiz-Lozada, Alexander	Temperature Control System for Pulse-Heated Kolsky Bar	EL (ARRA)
University of Puerto Rico	Osorio, Jose	The Study of Person Matching Algorithms for Healthcare	ITL
University of Puerto Rico	Rosado Rosado, Angel	Building the Graphic User Interface for the "Model-Based Testing Project"	EL (ARRA)
University of Texas Dallas	Keeler, Courtney	Effects of Dental Monomers and Initiators on Metabolic Activity and Biomass of Oral Biofilms	MML/NCNR Matls Science (ARRA)
University of the Sciences	Huon, Amanda	Modeling of the Transparency and Conductivity of Carbon Nanotube Networks	MML/NCNR Matls Science
University of Virginia	Olson, Eric	Characterization of Magnetic Nanoparticles for Biomedical Applications	MML/NCNR Matls Science
Virginia Polytechnic Institute and State University	Michalski, Mikala	Automation of the Microscope	ITL
Virginia Polytechnic Institute and State University	Strong, Arielle	Structure and Dynamics of Peripheral Membrane Proteins	MML/NCNR Matls Science
Washington University St. Louis	Draffin III, Cyril	Standardizing Building Codes for Unpredictable Winds	EL
Weber State University	Porter, Caleb	Investigation of Turmeric by Liquid Chromatography	MML/NCNR Chemistry
Weber State University	Smith, Nicholas	Radiative Absorption and Freezing Characteristics of Black Carbon Immersed in Aqueous Aerosols	MML/NCNR Chemistry

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Western Kentucky University	Johnson, Derrick	A Pallet Planner	EL
Western New England College	Jackson, Julie	X-Ray Photoelectron Spectroscopy Used to Map Compositional Variations in Combinatorial Thin Film Libraries	MML/NCNR Matls Science
Whitman College	Abrams, Nathan	The Effects of Helium Upscattering on the Neutron Life	PML
Williams College	Kealhofer, David	Setting Up a Four-Wave Mixing Experiment in Cesium	PML
Williams College	Knapp, Christina	Optical Squeezing and Laser Locking	PML
Worcester Polytechnic Institute	Nelson, Andrew	Evaluation of the Consolidated Model of Fire Growth and Smoke Transport (CFAST)	EL (ARRA)

- THE END -

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