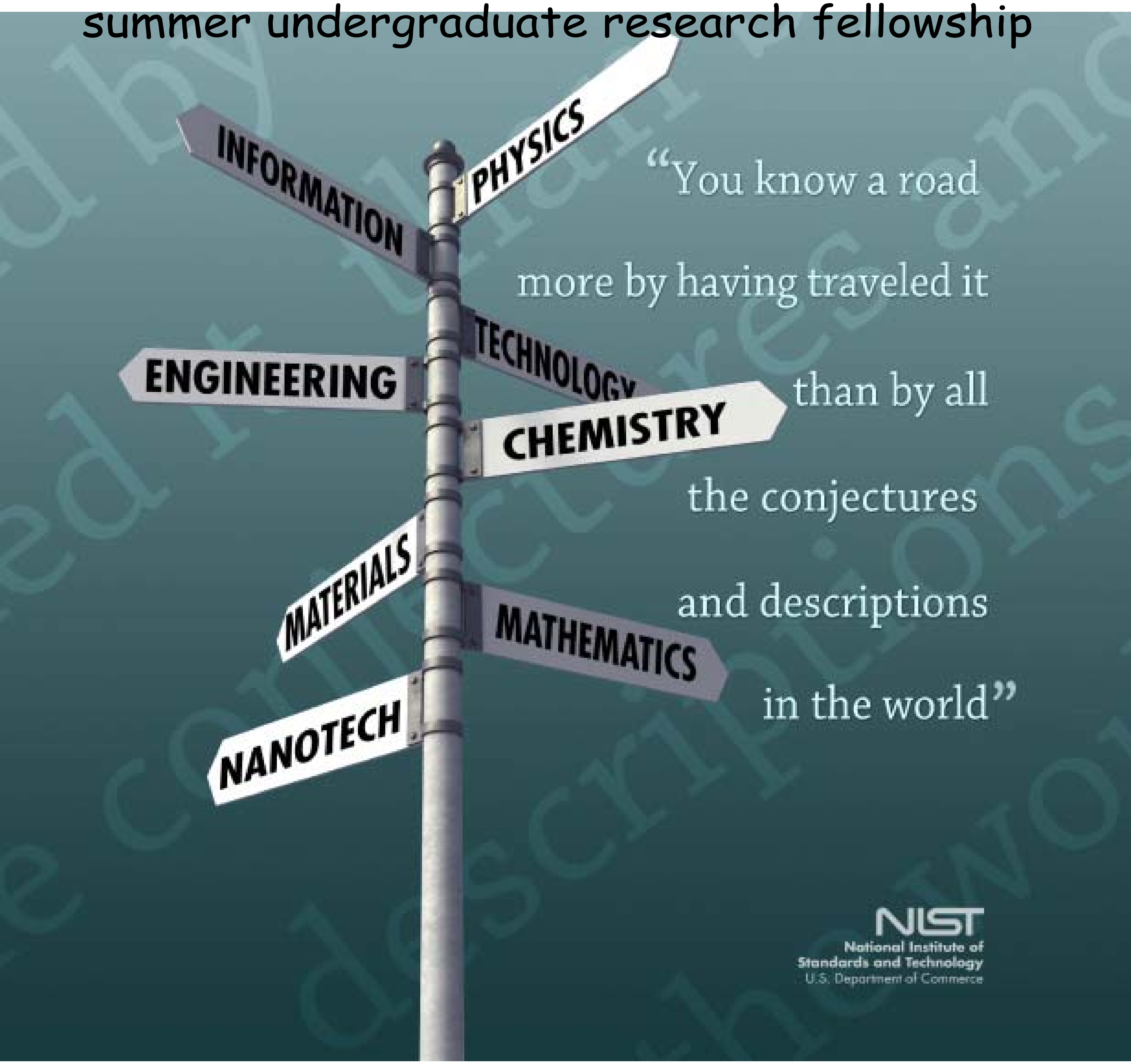
2010 SURF

summer undergraduate research fellowship



Program and Activities

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2010 SURF Summer Seminars and Tours

May 24 First official work day and orientation for SURF Session I students

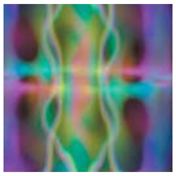
June 3 Dr. Marc Desrosiers
NIST Physics Laboratory, Ionizing Radiation Division

Radiation Accidents: How Bones and Teeth Are Used to Measure Human Exposures

Human skeletal tissues are composed of both organic and inorganic (mineral) portions. For bone and tooth tissue, ionizing radition (x-rays, gamma rays, high-energy particles) absorbed by the mineral component (hydrooxyapatite) results in a chemical change that can be measured by Electron Paramagnetic Resonance (EPR) spectrometry. EPR has been successfully used to quantify radiation overexposures to radiation accident victims where bone or dental tissues were available for analysis. The presentation included an introduction to EPR and radiation fundamentals, and described how this technique was used in two radiation accidents. The use of this technology to study Russian populations exposed to excessive radiation from Cold War nuclear weapons activities was also described. The data from these studies were used by the National Cancer Institute to assess the appropriateness of radiation safety guidelines for health care and industrial workers.

June 10 Professor William P. Reinhardt
University of Washington and Guest Scientist NIST Physics Laboratory, Electron and Optical Physics Division

A Tour of Real and Imaginary Universes: Jorge Luis Borges Meets Stephen Hawking



Scientific and mathematical images appear in "serious" literature, as in, for example, in the works of Borges and Thomas Mann. Scientists writing for a general audience have a great challenge in presenting quantitative mathematical ideas in verbal (nonmathematical and even nonpictorial) form.., Hawking's discussions of space and time being likely the best known, or at least the best sold. In this genuinely "liberal arts" talk, intended for students and scholars of all disciplines, some illustrations focusing on "what does it mean to be large or small?" "what is a long time? what is a short time?" "how big is the physical universe, versus the universe of the imagination?" and "what is the difference between information and knowledge?" are given from physical, literary, and mathematical, and even slightly political points of view. The talk includes an illustrated tour of a real (our own!) and an imagined universe (that of Borges…), and dramatic readings, some long, some very short, from texts by Thomas Mann, Herman Melville, Ray Bradbury, Paul Auster, John McPhee, as well as J.L. Borges.

June 14 & 15 ***Laser Safety Training***

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

June 17 Teri Gregory
Thermal Systems Lead, Space Servicing Capabilities Project,
NASA Goddard Space Flight Center, Greenbelt, MD

The Hubble Space Telescope and On-Orbit Servicing

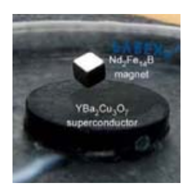
Since its launch in April 1990, the Hubble Space Telescope (HST) has been the

most scientifically productive program in the history of NASA. The rate of scientific discoveries has continuously increased over the life of the telescope through the design, development, and installation of state-of-the-art instruments during five on-orbit servicing missions to HST. In order to facilitate on-orbit servicing, the Hubble Space Telescope was designed with a modular architecture for Orbital Replacement Unit (ORU) change outs and with numerous internal and external astronaut handholds and foot restraints as crew aids during Extra Vehicular Actvities (EVAs).

This presentation described the development and execution of HST Servicing Mission 4, as well as a description of future on-orbit satellite servicing currently under study at the NASA Goddard Space Flight Center.

June 24 Robert M. Briber
Professor and Chair, Department of Materials Science and Engineering,
University of Maryland, College Park

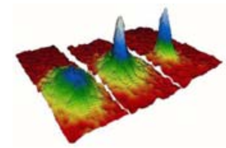
Materials for the Future



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 to many advances in technology and future advances in materials hold promise as the building blocks for future technological innovation. The talk provided an introduction to the field and gave examples of many advanced materials through hands-on demonstrations and audience participation.

June 30 Professor William P. Reinhardt
University of Washington and Guest Scientist NIST Physics Laboratory, Electron and Optical Physics Division

Solitons in gaseous BEC (Bose Einstein Condensate): History, Theory, and Experiment (most all at NIST!)



A brief introduction on Bose Einstein Condensate, including what Bose and Einstein thought and said; after that the whole story is at NIST, starting with Bill Phillips and laser cooling (Nobel Prize 1997); Prediction of Solitons created by Quantum Phase Engeineering, Reinhardt and Clark (1997); and THE EXPERIMENT: Phase Engineered Solitons are observed at NIST, which has resulted in the single most referenced paper in 'atom optics,' (Science, 2000).

July 1 Brian Weiss
NIST Manufacturing Engineering Laboratory, Intelligent Systems Division

Coming Up with the Tests: Frameworks to Guide Researchers in Developing Comprehensive Evaluation Plans

Advanced technologies are constantly emerging across a range of domains including those within the military, law enforcement, etc. Evaluating the performance of these systems is paramount to both (1) inform the technology designers of short comings and query end-user feedback so that modifications can be made in future iterations and (2) validate the technology's final capabilities so that buyers and technology users know exactly what they are getting. Many evaluation frameworks have been created to produce extensive test designs to capture the necessary quantitative and qualitative metrics of various intelligent systems. This talk will present several NIST-created evaluation frameworks including one that has been instrumental in designing over a dozen advanced technology evaluations while the other is still in development. Evaluation highlights will be presented to illustrate NIST's successful usage of test design frameworks.

July 8 Dan Englender
Program Director, Teach for America's DC Region

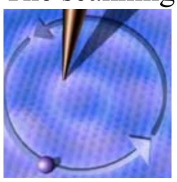
Teach for America

In low income areas, only 1 in 10 students will ever graduate from college. Teach for America hopes to build a movement to eliminate educational inequity by enlisting our nation's most promising future leaders in the effort. Since their inception 24,000 individuals have participated in Teach for America, impacting the lives of approximately 3 million students. The best hope for ending educational inequity is to build a massive force of leaders in all fields who have the perspective and conviction.

July 15 Dr. Joseph Stroscio
NIST Center for Nanoscale Science and Technology

Imaging Atoms at Ultra-Cold Temperatures

The scanning tunneling microscope (STM) enables a look into the nanoscale



world that is a billion times removed from our everyday senses. The technique is based on the quantum mechanical electron tunneling between a probe tip and a sample surface, which achieves atomic resolution measurements. Inherent in the electron tunneling process is sensitivity to the electron states in the sample under investigation, allowing imaging and spectroscopic measurements of electron systems in addition to imaging the atomic structure. In the talk, Dr. Stroscio described a new STM instrument recently completed at NIST that operates at ultra-cold temperatures down to 10 mK. He described some of the new physics tht becomes “visible” with STM measurements at these temperatures in the 2-dimensional carbon system known as”graphene.”

Also at the social that took place after the seminar, a video was shown called "Innovate Engineering Change" - complements of Dr. Bill Ott (the Deputy Director of the Physics Laboratory) who thought it would be of interest to the students.

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

August 3 Lunch: SURF Directors and special invited guests.

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

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

August 6 Last day for SURF students and farewell pizza party.

2010 SURF Summer Activities

It is difficult when you are 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 are 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 2010 – 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. Again, it worked out that the University of Maryland Materials Science Research and Engineering Research Experience for Undergraduates (REU) was touring NIST on the day of the BBQ and got to join the NIST SURFers for the goodies -- surely much better than that brown bag lunch they were planning to eat. It also gave the two REUs a chance to compare notes. NIST is always a top tour spot for the UMD REU to tour during the summer.

MSEL/CSTL/MSD Work-Life and Diversity Picnic

Food – just mention the word and it spreads like wildfire among the SURFers. NIST's Materials Science and Engineering Laboratory, Chemical Science and Technology Laboratory, and Technology Service's Measurement Services Division hosted a picnic and the SURFers joined in to enjoy the activities.

Take Me Out to the Ball Game

It is fun to see an Orioles or Nationals game up close and personal when you are in the area. It is even more fun when a relative's husband got pulled up to the Majors to play with the Florida Marlins. Boo…they were playing against the Orioles. Looks like the SURFers had a chance to see the Marlins beat the O's two out of three games.

July 4th in the Nation's Capital

Many of our 135 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 30 spectacular years featuring the most dazzling display of fireworks anywhere in the Nation. Many people arrive early 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.

Avatar – IMAX 3D

Avatar was advertised as taking you to a spectacular new world beyond your imagination, where a reluctant hero embarks on a journey of redemption and discovery, as he leads a heroic battle to save a civilization. The film broke several box office records during its release and became the highest-grossing film of all time in the U.S. and Canada and worldwide, surpassing *Titanic*, which had held the record for the previous 12 years. It also became the first film to gross more than $2 billion. Some of the SURFers felt it necessary to see the movie shown in IMAX 3D at the Natural History Museum in DC for a mere $15.

2010 SURF T-Shirt Design

T-shirts are always a popular way to remember where you've been, i.e., trip to Hawaii, that concert of your favorite band, but what is 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. This year's group was very industrious, designing two T-shirts. In addition to the "Mad Scientist," they designed a shirt to represent one of NIST's functions – standard reference materials. The note on the actual shirt on the back is SRM 1337. The numer 1337 represents the "geek" in all of the students. 1337 = LEET or elite and it is a computer language of sorts. 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 fourth NIST Summer Institute for Middle School Science Teachers was held from July 6 – 19, 2010. The workshop sponsored 18 middle school science teachers. The Summer Institute, 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 is 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.

NIST Survey of Usability Research on Passwords

Passwords are the source of many cartoons and office jokes. These cartoons and jokes are not based on good scientific data but rather on anecdotal evidental evidence. The usability researchers in ITL were conducting an independent research project with a survey on password usability. They were asking for input from the SURF students to provide a sound scientific basis that can inform the researchers in setting password policies in the future. The primary purpose of the survey was how passwords affect your job. As usual, the SURFers were always ready to jump in and help.

Gulf Oil Spill

The SURFers did not have to be in the midde of a crisis to be interested and learn. One of the SURF students received a cool video and description of what happenws in the Gulf with the oil spill! It is ironic that two scientists in the Math Department at University of North Carolina Chapel Hill worked on just such a problem 10 years ago. The proposal was submitted to the National Science Foundation to study the processes shown in the video but their proposal was rejected. So their video sat in a file somewhere until it suddenly became relevant to current events.

HELP!

SURFers are a close group of students and you could see a number of cries for "help" go out over the SURFevents email for help with different problems they were having with a project or looking for an item needed to work on a project. It was good to see that it was not very long before a thank you went out because someone in the group was able to help. Teamwork is definitely something the SURFers have down to a science!

The Future of a Scientist

Dr. Katharine Gebbie, Director of the NIST Physics Laboratory, offered to speak with any interested SURFers one-on-one about their future career plans. The Physics Laboratory initiated the SURF program back in 1993 with a group of only 20 students. This year we had over 130 students participating.

GRE® – Graduate Record Examinations®

For the second year in a row, SURF students organized a physics GRE study group to prepare for the test. The Graduate Record Examinations® (GRE®) General Test measures verbal reasoning, quantitative reasoning, and critical thinking and analytical writing skills. The GRE® Subject Tests gauge undergraduate achievement in eight specific fields of study. There was a variety of days so that everyone, regardless of sport or activity, could participate. You could go to as many or as few of the days as you like, but the format was generally either assigning problems or working on problems together and the group was fairly informal. What was needed – pencil, paper, and your freshman mechanics and E&M textbooks if you had them.

Urban Search and Rescue Robots

NIST has a US&R course and MEL resarachers Tony Downs, Brian Weiss, and Ann-Marie Virts gave the SURFers a tour of the facility. The test course is the world-standard obstacle course for testing uban search and rescue, and now bomb disposal robots. The course has been replicated througout the world and is the basis for the annual competition. It drives the development of mobil robot agility, sensing, navigation, and mapping capabilities.

Concerts

SURFers took advantage of the many concert venues in the DC area. SURF events email were getting groups together to see Jack Johnson, the groups Gold Motel, The Counting Crows, Owl City, James Taylor and Carole King, Weird Al Yankovic, and others.

Anime Convention

The Baltimore Convention Center hosted Otakon the last weekend in July. This is the largest aime convention on the East Coast, having a capped attendance of 25,000 people. Some of the activities at the convention incuded anime rooms, panels, workshops, meet/greets, video game rooms, masquerades, raves, dealers rooms, both live action and animated movies, and lots of other activities. It sounded like a group of SURFers made sure they were counted in that attendance cap if you happened to see all the "surf events" emails flying around.

Washington, DC Museums

How could you come to the Nation's Capital and not check out all the wonderful museums. They range from The Aircraft Museum, The Museum of Modern Art, International Spy Museum, Smithsonian National Air and Space Museum, National Museum-America History, National Museum-Natural History (make sure to check out the Hope Diamond), and the National Museum of Crime of Punishment (one that you might want to visit but never have your name associated with).

Bowling

Shady Grove 300, it is bowling – with a twist. What is the twist? A new action-packed playhouse that poses as a swanky bowling alley, bistro and bar all rolled into one -- state-of-the-art lanes, floor to ceiling video screens. I wonder if the SURFers still had to share someone else's shoes or if they were "pro" enough to have their own.

Rugby, Soccer and Volleyball

They may not have been wearing *DC United* soccer jerseys and had the trappings of 11 domestic and international champions dominating the NIST lobby, but the competition beween the teams was just as fierce. The group also played volleyball (probably not on the same scale as Misty May-Treanor and Kerri Walsh or in the same outfits). When it comes to rugby it is been a long time since the USA could claim a victory (1920 and 1924 games) but when you are having fun…you do not always have to win. You also did not have to know how to play the games when one type or another of the activities was available from your living room TV.

Drive-In Movies

Ah, how that word brings back fond memories. You could see the latest Disney movie or the latest shoot'em up featuring John Wayne. Unfortunately most of the drive-in theatres have gone by the wayside. But thanks to one of our SURFers, we found out there is still a drive-in movie theatre left in Baltimore. It has the largest movie screen in the United States and is celebrating its 55th season of continuous operation. On Friday and Saturday nights during the summer they show three movies, that change every week and the price of admission is only $8. That is pretty cheap for an evening of fun, even after the drive to Baltimore from Gaithersburg.

Drag Racing

It seems we had a drag racer in our midst and a number of SURFers who had never been to a motorsports event. Nathan Jacobson raced his car on Saturday, June 12 at the Mason Dixon Raceway in Hagerstown, MD. The Maxon Dixon Dragway is a ¼ mile NHRA dragstrip. Unfortunately Nathan lost by .002 of a second. 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 is more than just "putting the pedal to the metal" as the saying goes.

Trips

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

Cedar Point Amusement Park, OH

People throughout the entire world know about it. It is the number one rated amusement park on the planet. It is 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.

Hiking, Kayaking, Something Outside?

Some like to release the stress of work by working out in a gym, others have to be in the great outdoors. A few of the SURFers took to some local hiking spots to not only relieve the stress, but to also enjoy the scenery.

SURF Farewell Pizza Party

Every year the SURF Directors treat the students to a farewell pizza (40 pies this year!) party. Again this year the SURF T-shirt committee made a few dollars profit selling the summer's hottest fashion item – the SURF 2010 (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 is not to love.

Rita's Ice-Custard-Happiness

See ya!

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Student Abstracts
2010 SURF Program

American University

Transverse Motion of the Main Induction Coil in the Electronic Kilogram Experiment
John Geraghty

The kilogram is the last base unit in the SI that is defined by physical artifact (the International Prototype Kilogram) rather than fundamental constants and quantum references. The BIPM (Bureau International des Poids et Mesures) has shown the mass prototype copies are changing on the scale of 0.5 micrograms per year, creating an uncertainty in other physical constants based on the definition of mass. By improving the measurement of Plank's constant h using a watt balance system (ratio of mechanical power to electrical power), the Electronic Kilogram Experiment is able to provide an alternate definition of the mass standard.

The watt balance system employs an induction coil in the field of a superconducting solenoid that is suspended underneath the test mass pan. The system operates in two modes: one where the coil moves to generate a voltage and the other where a current in the coil generates an electrical force to balance the acceleration of gravity on a mass. The position and tilt of the induction coil relative to the magnetic field and gravity need to be measured to compensate for misalignment. In order to achieve this, new hardware and software for a laser positioning system is being upgraded. New 2D lateral detectors had to be calibrated to the system relative to voltage and laser beam displacement. The new software is an AC phase lock-in program, which detects the voltage/displacement signal coming from the now frequency modulated diode lasers. The program developed in LabVIEW, locks into the modulation frequency to pull out the displacement thus rejecting room light and background 60Hz voltage noise, common problems in the old system. The goal of implementing the new hardware and software is to reduce noise and to increase resolution of the lateral detection program.

Calibration of Transition-Edge Sensor (TES) for Applications in
Testing Bell's Test of Nonlocal Realism
Michelle Nadeau

In the famous EPR thought experiment, Einstein, Podolsky, and Rosen argued that quantum mechanics is flawed because the idea of local realism fails under certain conditions. They claimed that a correct theory of nature must include give objects predetermined properties. In 1964, John Bell developed a theorem that showed how to test the EPR paper's ideas and today's technological advancements allow us to finally carry out this test with indisputable results. By combining a two-photon source based on parametric down conversion and a transition-edge sensor (TES) with very high efficiencies, we hope to be able to test the viability of the hidden variable theory. At this time, the efficiency of the TES is known to be about 95% but we must verify its efficiency to better uncertainty to know that we can implement the above test of nature's most fundamental secrets.

Development of a Point Sesor to Measure Greenhouse Gases using Novel THz Spectroscopic Techniques
Virginia Perkey

Our research falls under the Greenhouse Gas Initiative, which aims to develop new standards, methodologies and technology to quantify greenhouse gases over a range of length scales. To meet these needs, a point sensor is being developed to detect and measure multiple species of greenhouse gases simultaneously. The sensor is designed to generate and detect chirped pulses at terahertz frequencies with ultra-low phase noise. The research approach is based on adapting recently-developed techniques in the microwave (2-40 GHz) [1] and extending them to the higher frequency terahertz regime (.3-3 THz) of the electromagnetic spectrum. New methods have been developed to generate well-isolated, harmonic-free chirped pulses at microwave frequencies (11 GHz), which are then multiplied by a factor of 48 using a cascaded multiplier chain to create terahertz pulses near 528 GHz . An artifact and harmonic-free chirped pulse in the microwave is essential for the success of our multiplication and detection scheme. The majority of the data to be presented shows the progress we have made using different mixing and filtering techniques to generate such pulses. The high-frequency chirped pulses were characterized at several harmonics (multiplication factors of 8 16, and 48) that were emitted from the cascaded multiplier chain. Detection was achieved by heterodyne mixing to down convert high frequency THz signal into the microwave, which is within the detectable range of our oscilloscope (DC-13 GHz). Future experiments and applications will be discussed in light of these developments.

[1]G.G. Brown, B.C. Dian, K.O. Douglass, S.M. Geyer, S.T. Shipman and B.H. Pate, *Rev. Sci. Instrum.* **79** no. 5 (May 2008), article # 053103

Appalachian State University

Calibrating Spectrophotometric Standard Stars
Cortney Bougher

Cosmological studies of the redshift of type-Ia supernovae and the search for Earth-sized extrasolar planets require greater measurement precision. Developing calibration techniques to lower uncertainties in absolute measurements of spectral radiance has become an essential goal. We are developing a method to improve the existing uncertainties: we calibrate a portable telescope at NIST with a laser-irradiated integrating sphere to obtain a correction algorithm for atmospheric extinction. We use this calibrated telescope alongside the Tilinghast telescope at the Whipple Observatory at Mt. Hopkins, Arizona and the FAST spectrograph so that we may apply a correction algorithm to the data taken by FAST. We took spectra of Vega and the spectrophotometric standard star HD 16459 along with spectra of a calibration source set up on the summit of the mountain. We created the calibration source using a laser system and an integrating sphere to produce a well known, optimal source. I am presenting the preliminary analysis of the spectra of Vega, HD 16459 and the source taken with FAST.

Simulation of High Reflectivity Photonic Crystal Mechanical Resonators
Luke D. Robertson

Mirrors are essential elements of many modern optical devices such as lasers, sensors and optical filters. Mirrors are most commonly made from metallic layers. To avoid absorption losses, most optical devices, such as semiconductor lasers, employ distributed Bragg reflectors (DBRs) which consist of many alternating layers of high and low refractive-index dielectric materials to achieve high reflectivity. However, these mirrors are unsuitable for applications such as radiation pressure cooling experiments due to their large mass and poor mechanical properties. In this work we design mirrors from a *single* dielectric layer of high index material with a photonic crystal etched into it. This photonic crystal may consist of, for example, an array of holes or a grating structure. These mirrors have extremely high reflectivities and mechanical quality factors, while at the same time are compact with low mass and high mechanical resonance frequencies. Possible photonic crystal patterns and their advantages over DBRs will be discussed, as well as the methods for simulating the theoretical behavior in order to predict experimental results in the laboratory.

Brown University

Data Acquisition and Analysis of Shim Arm Position During a 5 Degree Rod Drop Test

William Riedel

The NIST Center for Neutron Research (NCNR) owns and operates a 20 MW Research Reactor. This facility is used to generate neutron beams for experimental applications. The reactor engineering division at the NCNR performs maintenance and repairs on the reactor and confirms that all of its safety systems are operating correctly and efficiently. One of the most important safety systems for the reactor is the set of four shim arms that controls the fission process. The arms, located in the reactor vessel, absorb neutrons at a rate proportional to their degree of insertion into the reactor. The rate of reaction can be slowed by inserting the shim arms further into the reactor, or increased by drawing the shim arms out. In the event of an emergency, a reactor scram occurs, meaning the arms are rapidly inserted into the reactor to effectively stop the reaction. It is a requirement under the NCNR operating license for the reactor that all four shim arms must have fallen five degrees (out of forty) within 240 milliseconds of the initiation of a scram.

A data acquisition program was written in LabVIEW 8.6. It is used to gather position data of a shim arm during scram test procedures. The program plots the position of a shim as a function of time and performs the following functions: verify that the shim arm response adheres to the 5 degrees in 240 milliseconds requirement; record acceleration of the shim arm and time delay until physical clutch release; perform Fourier analysis on the input signal to allow for the examination of potential periodic noise; and aid in the investigation of any sources of impurity in the signal received from the reactor. A demonstration of the program was performed during a scram test at the end of July 2010 during reactor shutdown. The results of this demonstration will be presented.

Off-Line Two-Dimensional Separation of Proanthocyanidins in Botanical Standard Reference Materials

Jonathan Truong

Interest in secondary metabolites, organic compounds not directly involved in plant growth, has increased substantially ever since they have been found to have numerous health benefits. Proanthocyanidins (PACs), a class of polymers consisting of flavanol subunits, are known to have very high antioxidant properties capable of neutralizing oxygen radicals in the body. Recent studies have shown that different degrees of polymerization (DP) have different effects when consumed, such as antibacterial properties or improvement of cardiac recovery. As natural product dietary supplements become more widely used, manufacturers require more information on their efficacy and dosage. Thus, separation and characterization of these molecules in different foods is of great interest. The goal of this study was to develop a method to characterize and differentiate the amounts of PACs contained in various botanical Standard Reference Materials (SRMs).

Because the complexity of these polymers increases exponentially with each addition to the chain, a two-dimensional chromatographic method was developed to fully separate the distinct PACs. Adsorber technology with solid-phase columns was also explored to purify the extract before separation. Following a recent publication on the analysis of PACs in cocoa beans, normal phase liquid chromatography was used in the first dimension to separate the PACs according to the DP. Then, a reversed phase chromatographic method was developed for the second dimension separation of the individual components in each group. PACs were detected by their characteristic fluorescence excitation and emission wavelengths. Using an off-line approach allowed for an easy and relatively fast way that does not require complex plumbing compared to an on-line scheme. Additionally, this approach allows for the concentration of the fraction, enhancing sensitivity, and aids in the process of method development. In the end, a contour plot was generated detailing the separation of all the different PACs contained in the extract. This plot can be used to compare the PAC content of each SRM and to allow a way of collecting a specific PAC's information for therapeutic research. In later studies, electrospray ionization mass spectrometry will be used to characterize each PAC on the basis of their bond types and methods of quantification and end group analysis will be explored.

Bucknell University

Engineered Titania Nanoparticle Dispersions for Environmental Health and Safety (EHS) Applications

Daniel Markwalter

Engineered nanoparticles (ENPs) often exhibit distinct properties, different than those of the bulk material. This study seeks to develop a methodology for producing nanoparticle dispersions of P25 titanium dioxide in relevant biological media. The unique and potentially unknown risks posed by nanoparticles require these standard dispersion preparation techniques for appropriate risk evaluation. Particles are stabilized using bovine serum albumin (BSA) or citrate before being introduced into biological test media such as PBS or DMEM. Particle size is monitored over time using laser diffraction in the different media to monitor particle stability. Dispersed titanium dioxide nanoparticles are observed to have a 70 nm mean diameter. Comparative studies using DLS and XDC are also conducted to validate the laser diffraction results. Laser diffraction, being the most suitable technique for polydisperse samples, is the most effective technique for this type of analysis, allowing for the detection of agglomerates in the micron range upon destabilization of the suspension. Results indicate that BSA is an appropriate, biocompatible stabilization agent for P25 titanium dioxide nanoparticles, preventing agglomeration for up to two weeks. Without BSA, dispersions of P25 agglomerate within 24 hours when introduced to the biological media. In the end this research will guide standards for sample preparation used in further EHS studies.

Creating a Graphical User Interface (GUI): Comparing Technical Performance and End-User Utility

Elise Terrell

The Spoken Language Communication and Translation System for Tactical Use (TRANSTAC) is a Defense Advanced Research Projects Agency (DARPA) program focusing on the rapid development of two-way, free form, speech-to-speech translation systems. These systems are being designed to facilitate conversations between US military and non-English-speaking foreign personnel to communicate across a range of tactical dialogues without the need for an interpreter.

Since 2007, NIST has led the independent evaluation team for the TRANSTAC program. This requires designing test scenarios and analyzing extensive data that provides an assessment of how each technology and their constituent components perform. Two types of data, technical performance and end-user utility, are collected to ensure a complete evaluation of each system. The TRANSTAC systems are tested on their performance in sets of scenarios designed to mimic situations encountered in tactical environments. Utility data is collected through user surveys, demonstrating how system's users felt about their interaction with the technology.

While both of these areas are equally helpful in understanding the system's capabilities, the two sets of data have never been compared against one another. The goal of this project is to create a graphical user interface (GUI) that would bring these two sets of data together. Organizing the evaluation findings in a way that was clear allows the data to complement each other and illustrate general trends and patterns in the data. The GUI displays data populated from a custom built database and provides the user multiple comparison options. For further control and interaction, the user is also given the ability to select from various search criteria to view specific aspects of the data.

California State University Long Beach

Growth of Diamond Thin Films for Use in Investigation of Nanoscale Friction

Ramsey Noah

The fundamentals of friction at the nanoscale level are still not thoroughly understood. We propose an investigation of friction effects at this small scale using an atomic force microscope (AFM) and diamond thin films. Diamond has been chosen for many reasons. It has many potential applications in microelectromechanical/ nanoelectromechanical systems and many unique properties such as extremely high thermal conductivity, high hardness and wear resistance. We have produced diamond thin films using a hot filament chemical vapor deposition (HFCVD) technique. Although there are many established CVD techniques, including low pressure chemical vapor deposition and microwave plasma chemical vapor deposition, it is quite an art to grow diamond thin films. Some of our greater challenges have been creating an orientation for the film as a whole and growing films with thicknesses just under the mean free path of phonons in diamond (roughly 30 nanometers). In my talk, I will go into depth on the HFCVD process we used, how our standard operating procedure developed, the current state of the thin films and what is left to accomplish before friction measurements can be done using the AFM.

Additionally, I worked on testing and calibration for two other projects involving ultra high vacuum chambers. The first deals with nanostructured thermoelectrics, the second field emitters. The concept behind thermoelectrics has been around since 1821 when Seebeck first observed a current flow between two metals that were kept at different temperatures. This generation of electricity from temperature gradient is used commercially in some niche applications. The challenge today is to increase the efficiency (ZT rating) so that they can be used more widely and make a real impact on important energy issues.

Carnegie Mellon University

Raman Spectroscopy of Graphene Decorated with Copper Nanoparticles

Emily Gehrels

Graphene and copper nanoparticles are two of the most exciting materials in nanotechnology today. Graphene, a single-layer sheet of hexagonally arranged carbon atoms, has promising applications in electronics because of its unique properties, such as high electron mobility and intrinsic strength, while copper nanoparticles have been found to be powerful catalysts in a number of chemical reactions. The addition of copper nanoparticles to a graphene surface enables tunability in the electrical properties of the graphene layer, serves as an anchor for the growth of other nanomaterials, and leads to enhanced Raman spectroscopy.

Raman spectroscopy, the inelastic scattering of photons from vibrational modes of a system, is extremely sensitive to both graphene and copper oxide, an impurity commonly found on copper nanoparticles. It provides a rapid and non-destructive tool to probe the underlying physics of graphene including the number of layers present, the quality/defects of those layers, and electron-phonon coupling, just to name a few. Raman spectroscopy is also useful in identifying and quantifying the stoichiometry of copper oxides, providing important insight into the stability of the copper nanoparticles containing this impurity. When graphene is coated with copper nanoparticles the resulting Raman spectra provide insight into how the two materials interact and indicate changes in the properties of the graphene layer.

Copper nanoparticles have been deposited onto graphene substrates via two methods: (1) sputtering thin films of copper on graphene followed by high temperature annealing, and (2) chemically synthesizing and drop casting copper nanoparticles onto graphene. Raman, Scanning Electron Microscope, and Atomic Force Microscopy characterization of the graphene-copper complexes enables a detailed comparison of the two methods in order to determine the possible benefits of each method for use in future advanced nanostructured materials.

Controlling GPIB-Compliant Instruments Using a JAVA-Implemented Interface

David Jia

The purpose of this project is to develop a Java application in order to interface with and control measurement instruments connected to the computer via a GPIB (General Purpose Interface Bus). GPIB is used to send commands and receive data from various instruments. At first, several existing open-source software, such as Zephyr, a Java-based automated measurement program, were evaluated and eventually dismissed in the process. Commonly used programs to communicate through GPIB, such as LabVIEW and MATLAB, were also rejected for various complications. Finally, Java's JPIB library was selected as the mode of communication with GPIB-compliant instruments. A high-level control over the instruments was implemented in Java by creating text-based commands that encapsulate some of the instruments' GPIB commands. These high-level commands can be used to form scripts that can be run during experiments to accurately control procedures and record data. A graphical user interface was also created to ease the process of editing and running scripts. This software will be used to perform thermo-magneto-electrical measurements, such Seebeck coefficients and Hall effect, using a MEMS-based measurement platform. This involves controlling the temperature and magnetic field of a cryogenic probe station with a superconducting magnet, an additional temperature gradient, a semiconductor parameter analyzer and two lock-in amplifiers. Finally, the program has been written and documented to allow future expansion of the functionality of the currently supported instruments as well as the addition of new instruments.

Neutron Imaging of Rechargeable Lithium-Ion Batteries

Joshua Keller

Lithium-ion batteries are an important component of many modern electronic devices, and they are a leading candidate to drive electric cars of the future. However, Li-ion batteries decay in both charge capacity and power output over the course of many cycles of charging and discharging. The mechanisms behind this decay are not entirely understood. By performing neutron tomography on a Li-ion cell over several charge/discharge cycles, we can better understand these decay mechanisms. Neutron radiography is an imaging technology that has high sensitivity to light elements (hydrogen and lithium), complementing other forms of imaging. Since lithium has a large scattering cross-section with respect to incident neutrons, neutron imaging is an effective tool for observing concentrations of lithium. We observed the migration of lithium ions in rechargeable lithium-ion batteries with a spatial resolution of ~25 μm.

Characterization of Micro Electro Mechanical Sensors
Matthew Swisher

The purpose of the research is to determine the characteristics that apply to the motion of components of a specific type of Micro electro mechanical system (MEMS). The MEMS consist of a pad suspended above two electrodes by springs. The characteristics are important because they allow for the accurate calculation of forces being applied to the MEMS device. These characteristics include the geometry of the different components and the stiffness of the springs that are a part of the device.

MEMS have numerous practical applications; however they have limitations because there are few ways to control the motions of the components in the system. One of the most common methods to move components in a MEMS device is by creating a charge on an electrode, so as to exert an electrostatic force on the moving component, the pad. The component is attached to the springs which apply an opposing torque. This torque can be calculated as a function of the rotation of the spring and the stiffness of the spring. Additional forces come into play due to the design of the device. Once all of these characteristics are known, an additional force placed on the component can be calculated based on the response from the device. This enables the MEMS device to be used as a sensor for calculating small forces which are applied to it.

<u>City College of New York</u>

Quartz Tuning Fork Kelvin Force Microscope
Amandeep Chhabra

Kelvin Force Probe Microscopy is a technique to measure the surface potential of nanostructure devices. The surface potential is a function of the contact potential difference between a tip attached on a vibrating cantilever and the test sample with a small spacing between them. The periodic vibrations of the cantilever at a harmonic frequency result a current, which is directly proportional to the capacitance and the contact potential difference between the tip and the sample. The cantilever oscillates due the voltage applied to a piezo electric material attached to cantilever. The force experienced by the tip, when it scans over the sample, is recorded optically using a laser source and the acquired data is translated into topography images.

A quartz tuning-fork probe is being developed that vibrates and detects its own probe deformation as function of the displacement current, for application to Atomic Force Microscopy (AFM) and Kelvin Force Microscopy. Due to its high Q factor value, the resolution of AFM images improves.

To implement the quartz tuning fork probe, a quartz tuning fork was driven using a high frequency sine wave signal from a function generator. The displacement current was amplified by a current amplifier and then measured at a lockin amplifier to remove the EMI noise from the signal. A feedback loop was designed using a digital signal processor (DSP) to control the oscillations of the tuning fork. The displacement current measures both dissipative and reactive forces between the tip and the sample and the topography images are calculated from the measured current.

Studying Protein Clusters in Solution
Using SANS and Rheometry
Navjot Kaur

Aggregation or finite size clusters is a common process that has been observed for different types of proteins in biological systems. This process has been observed in many diseases such as Alzheimer's and Parkinson's. In addition, during manufacture, transport and storage of biopharmaceuticals protein aggregation can lead to problems with product specifications such as purity and safety. Protein aggregation kinetics depends upon various factors such as solvent conditions (pH, salt concentration, types of buffer), sequence of protein structure and protein folding and unfolding. Hence, it is critical to understand and control the protein aggregation in concentrated solution.

In this work, we have first aimed to understand the concentration change when filtering samples using different filter size as filtering is a common practice in many sample preparations. The protein concentration is determined using UV-Spectrophotometry at characteristic peak 280 nm. In addition, we have aimed to conduct a measurement of T_{cloud} as a function of protein concentration and concentration of added NaCl salt in preparing for our Small Angle Neutron Scattering (SANS) experiments. The rheology properties of the lysozyme protein suspension are studied as a function of temperature using stress-controlled rheometer. Finally, we have also conducted a joint study of concentrated lysozyme protein solution at different concentrations and temperatures using both SANS and rheometer.

Evaluating Changes in Physical and Mechanical Properties of Asphalt Binder
with Short-Term and Long-Term Aging
Dixitchandra Patel

Due to the tremendous cost saving benefits and the positive impact on environment, the amount of Reclaimed Asphalt Pavement (RAP) used in virgin mixtures has been increased from 10 % to about 40 % over the past years. The proper integration of increased RAP into virgin mixture requires better understanding of the physical and mechanical properties of the blended materials. Since the properties of recycled blend are highly dependent on the properties of the asphalt binder, this study focuses on characterization of asphalt binder as it ages.

The change in physical and mechanical properties of asphalt binder subjected to various accelerated aging processes and as extracted from RAP are being investigates. Two modes of aging will be simulated in laboratory. A short-term aging that resembles aging of asphalt prior to construction (during plant production, storage, and hauling) and a long-term aging that resembles the aging of asphalt during its lifetime (UV light exposure and oxidation). The short-term aging of asphalt was simulated using the Rolling Thin Film Oven test (RTFO) and by heating the asphalt in an oven for up to 6 hours. Long-term aging was simulated using a pressure aging vessel (PAV) and via the NIST SPHERE, which exposed asphalt samples to the equivalent of almost 15 years of UV field exposure.

The mechanical changes in asphalt with aging will be assessed by complex shear modulus (G*) that is measured using a dynamic shear rheometer (DSR) single frequency test in a constant stress model after the various laboratory simulation aging tests and ultraviolet radiation aging on asphalt binder were performed. The physical properties will be monitored using neutron scattering device. NIST Center for Neutron Research (NCNR), small angle neutron scattering (SANS) point outs the micelles that are spherical with average radii in the 50-100 A range, which is conveying the rheological properties of asphalt binders.

City College of New York Hunter

Temperature-Dependent Optical Properties of Semiconductor Colloidal Quantum Dots

Catherine Callo

Monitoring of tissue temperature is vital during clinical applications such as therapies involving tissue welding or hyperthermia, and imaging involving potential thermal damage to the tissue. Our particular interest is in developing techniques to measure temperature changes in microenvironments where traditional methods cannot be used. Our approach is based on semiconductor colloidal quantum dots (QDs). Main goal of this project is to demonstrate the correlation between the optical properties of QDs and the temperature of their surroundings.

QDs are colloidal semiconductor nano-particles that exhibit stable and unique photoluminescent properties. Upon synthesis, their absorption and emission spectra can be tailored by modifying their size and composition. However, these optical properties are known to be sensitive to their environment. In particular, change in the ambient temperature is expected to modify the energetics of the nanoscale arrangement and interactions of atoms in the QD, resulting in the change in its optical properties. We found that the emission peak wavelength changes as the temperature changes. These wavelength shifts have been proved to be reliable and reproducible. This feature makes QDs potentially useful for their application as local temperature sensors.

Temperature-dependent emission properties on several different types of QDs, including core-shell and core-shell-shell QDs, were studied in an effort to understand the effect of strain in the core-shell interfaces. Some theoretical models are also discussed to explain the mechanism of the temperature-dependent emission. We aim to explain how these multi layers affect the QDs' optical properties, such as the intensity of emission and absorption, and emission peak shift and width. We noticed that despite of the similar chemical composition of these QDs, their difference in structure seems to play an important role in the optical properties.

Clemson University

Electrodeposition of CdS-CdTe Photovoltaic Devices on Interdigitated Back-Contacts

Ryan Need

As the global demand for energy rises and environmental concern over the use of carbon-based fuels grows, the need for clean sources of energy is becoming increasingly apparent. Photovoltaic (PV) devices, also called solar cells, have the potential to meet these demands by converting the energy of photons in sunlight directly into usable electricity without any harmful byproducts.

In essence, PV devices are just semiconductor diodes. When light is incident upon the PV device, some of those photons will be absorbed by the semiconductor. The energy from these absorbed photons excites electrons from the valence band to the conduction band, thereby creating two charge carriers in what is known as an electron-hole pair. These charge carriers are then separated by the internal electric field which exists at the p-n junction of the diode. Those separated carriers can then be run through an external load to generate power.

While PV cells are a direct and elegant method of generating clean electricity, manufacturing costs and device efficiency currently limit their wide-scale application. In order to make PV technology a financially viable energy solution, the average cost-to-Watt ratio of solar cells must be lowered to below

$1.44/W before solar energy can reach parity with coal. Current first generation devices, which rely on the expensive and time-consuming growth of silicon crystals, have a cost-to-Watt ratio around $2/W. By taking advantage of direct band gap materials, second generation devices not only requires less material but can be produced using thin-film deposition techniques that enable roll-to-roll manufacturing. Together these two advantages have reduced the cost-to-Watt ratio to $1.07/W. The average cost-to-Watt ratio still lags behind these industry leaders at $4.18/W.

Third generation devices seek to lower the cost-to-Watt ratio of PV cells even further by utilizing 3D geometry. Here at NIST, Dr. Dan Josell and his team are working to put forth a platform for unambiguously measuring the performance of such third generation devices by studying the electrodeposition of CdS-CdTe devices on interdigitated back-contacts (IBC). IBC are a complex 3D structure that is generally difficult to manufacture, especially at the micron-length scale attempted here. Electrodeposition facilitates the formation of these complicated, 3D p-n junctions by enabling material to be selectively deposited on only one set of electrodes through the control of its potential. Dr. Josell and his team hope the work done here can serve as a guide for how PV devices with increasingly complex 3D geometry can be formed, measured, and understood.

College of William and Mary

Testing the Security of Android Applications

Kimberly O'Brien-Applegate

Applications for the Android platform, an OS created by Google for smart phones, may contain security vulnerabilities that need to be discovered and fixed before they are distributed for use. This is of particular importance if the US government and military choose to have them as a resource. Problems arise if the phone is somehow compromised, whether the phone is damaged, lost, stolen, or hacked. Methods need to be created to deal with these circumstances and safeguards preventing attacks must be put in place.

This project aimed to develop a testing lab to apply combinatorial testing techniques and to automate the testing process to efficiently assess the stability and security of Android applications despite any changes in the configuration of the phone itself. Software was used to generate test case data, convert the data into a series of files for the applications, and then execute tests via an automated testing tool for a virtual Android phone.

Precision Resistance Measurement Methods Applied to Magnetic Tunnel Junctions

Brian Richards

Resistance measurements of magnetic tunnel junctions (MTJs) are achieved using different methods including two-point measurements, four-point measurements, current versus voltage, and AC resistance measurements with a lock-in amplifier. MTJs, a device used for magnetic sensing and information storage within Magnetic Random Access Memory (MRAM), are micron scale electronic devices composed of two ferromagnets separated by an ultra-thin insulating layer. When the magnetic moments of the ferromagnets are aligned, a low resistance state is created; when the magnetic moments are anti-aligned, a high resistance state is created. These high and low resistance states represent a binary set that stores information, but must be precisely measured in order to distinguish the two states. The resistance of a MTJ is difficult to measure with adequate precision in a two-point measurement and when the device's resistance is much smaller than the connections. Four-point measurement techniques mitigate this issue by isolating the resistance from the surrounding circuit. Improvements are made by sweeping through a range of voltages and measuring the current versus voltage to determine the resistance via the derivative of Ohm's law, i.e. $R = dV/dI$. Further improvements are made by summing in small AC currents with a lock-in amplifier to measure the differential resistance of the MTJ. High precision resistance measurements of the MTJ establishes market viability by showing that any noise in measuring the resistance is most likely due to the measurement process instead of defects within the device.

On Estimating the Number of Leaf Nodes on Trees
Luis Valentin

Counting problems occur in many areas of study. Determining the number of perfect matchings in a bipartite graph, modeling protein foldings, and measuring the reliability of a network all involve difficult counting problems. Even the creation of popular games like crossword puzzles and Sudoku include counting. For any counting problem, a solution tree can be constructed, where every leaf of the tree corresponds to a valid solution. We approximate the number of leaves on this tree to get an estimation of the number of solutions to the original problem.

Knuth gives an algorithm to estimate the number of leaves in an arbitrary tree by taking one random path from the root node to any leaf and assuming the rest of the tree looks similar to this path. Unfortunately, this approach has high variance and does not converge to the correct answer quickly. Aldous and Vazirani give what they call the “Go With the Winners” algorithm for finding the deepest leaf node in a tree efficiently. These deep leaf nodes are the most influential to the Knuth estimations.

We introduce a new divide-and-conquer estimation algorithm that uses a “Go With the Winners” approach. We show that this algorithm has lower variance than the Knuth algorithm and, therefore, converges on the correct answer faster.

Colorado School of Mines

Theoretical Limits of RECIST in Medical CT as a Measure of Tumor Volume
Benjamin Galloway

RECIST (Response Evaluation Criteria in Solid Tumors) is a linear measure intended to predict tumor volume in medical computed tomography (CT). Using purely geometrical considerations, we establish limits for how well RECIST can predict the volume of randomly-oriented ellipsoids and randomly-oriented tumor models, each composed of the union of ellipsoids. The principal conclusion is that a change in the reported RECIST value needs to be a factor of about 1.2 to achieve a 95% confidence that one ellipsoid is larger than another, assuming the ratio of maximum to minimum diameters is no more than 2, an assumption which is reasonable for tumors based on comparisons with empirical studies. RECIST works less well on the more realistic tumor models than on ellipsoids fitted to their second moments. There is a significant probability that RECIST criteria will cause a radiologist to select a tumor other than the largest due to orientation effects of non-spherical tumors, an issue that can lead to incorrect diagnoses of patients and misevaluations of anticancer drug efficacies.

Stability of Novel Solitons on a Bosonic Lattice
Bryce Robbins

Classical traveling waves, which arise from linear partial differential equations, often exhibit dispersion and/or dissipation depending on the governing model. In the year 1834, an anomalous wave was discovered that did not exhibit either of these peculiarities [1]. Their persistence and extraordinary stability gave rise to its name, “solitary wave”. “Solitons” are solutions to various nonlinear partial differential equations such as the Gross-Pitaevskii equation (GPE) but are special classes of “solitary waves" that remain unperturbed upon collision and interaction with other solitary waves. Solitons naturally promote the transmission of data over long distances via optical fibers due to their non-dispersive propagation; they make high speed communication on the world wide web a reality.

In GPE theory, soliton solutions emerge as either bright (excess particle density) or dark (notch in particle density) depending on the nature of the potential. Following ideas introduced at NIST [2] we are currently investigating hard-core bosons (HCB) in one or two dimensional lattices. In this limit each lattice site is either empty or occupied making it convenient to map our problem into a spin coherent state. We show that the HCB limit supports two distinct types of solitons; a dark type that vanishes as it approaches the speed of sound in the condensate and a novel solitary wave that exhibits brightening and persists up to and past the speed of sound. In this generalization of the GPE formulation we also demonstrate that the dynamical evolution of the system is dictated by the particle-hole imbalance of the lattice. This novelty gives rise to both a quantum condensed fluid and a classical normal fluid that is completely driven by its quantum counterpart. These two constituents act in concert to produce these novel two-fluid solitary waves.

Upon numerical simulation in one dimension we show that various species of solitary waves interact and emerge unaltered in shape and velocity confirming their existence as solitons. My research in particular extends our formulation to a two dimensional lattice. In general, each species of solitons appear to be extremely robust. However, instabilities of different types may cause rapid or slow decay into vortices, which are interesting in their own right. Further testing has shown that setting up these solitons on a square lattice can also lead to instabilities depending on the angle of propagation with respect to the lattice; some angles, in particular, promote long term stability while others lead to rapid decay into vortex chains. We will show computer animations that highlight the features of these novel solitons interactions with each other and with the lattice.

[1] P. G. Drazin and R. S. Johnson (1989). *Solitons: an Introduction* (Cambridge University Press, 2nd ed.).
[2] R. Balakrishnan, I.I. Satija, and C.W. Clark, *Particle-Hole Asymmetry and Brightening of Solitons in a Strongly Repulsive Bose-Einstein Condensate,* Phys. Rev. Lett. **103**, 230403 (2009).

Converse College

The Effect of Electrolyte Concentration on Poly(ethylene gycol) in a Nanopore-Based Single-Molecule Mass Spectrometry

Julianne Casil

Biological nanopores demonstrate great potential for the future of chemical analysis and differentiation. These pores have been utilized in the analysis of polymers by measuring the change in conductance as a single polymer molecule enters and interacts with the nanopore. Each polymer molecule lowers the conductance of the channel during interaction and creates a distinguishable event that has a measurable magnitude of the change in conductance and duration the polymer inhabits the pore. A model that describes the blockade depth and residence times of the polymer poly(ethylene glycol) (PEG) as it interacts with a single *Staphylococcus aureus* alpha-hemolysin (αHL) ion channel was recently developed [1]. With the present model of PEG molecule interaction with an αHL nanopore, it is assumed that the electrolyte concentration correlates with the blockade depth and mean residence time of PEG in the channel. To better understand the present model, data gathered at varying salt concentrations maybe utilized to characterize the affect of electrolyte concentration and suggest possible improvements to the current model.

1. Joseph E. Reiner, John J. Kasianowicz, Brian J. Nablo, and Joseph W. F. Robertson. "Theory for polymer analysis using nanopore-based single-molecule mass spectrometry." *PNAS.* **2010,** *107*, 12080-12085.

Cornell University

Optimizing Performance in NGF Equipment Metadata Quality Assurance Tool
Colin Schmidt

The objectives of Next-Generation Factories (NGF) in the semiconductor industry are to reduce cycle times by 50 percent and cost by 30 percent. Significant cycle time and cost inefficiencies have been attributed to equipment downtime. Achieving NGF goals requires high quality deterministic data to provide fast and accurate knowledge which allows rapid detection, analysis, and resolution of system problems during the semiconductor manufacturing process. Equipment Data Acquisition standards facilitate equipment self-description to other factory software and equipment, and require consistent implementations. In order to assure compliance quickly, an automated tool was developed to evaluate equipment metadata against the EDA standards and ISMI guidelines to report errors and suggestions. The goal of this project is to develop and research software design optimization strategies for automated equipment data communication standards compliance validation. The tool was originally designed using a rule-engine, Drools. Drools is based on the Rete algorithm, which is optimized for handling large data sets. Despite the advantages to using Drools, there are circumstances where it incurs significant performance setbacks. Several methods were used to improve the speed of the tool, including optimization of the rule engine rules, implementation of certain types of rules in pure java, and introducing parallel processing. Overall the runtime of the tool on the longest set of metadata decreased by 77.5% without parallel processing. Parallelizing the code resulted in a further decrease of runtime by 30.8%. Further optimization of the parallelization may be possible by a more intelligent re-partitioning of the workload. This dramatic increase in performance will allow the equipment metadata to be validated and corrected rapidly, ultimately enabling equipment communication interoperability to expeditiously detect, diagnose, and resolve system problems in next generation factories.

Developing a R Package for Reading and Analyzing Medical Hyperspectral Images
Alexander Wang

Hyperpectral imaging, a type of multivariate imaging that takes images in a wide multi-wavelength spectrum, was first developed for remote sensing and satellite imaging but is now used by researchers for medical applications. Hyperspectral images capture light intensity data within a range of wavelength bandwidths of fixed bin widths. Hyperspectral image files are very large i x j x k data “cubes” of i rows, j columns, and k wavelength channels.

Because of the size of the cubes, it is impossible to find anything meaningful in the images from a simple visual analysis. Thus, a set of tools is needed to analyze these images in a quick and effective manner in order to extract important information. Using the R programming language, an open source language designed for statistical computation and graphics, a set of functions are developed for reading and analyzing hyperspectral images.

As an example, a set of hyperspectral images of a pig kidney taken at 3 separate time points and 126 wavelength channels have been processed, analyzed, and visualized using these R functions, allowing human eyes to detect biological indicators in the kidney such as oxygen levels easily. Using statistical methods such as k-means clustering and support vector machine (SVM) learning, images are segmented and classified into several tissue types so that researchers can identify important regions. Also, because the images contain redundant information in the wavelength channels, dimension reduction is achieved through singular value decomposition (SVD) and principal component analysis (PCA), which when applied to the matrix formed by the spectrum of the image, allows the most significant components of the image to be extracted and analyzed.

In summary, R functions have been written which will allow researchers to read and perform exploratory analysis of hyperspectral images. We hope to further test these functions on new data sets and make these tools available to other researchers in the medical imaging community.

Duke University

Automated Extraction of Cellular Features for Potential Robust Classification Scheme

Shwetadwip Chowdhury

The advent of new imaging technologies has allowed faster and higher-resolution cellular image acquisition. This has directly aided clinical research by allowing doctors and other researchers to better visualize cells and cellular components, which improves their ability to provide accurate prognosis, diagnosis, and treatment of a variety of diseases. However, a major bottleneck now is the manual evaluation of such images. Especially with the sheer amount of data being generated from these images, manual evaluation and analysis is becoming increasingly cumbersome. To address this concern, there has been extensive work researching methods to automatically extract cellular and subcellular features that give morphological and functional insight into the cell. Some examples include extracting size/shape of cell boundaries, texture features, density of mitochondria, expression level of proteins, nuclear/cell size ratio, etc.

Here, we specifically focus on techniques to robustly extract information about the cellular actin, myosin, and phosphotyrosene from fluorescent images. These proteins are known to be important components in the signaling pathways regulating cellular proliferation. Being able to quickly and automatically extract information about such proteins from raw images will greatly aid clinical treatment and research, especially on topics related to the composition and function of the extracellular matrix. Also, automated feature extraction is a promising tool for cellular classification. Future work can incorporate our feature extraction capabilities to classify a cell into categories with known feature parameters.

Cytotoxicity Study of Carbon Nanotube Treated Primary Normal Breast Cells, Normal Breast Cell Line, and Breast Cancer Cell Line

Anne Rohlfing

The use of nanomaterials in cancer treatments is a rapidly expanding area of focus in biomedical research, due to the materials' unique properties as well as their size. Antibody functionalized single-walled carbon nanotubes (SWNTs) present one possible treatment that has generated great interest, becoming the 6th most accessed article of the year for *BMC Cancer* (Y. Xiao et. al., *BMC Cancer*, 2009, 9:351). Antibodies that target HER2, an epidermal growth factor receptor overexpressed in certain breast cancers, were conjugated with SWNTs. Two unique properties of the SWNTs, their intense Raman signal and near-infrared (NIR) absorbance, were then exploited to detect and destroy the cancer cells. Upon selective attachment to the cancer cells via the antibody coating on the SWNTs, the antibody functionalized SWNTs were subjected to NIR radiation. The sudden increase in temperature led to selective photothermal destruction of the cells. The cells treated with antibody functionalized SWNTs also produced a strong Raman signal at 1590 cm^{-1}, allowing for the detection of the cancer cells.

In order to realize the clinical application of this treatment, cytotoxicity studies must first be conducted on the functionalized SWNTs. Our study measured the cytotoxicity of the functionalized SWNTs at the cell, protein, and gene levels. Cell viability tests were performed on three different cell types – primary normal breast cells, a normal breast cell line (MCF10A), and a breast cancer cell line (MCF7) – each treated with nonfunctionalized and functionalized SWNTs. The tests showed no cytotoxicity at the cell level for the nonfunctionalized and functionalized SWNTs. Enzyme-linked immunosorbent assay (ELISA) kits were used on the three treated cell types in order to measure levels of five proteins from the cytokine family, known to be signs of an inflammatory response from cytotoxicity. The SWNT-induced damage to the total genomic DNA was also assessed for the treated primary breast cells and MCF7 cell line.

Increasing Precision of a Small Mass Balance
Mark Strom

Newly developed mass sensors have the ability to sense mass changes in the zeptogram (10^-21 grams) region, with some studies claiming the ability to sense the mass of single gold atoms. These studies measure the change in the resonant frequency of a vibrating mechanical beam as extremely small amounts of mass are added. When a beam is oscillating at low amplitudes there is a simple relationship between its mass and resonant frequency, thus by measuring the change in a beam's resonant frequency, the added mass can be determined.

Despite the remarkable resolution of cutting edge mass sensors, the smallest NIST-certified test mass is 0.5 milligrams. Smaller test masses traceable to the international system of units risk having unacceptably high uncertainty, due to the precision limits of the electromechanical balances currently used for mass calibration. Frequency, on the other hand, can be measured to a high degree of precision with devices such as a quartz oscillator and an atomic clock. This gives an advantage to microbalances that rely on measuring frequency, such as the previously mentioned vibrating cantilever beam.

In the current design, a tuning fork is attached to a ceramic chip so that one prong and the base lie on the chip and one prong hangs off of the chip like a cantilever beam. The first step is to figure out this prong's cantilever beam spring constant, k, so that any mass can be measured by attaching it to the overhanging beam and measuring the beam's resonant frequency. To solve for the cantilever beam spring constant, the beam's resonant frequency is measured as small spheres of varying masses are attached to it. The mass of each small gold or ruby sphere is determined by using a microbalance to measure the mass of the tuning fork assembly before and after the sphere is attached.

It is necessary to obtain a very precise value for the mass of each sphere so that an exact relationship between the mass of the beam and the beam's resonant frequency can be calculated. To achieve a greater degree of precision, a robotic system was created to perform automated mass measurements of the tuning fork assemblies with and without the spheres attached. With the ability to perform hundreds of consistent mass measurements, a larger statistical sample of measured mass was obtained. This could provide a more well-quantified fit between beam mass and beam resonant frequency, making the tuning fork assembly a more precise mass-measuring device. These advancements could improve small mass standards in the future.

Franciscan University of Steubenville

Calibration and Evaluation of a Computer Vision System
Stephen Nowak

As useful as industrial robot systems have become over the past several decades, their utility is still hampered in many respects by their mostly-static control systems, especially with regards to robot safety. The MEL's Intelligence Systems Division has been researching and developing several potential solutions to these problems; of these, I have been working with a computer vision system, ARToolKitPlus.

ARToolKitPlus (ARTK+) is a vision system that can be used to calculate camera position and orientation relative to physical markers on an object in real-time. I created a software tool that implements the ARTK+ software. The ARTK+ implementation can track multiple objects independently. The software functions include a camera calibration function, a multiple-object tracking function, and a pose measurement function.

This presentation will focus on our progress in evaluating the performance envelope for object detection and tracking with this software, and will include a demonstration of our application's capabilities.

Franklin Olin College of Engineering

Creating Patterns of Glass Breakage Automatically
Poorva Singal

To improve safety, we need to move away from the current prescriptive design methods towards performance based methods for the design of structures under fire. We are studying this with the NIST Virtual Measurement and Analysis Laboratory using physics based codes for fire, thermal analysis, and structural analysis. But we also need to incorporate the breakage of windows in such a way that looks realistic. However, only the time of window breakage is specified by our codes, not the pattern or dynamic effects. We use a model of glass breakage we have created by analyzing patterns of breakage in the literature to create the pattern.

We have implemented this in a general Python-based program that allows the user to specify the parameters of the window breakage. The program then automatically creates the pattern and writes out the individual glass shards. Another student is using a physics engine to simulate the dynamics of the breaking glass using the shards generated by our program. The goal is to have these simulations incorporated into an entire visualization of the burning building in order to add realism to the model.

George Mason University

Improving Performance in FiPy with Mesh Partitioning
James O'Beirne

Partial differential equations pervade many scientific fields; materials science, financial mathematics, and quantum physics all rely on mathematical analogies in terms of PDEs. Solving these equations analytically is usually out of the question and conjuring up the numerical schemes necessary to approximate a solution is feasible but treacherous and repetitive.

FiPy is a finite volume partial differential equation solver implemented in Python; it greatly simplifies the usually arduous task of solving PDEs numerically by allowing users to express problems in simple Python. Once defined, problems are then solved using existing linear algebra packages, wrapped in interfaces cohesive with the FiPy environment. Once solved, results can be visualized effortlessly with FiPy's Viewer package: an interface to existing, established graphing tools.

Solving PDEs within FiPy, or any other numerical package, is often a computationally intensive affair; code can churn for weeks (or months) before producing usable results. Fortunately, lengthy execution can be alleviated by slicing the domain of the problem, or the mesh, up into overlapping pieces and distributing out the work of solving each region of the mesh to an individual processor. That is, we can save much time by solving the equation concurrently if we partition the mesh to be solved.

My work is in getting FiPy to properly partition unstructured meshes. In my talk, I will discuss the approach I took, the resulting modules added to FiPy, and, most entertaining, the performance gains suggested by profiling results from a fairly beastly anisotropic crystal growth problem. Comparative execution time, memory usage, scaling characteristics and other computational aspects of this new approach will be discussed.

<u>George Washington University</u>

Digital Image Correlation and the Influence of Speckle Pattern Characteristics

Nicole Messier

Digital image correlation (DIC) is a non contact method of measuring the shape of a deforming object using a specific pattern applied to the object surface. Patterns can range from grid patterns to random speckle coatings. Using high speed digital cameras, DIC has the ability to capture deformation under high-rate impact loading with high accuracy. The digital images can be used to analyze various aspects of a specimen such as full-field shape, deformation, and motion measurements. DIC becomes extremely useful when performing Kolsky bar experiments. The Kolsky bar is an experimental technique that can measure the deformation of materials at high strain rates in order to study rapid impact events like automobile crashes. The DIC method is used to measure the deformation in the specimen, which helps improve the accuracy of the data obtained in a Kolsky bar experiment.

The accuracy of the DIC shape measurement depends on the qualities of the speckle pattern applied to the object. In this project we used bullet and cylinder Kolsky bar test specimens with random speckle coatings to study how the speckle pattern characteristics influenced the accuracy of the shape and motion measurements from the DIC. DIC images were analyzed using a program called ImageJ, a freeware program which can analyze various characteristics of the images such as the average speckle size and the contrast. We also studied what type of noise the DIC may have. We then examined how various aspects of the DIC measurements, such as the total displacement, total displacement uncertainty, and correlation error, were affected by different patterns, lighting conditions and calibration procedures using images acquired from still objects and from moving objects.

Optical Phantoms for Oximetry Studies

Soohyun Myung

The goal of the project is to explore the challenge of translating bioimaging into the clinic. One of the ways to do so is to employ hyperspectral imaging. It can be used to study and measure the optical properties of oxy- and deoxyhemoglobin to determine oxygen saturation of tissue and organs. The hemoglobin will be encapsulated in alginate biopolymer beads and integrated onto a microfluidic platform for oximetry studies.

In this project, alginate hydrogels are chosen as the candidate biopolymer carrying material for the deposition of encapsulated cells, proteins, nanoparticles, fluorescent beads, and other polymer microstructures. Alginates are naturally derived polysaccharides composed of (1-4) linked β-D-mannuronic acid (M-units) and α-L-guluronic acid (G-units) monomers along the polymer backbone.

Sodium alginate is soluble in water and when dissolved forms a solution of variable viscosity dependent on the concentration and molecular weight of the biopolymer. In the presence of divalent calcium ions, sodium alginate solution is crosslinked ionically between chains to form a hydrogel. The calcium ions exchange with sodium ions on the G-blocks and binds together adjacent chains, resulting in gelation of alginate.

Here, alginate microbeads are engineered as a rudimentary optical phantom that is reproducibly fabricated. Alginate hydrogel microbeads may be formed with the direct cell writing dispensing system using an external gelation or diffusion setting method. In our experiment setup, a pneumatic controlled deposition system ejects sodium alginate droplets into a $CaCl_2$ bath.

This report will provide an overview of the fabrication of calcium alginate beads, future application of the beads and the spectral results of the beads studied; blank alginate beads and alginate beads with a textile dye for hyperspectral imaging; and alginate beads with myglobin as a representative model protein in oximetry.

Econmic and Environmental Impacts of Building Energy Efficiency
Nathaniel Soares

Building energy efficiency has become a key issue in recent years because it is one of the most cost-effectives approaches used to substantially decrease energy use and CO2 emissions across the US.

The energy efficiency of a building depends upon a huge variety of factors, including windows, insulation, heating and cooling systems, climate zones, energy prices, and more.

Furthermore, building energy codes vary by state. Increasing building energy efficiency requires performing many varying upgrades. By determining the costs and benefits of such upgrades, it is possible to determine the life-cycle cost of upgrading to different standards in different regions throughout the US.

It is also possible to determine various environmental impacts resulting from such upgrades. Lowering energy use has impacts on global warming, water usage, fossil fuel depletion, production of smog, and so forth. Through the inclusion of emission data for various energy types and across regions, one can evaluate the environmental impact of raising energy efficiency standards alongside monetary impacts.

Throughout the summer, my project has been twofold:

1) Accumulate and calculate energy consumption, lifecycle cost, and energy-related emission data
2) Design an interface to allow easy access to the results

My talk will review my approach and will summarize the results that I have generated.

Hamilton College

Filtering, Processing, and Analysis of aCORN Project Data
Andrew Portuguese

In neutron beta decay, the neutron decays to a proton, an electron, and an antineutrino. Using an improved method, the "a" Correlation in Neutron Decay (aCORN) collaboration seeks to measure the electron-antineutrino correlation in free neutron beta decay, which is characterized by the dimensionless parameter "*little a,*" and seeks to perform this measurement within 1% relative uncertainty. Experimentally, proton and electron detectors sit at opposite ends of a 3m long vacuum tube within a solenoid, through which a cold neutron beam runs. The cold neutrons decay, and coincident proton and electron detection allows measurement of the beta electron energy as well as the time-of-flight (TOF) of the proton. The configuration of the apparatus permits coincidence detection in two distinct decay cases, kinematically distinguished by the proton TOF, and the experimental asymmetry of these cases enables precise determination of a. Since many decays must be acquired, a data acquisition system with high throughput is necessary to acquire, filter, process, and store all gathered coincidence data in a usable form. The system must be robust enough to detect all coincident data from nineteen electron detectors that make up the beta spectrometer, eight backscatter veto detectors, and a proton detector; but agile enough to filter all off-coincidence signals in real time. After a specific number of detector events are digitized, the events are time sorted and coincidences are identified. Off coincidence and electron backscatter events are discarded. Each fully absorbed electron energy event and its corresponding proton TOF are stored. The principles of the aCORN data handling system will be discussed in this presentation.

Harvey Mudd College

Characterizing Quantum Dots in Fiber-Coupled Nanofabricated Waveguides
Robert Hoyt

Epitaxially-grown quantum dots (QDs) promise advancements in both classical and quantum information processing. Traditional measurements of QD emission using free-space optics are limited by total internal reflection due to the high refractive index of materials like GaAs, yielding collection efficiencies below 2%. We have proposed an approach using a micrometer diameter tapered optical fiber waveguide to out-couple the QD emission, and have calculated that efficiencies as high as 70% can be achieved if we fabricate a 160 nm wide waveguide around the QD. This approach introduces two new challenges: sensitivity to waveguide roughness and the need for fiber-compatible devices for wavelength selection.

Although an ideal rectangular waveguide produces high collection efficiencies, real waveguides will always have some variations due to errors throughout the fabrication process. Understanding how these variations affect the coupling efficiency is critical to understanding experimental data. Based on simulations employing the Finite-Difference Time-Domain method, sidewall roughness on the order of 5-10% of the waveguide width can reduce both the QD's radiated power and the overall coupling efficiency, especially at longer wavelengths.

The other problem is wavelength selection, where a QD's emission must be isolated from the background radiation from the surrounding material. An ideal solution would have high transmission, provide good isolation against background emission and be adjustable across a wide range of wavelengths compared to the current fiber-coupled bandpass filters. This is solved by collimating the fiber output into a free-space beam and using a tunable grating filter to select the desired wavelength. Circularizing the grating's output using cylindrical optics and focusing the beam back into a fiber achieved 25% transmission with good isolation. Further improvements in beam shaping and focusing could yield up to 40%.

Spintronic Effects in Nanomagnet Dynamics
Brian Soe

Spin transfer effects are of great interest in the development of technology such as magnetic memory. In a ferromagnetic material, electrical current can be polarized to carry angular momentum, which can be transferred to another nanoscale ferromagnet to flip its moment, as done when "writing" a memory cell. The critical current necessary to achieve this flip decreases as current polarization increases. In order to increase the current polarization of cobalt iron (CoFe) ferromagnet, the alloy was doped with varying levels of Germanium (Ge). The current polarization of the sample was measured using spin wave Doppler technique, in which a spin waves generated by a microwave antenna interacts with the polarized current as described by the spin transfer torque theory. This creates a shift in the spin wave frequency, from which the magnetization drift velocity and current polarization can be found. The current polarization was found to increase from 0.84+/-0.04 with no doping, to a maximum of 0.95±0.04 at approximately 25% Ge.

I have written a general purpose Labview program to verify resistivity findings as well as perform other measurements involving a single input and output. The resistivity measured in a Hall bar geometry was found to increase with the level of Germanium, which agreed with results from the devices used in spin wave Doppler measurements. A higher resistivity increases Joule heating, which introduces a potential source of uncertainty. A resistivity vs. temperature calibration was performed to determine the heating effect in the different samples. From the calibration, we determined there was no significant temperature change for the narrowest sample (2um wide) at current densities up to 1.5×10^{11} A/m^2.

Haverford College

The Effect of Manganese Particles on SH-SY5Y Neuroblastoma Cells: Oxidatively Induced DNA Damage

Jeff Schneider

Many varieties of nanoparticles are mass produced in today's society, yet little is known of their effects on health and the environment. For example, exposure to excess manganese (Mn) is known to cause a Parkinson like disease known as Manganism, but neither the mechanism, nor the effects of different forms of Mn are known. It is known that some nanoparticles can reach places in our bodies and cells that bulk particles cannot. In doing so, they may create an increase in reactive oxygen species within a cell that leads to an increase in oxidative damage to its DNA. The comet assay is commonly used to test for this, but this lab (DNA science group at NIST) has developed unique methods using gas-chromatography/mass spectrometry (GC/MS) to examine the specific chemical changes (lesions) that occur in the bases of the DNA. In this study, we focused on the effects of Mn ions on neurological cells.

Cultured SH-SY5Y neuroblastoma cells were exposed to 0 - 300 micro molar concentrations of $MnCl_2$ for periods of 0 - 24 hours. The extracted DNA was then washed with ethanol, solubilized in water, and derivatized before being analyzed by GC/MS. Isotopically labeled internal standards were added before such analysis in order to determine the lesions per million base pairs of each sample. The lesions analyzed were 4,6-diamino-5-formamidopyrimidine (FapyA), 2,6-diamino-4-hydroxy-5-formamidopyrimidine (FapyG), 8-hydroxyguanine, 5-hydroxy-5-methylhydantoin, 5-hydroxycytosine, trans 5,6-dihydroxy-5,6-dihydrothymine (thymine glycol).

Although previous comet assay measurements under the same conditions of exposure to Mn showed DNA strand breaks (oxidative damage to DNA), our preliminary data has shown no substantial accumulation of oxidatively induced lesions compared to controls in the absence of Mn. These results are necessary to establish a set of controls that can be used in future studies of Mn nanoparticles. Such negative controls will be critical in these studies.

Hood College

Effects of Sidechain and Backbone Structure on Semiconducting Polymers

Jessica Henry

This study examines the effects of side-chain and backbone structure on two semiconducting thermotropic liquid-crystalline polymers: poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene) (pBTTT) and poly(3,6-dialkylthieno[3,2-b]thiophene-co-bithiophene) (pATBT), with varying side-chain lengths. Dielectric relaxation spectroscopy was employed to characterize the frequency-dependent relaxation behavior of thin films (100 to 200 nm thick) over a temperature range of -130°C to 100°C. Understanding the relaxation properties of semiconducting polymers will allow for new and improved organic electronic materials and will provide fundamental insight into the dynamics of thermotropic liquid crystalline polymers. Organic materials in modern electronics promote cheap and simple device fabrication, large area applications, flexible substrates and rapid prototyping.

OMCE Merging
Nathan Jacobson

NIST has developed the Open Monte Carlo Engine (OMCE) as a tool to be used within other softwares. OMCE is a mathematical simulator that generates histograms of mean values and standard uncertainties. It reads in an XML file, runs a simulation, and then saves the results. Over the summer, I wrote a Python program that combines multiple XML structured files into one. This allows us to be able to run inputs from multiple files with the OMCE tool, which had been designed to handle a single file only. The program has to analyze the content of the XML files to decide how to handle duplicate entries and whether to delete them or rename them. Monte Carlo simulations are very important because there are so many equations that one wants to solve yet can not be done analytically or there is not enough time. Monte Carlo helps one get answers when not possible otherwise. The NIST software is very important because it validates Monte Carlo simulations. I was able to improve and expand the data handling of the bookkeeping capabilities of the validator.

Jackson State University

Smart Polymer Surfaces for Controlling Interfacia Adhesion
Kandice Williams

From cell attachment, to functional coatings, to pressure sensitive adhesives, controlling adhesion of an interface is a very important problem that has implications in many different technologies. One approach to controlling adhesion and release is via the development of a responsive wrinkled surface. This control has been suggested to be related to the coupling between the length-scale of the wrinkle patterns with a natural length-scale defined by the properties of the interface. In this work, we seek to better understand the contributions of wrinkle wavelength and amplitude in controlling adhesion with a soft material interface. A contact mechanical-based approach is used to quantify the adhesion of wrinkled surfaces. For smooth interfaces, the theory of Johnson, Kendall and Roberts (JKR) can provide quantitative measurements of the adhesion energy from a single indentation experiment by bringing a lens into contact with a surface while monitoring the load, displacement, and contact area during the test. This theory is difficult to implement for patterned interfaces such as wrinkled surfaces. To quantify the adhesion energy for wrinkled surfaces, we have developed a new measurement approach that does not rely on established contact mechanical models such as the JKR. To demonstrate its utility, we apply this new approach to quantify the adhesion of smooth model elastomers and compare the results predicted by the JKR model. Finally, we use this approach to quantify the adhesion of wrinkled surfaces and relate their adhesive performance to the length-scales of wavelength and amplitude.

Johns Hopkins University

Combinatorial Methodologies Applied to Thermoelectric Materials Development
Howard Joress

Thermoelectric (TE) devices show great promise as a means to reduce our reliance on oil and other forms of costly and unsustainable electrical power generation by capturing waste heat and converting it into electrical power. TE materials (such as Bi_2Te_3) also have important solid state cooling applications. Unfortunately, there currently is no material that can convert energy efficiently enough to make such devices practical beyond a few niche applications. Combinatorial methods can be used to accelerate this search. These methods have the ability to quickly create and screen compounds for desirable properties, greatly decreasing the time and cost of research and development.

In order to study the correlations between structure and TE properties of oxide materials, which have thermal stability at high temperatures, we have manufactured a continuous, binary, combinatorial library of $Ba_2Y_{1-y}Gd_yCu_3O_{6+x}$ using pulsed laser deposition (PLD). By scanning the library using x-ray diffraction we observed the lattice parameters of the crystal changing as a function of composition, y. The library was also used to demonstrate the feasibility of utilizing our thermal conductivity tool for screening combinatorial libraries. In addition, using our Seebeck coefficient screening tool, we have demonstrated the variation of the Seebeck coefficient of a single crystal $Bi_2(Te_\delta S_{1-\delta})_3$ along the concentration gradient δ. In order to verify the existence of the gradient we calculated the carrier concentration through the use of Hall resistance measurements data.

Juniata College

Neutron Reflectivity and Magnetization Reversal in Heusler Alloy Spin Valves

Theresa Ginley

Read-head sensor performance is based in part on the spin polarization in the magnetic layers forming the spin valve. Heusler alloys, which are half-metallic ferromagnets, are currently among the most promising class of materials used in spin valves. Here, we study spin valves (glass/3nm Ru/3nm Cu/FREE/5nm Cu/0.5nm $Co_{50}Fe_{50}$ / 4nm CMG/1nm $Co_{50}Fe_{50}$ /6nm $Ir_{20}Mn_{80}$/12nm Ru) with the Heusler alloy $CoMnGe_2$ (CMG) in the free layer. Transport studies demonstrate that when 0.5 nm CoFe layers are added to the top and bottom sides of the 8 nm CMG free layer, the magnetoresistance increases by 25% relative to that measured in spin valves with CMG alone. Magnetometry experiments show that the transition between the nominal parallel and antiparallel states near 5 mT is sharp for the CoFe/CMG/CoFe combination, but the same transition is smeared over a large field range for the CMG free layer alone. To understand the origin of this transition difference, we used polarized neutron reflectivity (PNR) to probe the interfacial magnetic structure of the free and pinned layers. PNR is a unique measurement tool because of its sensitivity to the depth-dependent magnetic structure of ferromagnetic layers on a nanometer length scale. PNR at 5 mT on the CMG samples have spin-flip scattering, indicating that a component of the magnetization is perpendicular to the field, contrary to expectations. (Specifically, the free layer magnetization is canted at an angle of approximately 50° relative to the field.) This spin-flip scattering gradually diminishes as the field is increased from 5 mT to 52 mT. Our results demonstrate that in spin valves with CMG alone, the free layer reversal proceeds via gradual coherent rotation rather than domain formation. In contrast we found no indication of spin-flip scattering for the CoFe/CMG/CoFe sample at any field measured. In addition, the spin valve with the CMG free layer alone showed in x-ray scattering an increased interfacial roughness with the neighboring Cu layer that was not present in the CoFe/CMG/CoFe sample. It is thus possible that the increased roughness is, in part, responsible for the undesirable reversal behavior and for the subsequent reduction of the magnetoresistance.

Lebanon Valley College

Characterizing Anomalies in Retroreflective Sheeting Material Using Goiometric Scanning Techniques

Matthew Thiesse

The study of retroreflectivity is of great importance in practical applications such as traffic signage as well as safety reflective tape. While nighttime characteristics of such materials are very well characterized and understood, daytime characteristics are more complicated and variable. Current guidelines for daytime measurements have been surpassed by the technologies that make up these materials. There are several technologies currently being utilized in retroreflective materials manufacturing including spherical bead coatings and, more interestingly, microprisms. For daytime measurements, the annular or circumferential 45°/0° (or 0°/45°) geometries are used. However, when observing a retroreflective surface at 45 degrees from the illumination angle, anomalous bright spots appear in symmetric increments along the entire annular ring for certain types of material. Two related yet individually important experiments are discussed.

For different types of retroreflective materials, the described anomaly is characterized and quantized using goniometric measurements. For even the best goniometers, an entire run of data-collecting could take hours to complete. To optimize this time without sacrificing the accuracy of the results, it is possible to decrease the angular spacing between measurements (thereby decreasing the total number of data points taken) while creating an acceptable amount of resultant uncertainty. Currently, the Illumination Engineering Society (IES) and the American Society for Testing and Materials (ASTM) have guidelines dictating the angular spacing required for such measurements for certain types of luminaires but these guidelines do not include uncertainties resulting from these geometries. For various spherical angular spacings, different uncertainties were found computationally using the Mathematica software package. This information can be generalized to any application utilizing goniometric measurements.

Data was then taken on the NIST five-axis goniometer for angle sets that represent portable reflectometers for several types of materials. The resulting bi-directional reflectance data was then integrated to match different portable reflectometers manufactured by multiple vendors. Significant differences were found suggesting the need for a revision of current daytime retroreflectivity measurement techniques. Future work to help determine new daytime techniques will be presented.

Lehigh University

Interaction of Single-Wall Carbon Nanotubes with Biomolecules in Aqueous Solutions

Melissa Goleb

Individual single-wall carbon nanotubes (SWCNT) show great potential for many nanotechnology applications. They have unique electronic properties, great tensile strength for their size, and they are efficient heat conductors. Semiconductor type SWCNTs show extremely stable photoinduced band gap luminescence in the near-infrared (NIR) range. Applications of SWCNTs include single nanotube field effect transistors, transparent conductors, biosensors, and fluorescent probes. Detailed understanding of SWCNTs interactions with biomolecules, specifically proteins, is crucial for the development of nanotube-based technologies.

Dynamics of SWCNTs and proteins in solution can be observed by techniques such as dynamic light scattering (DLS) and fluorescence correlation spectroscopy (FCS). Both methods detect diffusion coefficients of the dispersion constituents, the former relying on the scattered laser light and the latter detecting fluctuations of nanotube fluorescence in a confocal detection volume. In combination with absorption spectroscopy, we can create a comprehensive optical characterization of protein-dispersed nanotubes in aqueous solutions.

SWCNTs grown by the cobalt-molybdenum catalyst (CoMoCat) method were dispersed by sonication in bovine serum albumin (BSA) solution in phosphate buffered saline (PBS) with various initial concentrations of nanotubes and BSA. Individual NTs were separated from residues by centrifugation. Remaining NT mass content was measured by the visible-near-infrared (Vis-NIR) absorption spectroscopy and the presence of individual nanotubes was confirmed by the NIR fluorescence spectroscopy. The ratio of free protein molecules to the nanotubes in dispersion and the mean nanotube length was measured by DLS and FCS. The effect of adding of surfactants was also explored.

Marquette University

Topography Measurements and Correlations for NIST SRM 2461 Standard Casings
Charles Janicki

When a bullet and casing are discharged from a firearm, both the bullet and the casing receive markings that are characteristic to the overall class of the same type of firearm as well as markings that are uniquely characteristic to the individual firearm. When a bullet or casing is recovered from a crime scene, a ballistics examiner uses an Integrated Ballistics Identification System (IBIS) to acquire a digitized optical image of the signature markings on the bullet or casing. These digitized images are then stored in the National Integrated Ballistics Information Network (NIBIN) and compared with other digitized images of bullets or casings obtained from crime scenes. In the process, high-confidence candidates are identified.

To maximize the probability of a match, reference standards and quality control procedures must be established. IBIS stations across the United States need common standard bullets and casings for use in calibrations and quality control, which leads to the discovery of differences in their image capturing and correlation. Currently, the National Institute of Standards and Technology (NIST), in association with the Federal Bureau of Investigation (FBI) and Bureau of Alcohol, Tobacco, Firearms, and Explosives (ATF), have developed Standard Reference Material (SRM) 2460 bullets and 2461 prototype casings. The SRM casings are produced using a master casing, fired under standard firing conditions at ATF, through an electroforming process. Through previous analysis of the first three production shipments, the electroformed casings have demonstrated very small decay factors and thus, high reproducibility of the surface topography of the original casing.

To ensure that the one hundred and five casings from the fourth production shipment have similar surface topographies, 3D measurements of the firing pin impression and breech face markings are made using a Nanofocus confocal microscope. Correlations, emphasizing the Cross-Correlation Function Maximum (CCF_{max}) and the NIST developed parameter of Topography Difference (D_s), are then performed on the firing pin and breech face measurements. As of now, the accepted CCF_{max} cutoff is 95% but recent results demonstrate that further analysis of the accepted long wavelength cutoff of the Gaussian filter is needed to accurately assess the reproducibility of the SRM casings.

Massachusetts Institute of Technology

Mechanical Properties of the Active Layer in Organic Solar Cells
Bethany Lemanski

Organic solar cells are emerging as a promising source of renewable energy. These devices are an attractive alternative to traditional inorganic solar cells (e.g. silicon-based) due in part to their ability to be processed at room-temperature on low-cost plastic substrates using roll-to-roll manufacturing methods. Although organic solar cells are relatively inefficient (< 10 %), the low-cost production may make them an economically competitive energy source. However, before companies can begin roll-to-roll manufacturing of devices on a large scale, they must understand how processing parameters affect not only the device performance but also the mechanical properties of the active layers.

In this study we focus on a widely studied bulk heterojunction organic solar cell with an active layer that consists of a blend of regioregular poly(3-hexylthiophene) (P3HT), and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). The mechanical properties of this material system are studied under varying processing conditions, forming different film morphologies. We use a buckling based metrology to determine the Young's modulus (a measure of stiffness). We then measure the crack onset strain by placing the films under tension to examine brittleness. Along with measuring the mechanical properties, organic solar cells are fabricated to compare the mechanical properties to device performance. From this analysis we correlate device performance to mechanical properties and suggest avenues of producing efficient solar cells that have favorable mechanical properties.

Miami Dade College

Software Validation and Verification
Thomas Silva

The NIST Weights and Measures Division uses a number of Microsoft® Excel(TM)[1] spreadsheets in training seminars and as job aids that are associated with calibration procedures and proficiency tests/interlaboratory comparisons. Formal verification and validation methods need to be studied and implemented for these Excel spreadsheets as they are posted online and available to State Weights and Measures laboratories and industry. In addition, training and references on software verification and validation are provided to NIST customers. This project included:

1) reviewing and updating of a Standard Administrative Procedure (SAP 10) based on literature review and best practices from State laboratories;

2) updating a software evaluation checklist/form and laboratory inventory file also based on literature review and best practices from State laboratories; and

3) reviewing three sample Excel spreadsheets for performing double substitution (Standard Operating Procedure,

4) using
  a) SAP 10;
  b) sample data sets from published data, hands-on measurements, and extreme data; and
  c) the software evaluation form.

[1] No approval or endorsement of any commercial product by the National Institute of Standards and Technology is intended or implied.

Miami University Ohio

Measuring Optical Detector Linearity
Alexis Denton

Radiometers are vital in measuring solar spectral reflectance, radiance, and irradiance in applications of General Field Spectrometry and Oceanography, but one remaining problem of interest with optical detectors is their nonlinearity. For instance, the Hubble Space Telescope must deal with nonlinearities in its internal optical detectors, which, if not accounted for, may lead to inaccurate readings of signals from stars and other celestial bodies. To investigate these nonlinearities, the responsivities of the Analog Spectral Device, Compact Array Spectrometer, and basic Silicon detector were measured with a beam attenuation method. The Beamconjoiner III, developed at NIST, splits the beam of an incoming light source, passes it though a combination of three filters, each with 8 different transparencies, re-attenuates the beam, and passes the radiation through to the optical detector. With 120 possible filter combinations, 120 signals and 30 dark signals were recorded for a Tungsten Lamp and a 515 nm Class IV Argon Laser, and the responsivities of each detector were plotted against the input signals to examine the linearities.

The ASD, an ideal remote sensing device due to its portability and spectral range (350 nm to 2500 nm) is commonly used by researchers measuring reflectance in deserts and crop fields. The importance of corrections to the internal linearity of optical detectors will be discussed in terms of the effect they have on data taken by these researchers, for example the effect these coefficients might have on the determination of the health of vegetation.

Understanding Kinematic Positioning of an X-Ray Optic using 3-Dimensional CAD Modeling
Nicholas Helmulth

The Parallel Beam Diffractometer (PBD) of the Ceramics division is the most accurate X-ray diffraction measurement instrument in the world and is used to calibrate all other diffractometers through certification of NIST Standard Reference Materials (SRMs). NIST uses the PBD to characterize lattice spacing of SRMs to very low uncertainties and this is achieved through a systematic and comprehensive approach to alignment of the PBD. Nearly every component of the PBD has the capability of being rotated and translated to near perfect alignment so that the uncertainty of data gathered through experimentation can be estimated and minimized. Optimal alignment of the components is often achieved through kinematic adjusters, or mounts that ensure the attached body is not over-constrained through its degrees-of-freedom. Thus, properly constraining the body requires exactly six points of contact, one for each degree-of-freedom. This principle not only inhibits undesired movement of the body during positioning, but prevents stress from being introduced to the attached body, making kinematic mounts appropriate for mounting and adjusting the PBD optics.

Several commercially manufactured kinematic adjusters are available and designed specifically for the mounting of optics. In particular, the Five-Axis Aligner Model 9081, manufactured by New Focus*, is used to position a graded, parabolic mirror within the PBD. This mirror is the first conditioning optic for the X-rays used in the PBD. Nominal specifications for linear travel, angular range, along with linear and angular resolution are provided through the manufacturer. However, a greater understanding of the device and its interaction with other components is necessary. In this presentation, I will show the results of constraining of a 3-dimensional Computer Aided Design model of the mount and the surrounding system. This modeling made it possible to determine practical limitations for experiments by studying the system in the simulated environment. I will present deviations between the nominal specifications and the actual Five-Axis Aligner behavior. I will also show the possible range of motion for the adjuster and will conclude with future modifications to the mirror housing determined through this range of motion study.

*Certain commercial equipment, instruments, or materials are identified in this document. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the products identified are necessarily the best available for the purpose.

<u>Middlebury College</u>

Automated Logical Inference and Reasoning
Derek Campbell

Automated logical inference systems and reasoners have applications in defense, medicine, manufacturing, and many other fields. Relying on a small set of rules, an intelligent system can derive large amounts of new knowledge from facts supplied by a user. Two primary challenges arise. The first is to find a way to represent knowledge about the real world in form usable by an automated system. The second is to construct such an automated system that can infer new knowledge in an efficient manner.

The language of First-Order Logic will be discussed as a tool for representing real-world information. An overview of an inference strategy will be given, and the problem of unification will be addressed. Unification with individual variables is a well-understood problem, with more than one highly efficient (linear-time) solution in existence. Languages involving sequence variables can be much more expressive than languages restricted to individual variables, but unification with sequence variables is a more difficult problem. Possible solutions to this problem will be discussed.

WRed: Data Reduction in a Web-Based Environment
Joseph Redmon

The NIST Center for Neutron Research (NCNR) is a user facility in which scientists come from around the world to perform experiments. The center currently provides a suite of data reduction programs through the DAVE project to aid new users in data reduction and to speed the workflow of experienced scatterers.

The focus of this project was to explore web-based data reduction of triple axis neutron scattering data. Web-based data reduction offers several advantages over traditional desktop based data reduction. Portability is one obvious advantage to a web-based system. NIST is currently platform agnostic, so it must distribute working programs for Mac, Windows, and Linux operating systems. A web-based system developed for W3C standards-compliant browsers bypasses this portability issue, and will operate the same regardless of operating system or web browser. Web development also solves the version control issues. If there is a bug in a release of local software we can patch it in the next release, however users may not update to the current version for some time (i.e. IE6). With web-based software, bugs can be patched for all users simultaneously. Also, as data sets get larger, then specialized hardware such as GPUs and clusters become necessary to process the data in a timely fashion. Web-based development allows us to hide that complexity from the user and allows them to focus on their data reduction needs.

In this project, I implemented several key features:

1) A RESTful architecture, which allows for live updating of data as it comes off the instrument. It also allows for easy scaling and deployment as the project progresses.
2) Graphical reduction pipelines. We can envision the reduction of data as a flow through a pipeline of reduction steps such as adding files to increase signal, subtracting background files, applying detailed balance corrections, etc. We allow the user to create such pipelines graphically, and inspect their data after each step. This allows users to easily create reduction templates and quickly identify any problems that arise in any step of the process. Furthermore the pipeline is updated automatically if live data comes in off the instrument.
3) Extensible fitting. Several basic data fitting algorithms are already implemented, and a generalized fitting template allows for additional fitting algorithms to be added as necessary.

Real-Time Person Tracking in Video Streams for the Smart Space Project
William Westling

Tracking objects in video feeds in real-time is a challenging engineering task. Fortunately, the problem can be split into many distinct parts, including foreground segmentation, connected component computation, and statistical tracking, which can be spread across available processors. The person tracking pipeline for the Smart Space project was built on top of the NIST Data Flow System II distributed computing architecture. Each step is run within its own module, potentially on its own networked computer, while NDFS II sends data from one module to the next. This modular approach also allows one to interchange algorithms in order to find the best balance of speed to accuracy or to take advantage of advances in the field.

The person tracking pipeline was designed to be integrated into the larger Smart Space project using a blackboard architecture, which will employ a multi-camera setup to additionally obtain the subject's face identification.

Millersville University of Pennsylvania

Developing a Real Time Face Identifier for the Smart Space Project

William Killian

Properly identifying people in real time from a multiple video feeds is a non-trivial task. Better results for face identification occur when using more elaborate algorithms that have time to analyze all components of a face, but those algorithms are far too slow to run in real-time. We substituted using slower algorithms with distributed computing across multiple computers and processors. The algorithm used to develop a real time face identifier has two primary parts; the first part determines the feature set of the face using Eigenvectors while the second part uses a Support Vector Machine (SVM) as a classifier. After the system is trained on a known set of subjects it can be applied to predict a face identity. This algorithm has been incorporated into the NIST Data Flow System II, a distributed computing architecture capable of processing large volumes of data. The identification rate of the algorithm in a single view environment has been evaluated. Future incorporations of the identifier may include utilizing a multi-camera environment to identify all individuals in a given scene. There has been a strong emphasis on integrating the face identifier into a complex Blackboard architecture. This usage of a distributed system can result in meeting reconstruction, recording, and a better overall understanding of events occurring in a scene.

Montana State University

Research for the Revision of National Fire Protection Association 1982 Standard on Personal Alert Safety Systems

Cassandra Knierim

Personal alert safety system (PASS) devices, which sound an alarm when activated, are worn by many firefighters in dangerous environments. These devices are generally required to comply with the National Fire Protection Association (NFPA) 1982 Standard, which is currently under revision to add requirements regarding the alarm sounds and patterns. The ideal PASS alarm would be one that is easily localized spatially, easily heard over common fireground sounds, and if possible, psychologically/physiologically draws attention and instills a sense of urgency. Little experimental work has been done with PASS alarm sounds themselves, but there is preexisting work regarding psycho-physical responses to specific sounds, sound source localization, sound transmission and obstruction, and sound characterization and measurement. The search and review of this literature will be used in the formulation of a scientifically-supported PASS alarm, designing any further experiments, and finally, in the actual revision of the standard.

Mount Saint Mary's University

Analysis of the Nanomechanical Properties of Biocompatible Coatings on Gold and Silver Nanoparticle Surfaces

Carly Geronimo

Coatings on nanoparticles (NPs) enable a range of applications, and are typically characterized by integrative techniques. However, it is challenging to characterize molecular coatings on NPs with single NP resolution. Therefore, this work sought to explore the nanomechanical properties of a range of molecular coatings on NPs, with AFM force spectroscopy as the primary characterization technique. It was hypothesized that the adhesion force between an AFM tip and a coated NP should depend primarily upon the NP's surface coating. NPs with different coatings were engineered to study their effects. Five different coatings were selected for characterization comparisons: PEG-SH (5K), PEG-SH (20K), Polyvinylpyrrolidone (PVP), Dextran, and Bovine serum albumin (BSA). Thus, for comparison of core metal NPs, commercial gold nanoparticles (AuNPs) and lab synthesized silver nanoparticles (AgNPs) were used. Finally, this study explored aptamer-coated AuNPs. Aptamers, special DNA sequences that adopt unique and well-defined 3D structures, attached to NPs are currently being investigated for applications ranging from biosensors to targeting ligands for drug delivery. In particular, aptamers are of great interest as a cost effective alternative to antibodies for increasing the uptake of NPs to specific organs and tissues. Other advantages of aptamers include their capability to bind to specific target antigens with high affinity and specificity, smaller size, lack of immunogenicity, and ease of isolation. However, little is known about the behavior of aptamers on NP surfaces and its effects on colloidal properties. In conclusion, this work will summarize the feasibility of using AFM force spectroscopy to identify and characterize surface coatings on single AuNPs and AgNPs.

Controlling Agglomeration Sizes of Silver Nanoparticles with Different Polymer Coatings: Effect of Coating on Agglomeration and Cytotoxicity

Melissa Halter

We live in a society that is driven by advancements in science and technology. Widespread interest in nanotechnology has made nanoparticles a popular area of study. Nanoparticles range in size from ~1 nm to 100 nm in diameter. They can be found in many common consumer products such as makeup and sunscreen. Nanotechnology has a vast range of applications from creating new materials to being used in medical devices. One obstacle in the advancement of nanotechnology is the unknown toxicity of nanoparticles. It is very difficult to perform reproducible toxicity studies on nanoparticles because of their uncontrolled agglomeration that arises from van der Waals forces.

Controlling agglomerate sizes of silver nanoparticles with different polymer coatings helps achieve reproducible results and enables study of the effect of agglomeration on toxicity. Several factors, including nanoparticle concentration and mixing rate, have been found to be crucial for accomplishing reproducible agglomeration. Here, we analyzed silver nanoparticles with different polymer coatings by adding them to cell culture media where some agglomerated. Bovine albumin serum, a protein, was then used to coat the nanoparticles to stop agglomeration once they reached their desired size. Dynamic light scattering and ultraviolet-visible spectroscopy were used to confirm agglomerate sizes.

We were able to successfully control agglomerate sizes. The agglomerated silver nanoparticles will be used in cytotoxicity studies. It is hypothesized that increasing the agglomerate size of the silver nanoparticles will decrease their hemolytic toxicity.

Muhlenberg College

Accurate Optical Models for OPV Device Performance
Jake Herb

Nanostructured organic photovoltaic devices (OPVs) composed of a photoactive polymer and a fullerene derivative hold promise as being cheaper and easier to process than current silicon solar cells. With the possibility of roll-to-roll production and the ability to create flexible solar cells, OPVs are quickly becoming attractive alternatives to silicon cells. OPV device performance is determined by a combination of optical and electronic/transport effects in the bulk heterojunction (BHJ). For example, while simple models predict that performance should monotonically increase with active layer thickness, the performance of real devices typically exhibit an 'optimum' thickness (due to transport limitations) and can show oscillations in performance with thickness (due to optical effects). We are exploring if accurate modeling of the optical effects in devices will facilitate insight into the transport limitations of devices.

OPV devices have been fabricated OPV with two polymers: poly-3-hexyl thiophene (P3HT), the earliest high performance OPV material, and poly-3-octylphenyl thiophene (POPT), a material designed for better performance. Spectroscopic ellipsometry is performed on reference films to develop accurate optical models. Device measurements, both as a function of incident wavelength (external quantum efficiency) and as a function of electrical load (power conversion efficiency) are performed as a function of active layer thickness in the (30-200) nm range. Reliable device fabrication is a challenge. Trends suggest that one can separate poor exciton separation kinetics from transport limitations, as well as identify the limiting carrier (electron or hole) from characteristics in the thickness series.

North Carolina State University

Electrical Characterization of Soluble Organic Materials
Andrew Hewitt

Organic molecules are of great interest both academically and for their potential industrial applications. Organic electronics have great potential to be used in low-cost, flexible, and easily fabricated devices. Specifically, organic field-effect transistors (OFETs) are of particular interest because they allow us to begin to access the intrinsic electrical properties of the organic material. We have characterized newly synthesized material generated by a collaborator at the University of Kentucky, John Anthony, via spin and drop cast methods and single-crystal growth. Electrical properties, such as mobility, on/off ratio, voltage threshold, and swing voltage, are presented and their sensitivity to processing techniques such as substrate preparation, spin speed, solution concentration, and curing are discussed. Assessing how these processes affect electrical properties is vital for advancing the field of organic electronics.

Analysis of Marginally Trapped Ultra-Cold Neutrons for Neutron Lifetime Experiment
Daniel Marley

The neutron beta-decay lifetime plays an important role in providing a test of the Standard Model and in theoretical predictions of the primordial abundance of ^{4}He in Big Bang Nucleosynthesis. The decay of a free neutron is a product of the weak interaction and results in a proton, an electron, and an anti-neutrino. At the National Institute of Standards and Technology Center for Neutron Research (NCNR) there is currently an ongoing experiment aimed at improving the current value for the neutron lifetime. The neutron lifetime experiment uses ultra-cold neutrons, cooled using a superthermal process, magnetically trapped within a cell to measure the lifetime. When a neutron decays, the electron from the decay ionizes the liquid ^{4}He, producing scintillation light that is detected using photomultiplier tubes. In order to ensure that an accurate measurement of the neutron lifetime is made, much analysis must be done on the systematic uncertainties associated with the experiment. One of the largest sources of uncertainty stems from marginally trapped neutrons remaining in the cell. A neutron is marginally trapped if it has energy greater than the trap depth of the magnetic field, but has an orbit through the cell such that it remains in the trap. The orbit of neutrons can change over time in the cell and as a result there can be wall interactions that cause upscattering, absorption, or reflection of the neutron on timescales similar to the neutron lifetime. Consequently, the neutron lifetime calculated from data consisting of permanently trapped and marginally trapped neutrons will be systematically shorter than the actual lifetime of the neutron. The materials lining the cell contribute to the factors listed above through both the real and imaginary parts of their nuclear potentials. The imaginary portion of a material's potential represents the absorption and incoherent scattering of the neutrons while the real portion describes reflection. Analysis is done concerning the values of each material's potential to determine the effect of marginally trapped neutrons using a Monte Carlo simulation and the corresponding results will be presented.

Oklahoma State University

Three-Dimensional Phase Reconstructed Data Cube
Bryan Sudbrink

Despite fundamental assumptions in surface analysis, that the surface is representative of the whole and the analysis area is homogeneous at sampling depth, concrete remains a heterogeneous material. In order to track and summarize the change in composition with depth, a method was developed using X-ray spectrum imaging. To test this, X-Ray spectrum images were taken using an Eagle III micro XRF (µXRF). After each scan a 30 µm depth was ground off and then the sample was rescanned, holding the analysis area constant. The data from each scan were then used to develop Composition Simility models for cement and concrete analysis. Alteration in the aggregate phases occurs gradually, whereas alteration in the cement phases can occur immediately. X-ray spectrum imaging provides a compositional summarization which, contrary to assumptions made in surface analysis, confirms that phases will appear and change location within a sample on the order of tens of microns.

Pennsylvania College of Technology

Production and Evaluation of a 5-Axis Test Artifact
David Blumenfeld

Characterizing 5-axis coordinated motion is an important concept for optimizing performance of a 5-axis machine tool. One way to do this is through the machining of a test artifact. The goal of this project is to create a machining and metrology procedure for inclusion in an ISO standard (10791-7 - Test conditions for machining centers -- Part 7: Accuracy of a finished test piece) for machining centers. These procedures are meant to test the capabilities of a machine tool’s controller and the machine’s kinematic errors.

The machining procedure includes both the programming parameters and the set-up parameters. Both of these parameters are complicated by the fact that the test artifact is mounted at an angle in the work volume. The set-up procedure uses a spindle mounted touch probe program to determine the work piece coordinate system. The machining program is made using a commercially available computer aided manufacturing (CAM) package. The measured defects in the part will be used to characterize the capabilities of the machine tool controller. The metrology procedure is based around the use of a coordinate measuring machine (CMM) to measure the accuracy of the machined part. The CMM was used to both scan the outside (machined) surface of the test artifact and probe individual points on the circumference of the test artifact.

Lessons learned through this project will provide a better understanding of the issues involved in the metrology procedure. These lessons will be communicated to the ISO standards committee and will hopefully result in a in a stronger standard.

Initial Research Toward the Development of a Uranium Glass Analogue
Matthew Cox

Under the generic banner of "Glass" exists a multitude of unique and specialized materials. These materials range from simple soda-lime glass used in windows and soda bottles, through borosilicate based scientific glasses, to exotic glasses such as uranium-doped glass for glass-to-metal seals in electronics applications. This research project focuses on the initial investigations required for the production of an analogue for uranium-doped glasses formerly used in electronics production.

Uranium glass possesses a series of unique properties that give it a successful niche in the modern glass shop, even though large-scale production seems to have ended in the early 1950s. Of these properties, four were chosen as benchmarks for the evaluation of a successful uranium glass analogue, with an additional property chosen as a failure condition. The four benchmark properties were: Ultraviolet (UV) fluorescence, ability to wet to scientific metals, color, and coefficient of expansion. The property determining failure was a level of radioactivity significantly above background levels.

The majority of the research was devoted towards the development of a method for investigating and reproducing the UV fluorescence. In this method a series of glasses possessing various levels of a non-radioactive doping agent were produced and then examined under a UV light source to determine a concentration that produced the maximum fluorescence. These test glasses were then compared to samples of production uranium glass to find a dopant concentration that best simulated the uranium glass fluorescence.

Using Machine Vision Systems to Improve Part Quality in Additive Manufacturing
Patrick McCormick

The purpose of this research is to test the application of a machine vision camera system in layer type additive manufacturing processes. The vision system can be used to measure parts in-situ (i.e., in the place). This will allow for measurements of geometries that otherwise would be impossible to make. Some examples of these geometries would include casting cavities and internal structural supports.

To test this concept, a commercially available three dimensional printer was utilized with a camera system. The printer used layers of fine powder and an inkjet print head that would fuse the powder with a liquid binder. Because these layers were exposed after printing, it was possible to modify the printer to stop after printing a layer and allow the vision system to take a digital image of the printed layer. The camera was calibrated to provide accurate dimensional measurements.

As research progressed many variables arose. While the linear dimensions remained very similar and accurate between the layers, the overall placement of the layer began to deviate. In addition, printed parts are often processed after printing. The post processes include baking and methods of hardening the part. A coordinate measuring machine was used to measure the changes in parts and to quantify the measurements taken from the machine vision system. A combination of the results from the machine vision measurements and the coordinate measuring machine measurements allow for part size predictions to be made.

Aspects of Micro Manufacturing
Michael Vandervort

This project will give introductory guidance to U.S. industry and government of considerations into all aspects and ideas about micro manufacturing. This entails a compilation of subjects and objects that need to be considered before, during, and after implementation of micro manufacturing. Some ideas that need to be considered are: all routes of manufacture before budgeting, the range of machine capabilities, and all the manufacturing environment details before purchasing equipment. These key ideas will let a company know the most cost affective, flexible, and reliable method to use.

Micro manufacturing is the broadest area of any manufacturing scale. Since micro-scale is between two scales, macro and nano, it can be approached from both means of manufacturing. Finding the most efficient method for manufacturing a micro-scale part can be difficult and time consuming in of itself. Focusing on traditional material removal methods (e.g., milling, turning, electrical discharge machining (EDM), and laser) for micro manufacturing is a way to get the U.S. industry interested in micro-scale manufacturing. The reason for only researching material removal methods is for the fact that most established U.S. industry does not like major changes. The U.S. industry seems to be resistant to completely change the way of manufacturing and with the current economy most do not want to take the risk because of micro manufacturing's high initial cost. With material removal methods, companies can purchase scaled-down or high precision models of there macro scale machines. Many of the methods use the same theories as macro manufacturing, but with great delicacy and cleanliness. The goal is to present ideas of what is involved to industry, so they can independently decide whether to pursue micro manufacturing based on the feasibility of each component.

<u>Princeton University</u>

Using Mathematica to Compute the Geodesic Path Between Cell Shapes
Tegan Brennan

Image cytometry is a valuable tool for understanding cellular responses to pharmaceuticals and environmental toxins as well as discovering correlations between cellular responses and the cell phenotype. Cell shape, for instance, is an important morphological feature used in understanding cellular activity. A population of identical cells exhibits a population of shapes, which for statistical purposes is important for analyzing and comparing cell colonies.

To compare cell shapes, we have worked on a program to calculate the geodesic distance and a geodesic path between two cell shapes, using what is called the Shooting Method. The Shooting Method is defined on the space of closed curves (cell boundaries) where rotations, translations and reparametizations of the same curve are identified. A Riemannian metric can be defined on this space and with this a measure of distance can be defined. The geodesic path is the shortest path between two curves in this space which can be found by implementing an iterative numerical routine. To carry out this computation, we worked on a Mathematica package which can execute the Shooting Method. The program takes two curves as arguments, calculates and plots the geodesic path between them, and outputs the associated distance. One application of this program is to determine if the resulting shape distributions of a certain cell type grown on a variety of substrates differ, i.e. is there a substrate effect. In this way, we can measure the extent to which environments affect the shape of a cell.

Rensselaer Polytechnic University

Development of a Feedback Controller for a Droplet-Forming Microfluidic Device
Johannes Kutten

Microfluidic devices have the potential to function as small-scale, high-speed chemical assays. This application requires that reagents be mixed in very precise amounts. Our devices are designed to create uniform droplets of water in oil in order to demonstrate how microfluidic channels can accurately control reagent volume.

Microfluidic T-junctions were constructed from PDMS using standard soft lithography techniques. In these devices, a channel containing a dispersed phase of deionized water intersects a channel containing the continuous phase of silicone oil at a T-junction. The shearing flow of the continuous phase created at the junction causes the dispersed phase stream to neck and pinch off into discrete, uniform droplets. Droplet size is determined by a number of factors, including the fluid viscosities, the channel surface conditions, and the junction dimensions; however, dynamic control of droplet size is only possible by adjusting the flow rate ratio between the two streams ($\varphi = Q_d / Q_c$) and the magnitude of the two flow rates.

This project had two aims: first, to characterize the relationship between flow rate parameters and droplet size at a variety of flow rates for a number of microfluidic geometries; and second, to use this characterization data to create a LabVIEW program which can reliably control droplet volume by adjusting flow parameters. Droplets size increases with increasing φ with a logarithmic functional dependency. Qualitative observations show that time to steady-state droplet size following a change in φ is dependent on flow rate, and lower flow rate ratios result in more uniform droplet sizes.

Roanoke University

The Human and Robotic Team: Adding Humans to USARSim Aide Research
Steven Nunnally

Robotic research is very important. Robots can be used to manufacture products more efficiently, enter unsafe areas, and help advance humankind for a more technological future. To make the research more efficient, NIST has led an open source project to develop a physics based, validated robotic simulator called USARSim (Unified System for Automation and Robot Simulation). This allows many researchers to work in this field that would otherwise be unable to because of the expensive nature of robotic technology.

People are going to be a big part of robotic research in the near future. In a manufacturing setting, people must currently avoid a robot at work, but in the future it is envisioned that humans and robots can work side by side creating an efficient team to produce more effectively. Currently, the robot does not know the difference between a human and a box, and therefore significant injury could occur. In an urban search and rescue environment, robots must interact with victims and other rescuers to accomplish their mission of finding survivors and protecting rescuers. In either of these examples, it is apparent that humans are a necessary part for USARSim to continue its effectiveness as a robotic research tool.

The project this summer was to add a controllable human to USARSim to enhance the tool’s ability to aid researchers in accomplishing these goals. The human was built to be as realistic as possible and be able to perform many tasks in a manner that a real human would. The human is not yet complete because the controls are still very basic, but some sample scripts are created so that the human can walk. This becomes an outline to allow other researchers to program the human as they wish following the steps learned throughout this summer project.

Saint Mary's College of Maryland

Determining the Differences in the First Steps of Hyaluronan Mediated Cell Adhesion Under DEP Conditions

Colleen O'Neil

The combination of dielectrophoresis (DEP) with microfluidic systems can allow for the rapid trapping, patterning and further studies of cells processes. However, the conditions in which the cells are maintained may affect the ability of the cells to adhere to the surface and be viable for periods long enough to study processes such as cell differentiation. It is known, for various cell types, that the first events of cell adhesion are mediated by an extracellular coating consisting of, among other components, hyaluronan, a linear glycosaminoglycan of 1 to 10 MDaltons. Previously, we have observed differences in cell adhesion when carrying out DEP experiments using either positively or negatively charged polyelectrolyte multilayers (PEMs) as adhesive material. In this work we studied the first events of cell adhesion mediated by the cell membrane-bound hyaluronan. Using total internal reflection fluorescence microscopy (TIRFM) we determined the dynamics of hyaluronan interactions with opposite charged PEM surfaces under DEP conditions. This study shows that when the NIH-3T3 cells are suspended in sucrose, a commonly used medium when carrying out positive DEP experiments, the hyaluronan interactions with the PEM surfaces are weaker when compared with cells suspended in cell growth medium. We also see defined hyaluronan structures appear faster and more prominently when cells are seeded in cell growth medium. In addition, a smaller number of cells are observed, after the fixing treatment, under sucrose conditions versus cells suspended in cell growth medium. In general, the first events of cell adhesion under DEP (sucrose) conditions seem to be affected by the medium in which the cells are seeded. Nevertheless, the forces applied to the cells by the non-uniform DEP field to trap them are strong enough to ultimately allow for the final anchorage of cells even under flow conditions.

Human-Computer Interaction Performance Testing on Medical Interfaces

Lucia Randazzo

The National Institute of Standards and Technology (NIST) was involved in usability and accessibility testing in conjunction with the Help America Vote Act (HAVA) in 2002, the goal of which was to help realize nationwide improvements in voting systems. Currently, NIST is involved in a similar research activity: human-computer interaction performance testing with newly developed medical interfaces. The U.S. Food and Drug Administration (FDA) and the Association for the Advancement of Medical Instrumentation (AAMI) have set standards for human performance testing with the medical interfaces.

Human performance is measured by creating simulated or real-life tests to measure the usability and accessibility of the system. These measurements are based on the pass/fail criteria determined by using formulas to measure various aspects of human performance, such as effectiveness, efficiency, and safety. These measurements are then compared to previously decided benchmark measurements.

We are in the initial phases of determining what factors are important to measure and planning how to manage the testing and result collection. Currently there is a great deal of ongoing background research exploring the various types of performance tests and metrics. This summer, I assisted with this research and in creating formulas to help measure the usability of the medical systems to be tested.

State University of New York Albany

Synthesis, Characterization and Neutron Studies of a Spin-1 Frustrated Kagome Lattice
Magdalen Lovell

In geometrically frustrated materials, magnetic exchange interactions cannot all be simultaneously satisfied due to the shape of the lattice, leading to a highly degenerate set of classical ground states. In low spin frustrated systems, quantum fluctuations can destabilize simple long range magnetic order allowing for novel quantum states such as the quantum spin liquid state.

The kagome lattice, a system of corner-sharing triangles, is a particularly frustrated lattice. Quantum spins coupled antiferromagnetically on the kagome lattice have long been considered a promising situation in which to find spin liquids. Although a few materials have recently been suggested as candidate spin-1/2 kagome lattice materials, there is a significant lack of experimental realizations of spin-1 kagome lattice antiferromagnets. Thus we attempted to synthesize Nickel analogues to the Copper-based naturally occurring minerals volborthite and vesignieite.

Hydrothermal synthesis methods have produced powder samples of BaNi3V2O8(OH)2, the nickel version of vesignieite. X-ray powder diffraction measurements find that the sample displays a monoclinic crystal system, with Ni ions occupying a slightly distorted kagome lattice structure. SQUID measurements find that the sample is antiferromagnetic, with a Curie-Weiss temperature of roughly -20 K. The lack of long range order at a temperature comparable to the Curie-Weiss temperature demonstrates the effects of frustration in the system.

State University of New York Binghamton

Modeling and Simulation for Sustainable Machining
Eric Chernow

Modeling and simulation techniques have frequently been utilized in the last decade to replicate manufacturing processes. In examining Numeric Controlled (NC) machines, simulation has been preferred to physical testing of programs due to the potential savings of time and money. By validating these NC programs in the virtual environment, damage to valuable machines and cutting tools can be prevented, and production will not be interrupted in the factory. Recently, sustainable manufacturing has been identified as one of the focus areas by industry for minimizing energy usage, reducing material resources consumption, and improving environmental impact. However, little work has been done applying the modeling and simulation techniques to analysis of sustainable manufacturing systems.

This project provided a traditional virtual NC machining model with a new capability – to quantitatively analyze the environmental impact of a machining system. Aspects of sustainable machining that were modeled and evaluated included energy consumption, coolant and lubrication usage, and waste management. The technique of Life Cycle Assessment (LCA) was applied to help perform this task. The objective of this methodology is to quantify the sustainability impacts of a process or a product from cradle-to-grave. Dassault Systèmes DELMIA V5/V6 simulation software was used to create the virtual machining model. The sustainability impact modules were developed and integrated to this machining model. The outputs of this system included the virtual machined part that was used to examine the NC program for errors, the NC validation report detailing any collisions between the tool and machine, and the sustainability report outlining the environmental effect of that particular operation. It is hoped that this research project can help the manufacturing industry have a better understanding of the issues surrounding sustainable machining and, in turn, companies can take actions to reduce their negative environmental impacts.

Development of Resistance Standards in the 1 MΩ to 1GΩ Range Using Hamon Transfer Methods
Wesley Chiu

The development of highly accurate and stable standard resistors and the ability to accurately define values of resistance is the goal of Resistance Metrology. This allows for the dissemination of resistance values with low uncertainty to commercial labs that may then calibrate electrical equipment. High Resistance Metrology deals with resistance in the 1 MΩ to 100 TΩ range. The development of automated bridges and new techniques in the creation of standard resistors has greatly improved the accuracy of measurements of high resistance. The guarded Hamon technique has been used to reduce leakage currents and allows for accessible resistance scaling between nominal decades (i.e. 1 MΩ, 10 MΩ, 100 MΩ) made by reconfiguring the Hamon standard. Although film resistors exhibit measurable voltage coefficients, they are used in place of wire-wound resistors because of their shorter settling times. Modern film resistors also have improved stability and no inductive properties. Glass to metal seals are also used to further reduce leakage currents. Initial measurements have shown that this new construction method has lower uncertainty and may perform better then previous standards.

Durability of Adhesives in Salty Environments
Michael Imburgia

Adhesive bonding is a growing option in many structural applications, serving as a substitute for the traditional types of bonding such as welding, bolting, riveting, etc. A common concern with using adhesives is the durability of adhesives in hostile environments. Understanding the mechanical performance of adhesive joints in wet, salt-rich environments will provide needed information for marine, harbor and other sea water applications. This research aims (a) to develop sound short-term accelerated test method based on fracture mechanics approach to assess the durability of adhesive joints, and (b) to use this test method to understand the effects of salt on the adhesion of various adhesive systems, including epoxy/glass oxide, epoxy/aluminum oxide, and an epoxy/polyimide interfaces. The study uses dynamic mechanical thermal analysis to assure the optimal curing conditions for the epoxy, attenuated total reflectance Fourier transform infrared spectroscopy to identify the chemical composition at each failure interface and contact angle measurements to determine the thermodynamic stability of the interfaces in wet, salt-rich environments.

Residential Appliance Energy Research
Joseph Shamah

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.

Our work this summer was divided into two separate phases. The first of which involved an assessment of all publically available survey data on the usage of consumer appliances. Various companies and organizations were contacted to determine what data was available. Any relevant public data was obtained and documented. The data was then analyzed to acquire the desired information. This information will assist in the revision of the test procedures to accurately reflect current consumer usage habits.

The second phase was the design of a new residential appliance test facility at NIST. The test facility will include a number of representative appliance models, as well as data monitoring equipment. A future goal is to implement automation of the test facility, and the requirements for this task were investigated. The test facility will enable NIST engineers to analyze and verify proposed test procedure modifications before they are published.

Swarthmore College

DMIS Test File Reducer
Steven Hwang

DMIS (Dimensional Measuring Interface Standard) is the only standard machine control language for CMMs (Coordinate Measuring Machine). The DMIS language unlike other programming languages includes commands which execute one of the following: defining geometry, defining tolerances, directing machine motion, flow of controls and other miscellaneous useful functions. Companies that use CMMs use the DMIS language for writing programs primarily, because it facilitates the interoperability of code. However, presently there is no interoperability of DMIS code between systems from different vendors since some vendors provide software for writing DMIS programs that are incompatible with other systems. Either the software does not write in real DMIS, or it uses different portions of DMIS than other systems.

The NIST DMIS Test Suite has been created to help solve this issue of incompatibility. The Suite is intended to help users and vendors use DMIS 5.2 and provide conformance testing utilities. For a vendor building an execution system for DMIS files, a set of test files would very useful for evaluating vendor's software which is used to read the DMIS files. Provided that the test files are compatible with the implemented Conformance Class, any error that may occur while a test file is fed into the vendor's systems would denote a failure of the system's parser.

I built a File Reducer that takes a description of a "Conformance Class" and a set of test files known to be for full DMIS and generates a set of test files. This generated set of files is meant to be dealt with by a system that implements the specific Conformance Class which denotes which portions of DMIS would need to be accessible to the system. A vendor could use the File Reducer to generate files geared specifically toward his system's Conformance Class. These files should run without error on the vendor's software.

Characterization and Compensation of Micro-Scale 3-Axis Milling Machine
Julian Leland

All machine tools exhibit some degree of error in their motions: a specified relative motion between the workpiece and the tool tip will be affected by these errors, reducing the quality of parts produced. These errors can be minimized by characterizing each error with specified measuring methods and using the machine controller to compensate for each. Micro/Meso-Scale machine tools exhibit the same type of positioning errors as traditional-scale machines. However, because of their small work volume and higher specified positioning performance, they present a challenge for the machine tool metrologist. Metrology hardware is generally too large for the small machine work volume and custom fixturing must be designed to accommodate each measurement set-up. Additionally, some errors contributing to each measurement are of the same order of magnitude as the specified machine performance making the uncertainty in measurement very significant.

The positioning performance of a micro-scale 3-axis milling machine designed and built by NIST in 2005 is measured in accordance with international standard ISO 230-2 - Test code for machine tools -- Part 2: Determination of accuracy and repeatability of positioning numerically controlled axes. Critical machine design information is compiled and used to generate both a mathematical kinematic error model and virtual three dimensional solid model of the machine. A measurement uncertainty analysis (with accompanying sensitivity analysis) is conducted to identify sources of measurement error optimize measurement procedures. Custom fixturing is also designed and manufactured to accommodate each measurement set-up. Linear positioning accuracy and repeatability of the X-, Y- and Z-axes is measured using a single-pass heterodyne displacement-measuring interferometer (DMI) system. Error compensation tables for each axis are generated from the measurement data and incorporated into the machine controller to reduce positioning errors. Last, the linear positioning measurements for each axis are repeated to verify the compensation of the positioning errors. This talk will present the characterization and compensation procedure in greater detail, and will discuss the results of the compensation as well as avenues for future work.

Towson University

Design and Control of a Bi-Directional Microscopic Robot
Joshua Giltinan

Microelectromechanical Systems (MEMS) are devices with sub-millimeter features that combine the electronic function of computer chips with mechanical function. Examples of well-known MEMS devices are the sensors that decide when the air bag on your car is deployed and the array of mirrors used in a DLP projector.

The MEMS device worked on in this project is a type of untethered scratch drive actuator (USDA), a type of microrobot, featuring bi-directional capability. A unique feature of the USDA is that it is not permanently attached to a surface, but rather is free to move in one or more dimensions. Previous research demonstrated USDAs which can move linearly as well as pivot about a fixed point. The microrobots in the current project use a bi-directional USDA to move forwards and backwards.

At the micrometer (10^{-6} meters) scale, the dominant environmental force is not gravity, but intermolecular forces, such as friction and Van der Waals forces.

A USDA is driven by a varying electrostatic force created by a series of flat electrodes that are tens of micrometers wide arranged on a “field” of operation. These electrodes provide an open circuit on which the robot can act as a capacitor. A charge that builds up on a flexible portion of the robot, which is attracted to the electrodes, and the robot flexes downward towards the electrodes in what is called capacitive actuation. When the voltage is removed, the robot relaxes to its original shape, but displaced by approximately ten nanometers.

Motion of a bi-directional USDA is facilitated by choice of a correct robot “arm” using a nested hysteresis loop of operating voltage; these loops can be represented as a finite state machine with three binary variables, seven of the possible eight states are used in operating the robot; the needed hysteresis loop was modeled as part of this project. Although the robots had been designed and partially fabricated before the start of this project, two masks were designed and fabricated. One allowed for accurate handling of the chip containing the robots; the second was to define where stress material, chromium, would be placed on the robot. Additionally, the effect of the chromium on the polysilicon of the robots was modeled to determine the chromium thickness to be applied to the robots.

University of California Irvine

Absorption Coefficient Measurements of Aerosolized Nigrosin Particles Using Laser Heating
Sara Hariri

Aerosol particles in the atmosphere exert thermal effects on the climate through direct and indirect absorption and scattering of solar radiation. Measurement of these aerosol optical properties is dependent on the size, shape, composition and concentration of the particles. A variety of techniques are used by the climate community to measure the aerosol optical properties, namely particle absorption and scattering. Today, such techniques are used to monitor the optical properties of atmospheric aerosols from ground stations to satellite in orbit around the Earth. Many of the absorption techniques evaluate aerosol properties from particle-laden quartz filters that were exposed previously to the atmospheric. However, it has been shown in the literature that the presence of the filter can result in an artificially enhanced measurement of absorption due to scattering by the filter fibers back onto the embedded aerosol particles. Understanding better such biases is important for obtaining reliable data, which can then be used as input to aerosol algorithms under development for climate models.

To address the issue of absorption enhancement, a novel rapid laser-heating technique is being developed at NIST to determine the absorption properties of collected aerosol particles, by monitoring the sample thermal behavior and solving the energy conservation equation. The objective of our work was to develop a calibration protocol to ensure precise determination of particle absorptivity, and to compare results with other values published in the literature. To this end, we used aerosolized nigrosin, which is a mixture of synthetic black dyes used to make Indian ink. The nigrosin particles were packed tightly in a copper pan to simulate a uniform bulk material. The laser-heating technique consists of placing sample material on a thermocouple that sits in the middle of a copper sphere. The copper sphere provides uniform heating of the sample through radiation heat transfer. Heating is achieved rapidly with a continuous-wave infrared laser. The thermocouple monitors the sample temperature with time, which is recorded with a data acquisition system and computer. The measurement protocol involves perturbing the sample temperature from its steady-state temperature, and monitoring the response during the temperature decay back to steady state after cessation of the laser heating. The monitored change in sample temperature with time is used to solve for the absorptivity in the energy conservation equation.

University of Colorado Boulder

Approximating the Number of Toplogical Sorts
Amanda Crawford

Topological sorting is used in a variety of applications, one of the most important being scheduling problems in computer science. Brightwell and Winkler determined that counting the number of topological sorts of a directed acyclic graph (DAG) is #P-complete, providing reason to approximate (rather than count) the number of topological sorts. Currently, the main method used to do so is Markov Chain Monte Carlo (MCMC). MCMC methods are well studied and therefore much theory has been developed in this area. Brightwell, Winkler, Bubley and Dyer are among many who have used MCMC to approximate solutions to this problem. We chose to go a different route, and developed a method based on sequential importance sampling (SIS). While this method appears to be much faster than MCMC in general, it is a rather new technique and consequently little theory has been developed in this area. Because the sample variance of the SIS method does not always accurately approximate the true variance, it is necessary to find a new technique to approximate the variance, and so we also developed such a technique and used it to compare different importance functions. Additionally, we discovered an aggregation technique and used SIS to speed up the MCMC method.

University of Connecticut

The Effect of Temperature Change on Plasma Etching Processes
Joshua Leibowitz

Plasma etching is a process in which material is selectively removed from a wafer to fabricate mico/nano scale patterns on its surface. These patterns are then generally used to create integrated circuits for use in semiconductor devices. The plasmas, or ionized gases, used in plasma etching are typically generated by a radio frequency (RF) electromagnetic field applied to the electrodes in a vacuum chamber. In the plasma, ions, free radicals, electrons, photons and other excited particles are produced. These high energy plasma species react with the surface to form a vapor phase byproduct, which removes the surface substrate.

Since plasma etching is a chemical reaction, the electron temperature and energy at etching plays a key role in the process. When the same etch is performed at a different temperature, properties such as the etching profile, etching rate, and selectivity will change. By modifying the temperature, one can create etched substrates with ideal properties. Plasma Etchers at NIST have the ability to go to lower temperatures, and etch with better parameter accuracy than many etchers, allowing for better control of results.

Temperature control in plasma etching is not easy, however. Several factors such as the chuck temperature, the ion density, the ion energy and the exothermicity of the etching reaction affect the surface temperature. Scanning electron microscope (SEM) was used to monitor the etching profile and surface while Optical Emission Spectroscopy was used to attempt find a correlation between the chuck temperature and the electron temperature, as well as provide insight towards the chemical reactions that occurred.

University of Delaware

Investigating Lamellar Structures in Hydrated Nafion Thin Films
Andrew Baker

It has been previously observed that lamellar structures, which consist of alternating water-rich and Nafion-rich layers, exist at the interface between thick hydrated Nafion films (~500Å) and silicon substrates, while the remainder of the films exhibit bulk-like characteristics. It is proposed that these lamellar structures can be isolated by depositing films with thicknesses equal to that of the lamellae (~70Å). If these structures do exist within the thin Nafion films, there are many potential applications, especially if the lamellae terminate with a water-rich layer. This outer layer can be used to support phospholipid bilayer samples in a vapor environment, instead of in a liquid environment, which can allow researchers to gain more information about the structure of proteins embedded within these samples.

In order to determine if these structures exist in thin films, various films were deposited at thicknesses between 20 and 300Å and characterized using neutron reflectometry to determine their structure. Reflpak software was used to fit the data to various lamellar models as well as uniform layer models for each of the samples. Preliminary results indicate that hydrated films measuring 55 and 90Å thick are composed entirely of 3 and 5 layer lamellar structures, respectively. Additional data must be fit for films exposed to H_2O and D_2O vapor at 90% relative humidity in order to verify these results.

University of Maryland Baltimore

Developing a Root-Based Semantic Vocabulary
Laura Anzaldi

Information related to medicine, biology and chemistry is stored in a number of different databases, each of which uses a different vocabulary. This makes combining or sharing information very difficult, as for literal, pattern-matching computers, different vocabularies are completely different languages. Therefore it is necessary to develop a root-based vocabulary (mirroring Latin) to act as a standard. This is advantageous, as once a common set of roots has been established, the meanings of compound words become intuitive. For example, the Latin word "biology" is formed from two roots: "bio" (meaning life) and "ology" (meaning study of). The prefix of "bio" can be appended to an infinite number of other roots to create logical vocabulary terms—*bio*technology, *bio*medical, *bio*informatics. Adding vocabulary, which is essential for the exponentially growing field of biology, could not be easier. New vocabulary can be formed by combining different root words, or if need be, creating new ones.

In order to form this new vocabulary, specialists in biology selected a diverse, extensive and representative collection of ontologies, unfortunately encoded in incompatible formats (OBO and OWL). We converted each ontology into XML using Perl and loaded them into Oracle database tables, where they were manipulated to create hierarchical trees of vocabulary words. We recorded the counts of each word at each level of the tree, and recorded this data for each of the ontologies into a combined table. These counts will be used to aid the analysis of determining which words would serve most naturally as roots. The final part of this project involves developing a website using Perl CGI which will enable biologists to query the combined table. These experts will be able to do what computers cannot…judge how suited a word is to serve as a root. Proper root words are easily concatenated, easy to say, and usable in a wide variety of contexts. A standard root-based vocabulary will streamline communication and facilitate unity in information between different scientific companies and organizations.

Homogeneity Analysis by Way of Laser Ablation Solid Sampling Coupled with Inductively Coupled Plasma Mass Spectrometry for the Assessment of Micro-Scale Sample Homogeneity
Naomi Bier

Standard Reference Materials (SRMs) are materials that have been thoroughly characterized and certified by NIST for properties such as elemental composition and homogeneity. These materials are used by customers in industry, academia, and other sectors, for a variety of purposes. For example, SRMs can be used for calibrations of instrumentation, validation of in-house methods, and for quality control. It is crucial that SRMs be homogenous in composition, both at the macro- and micro-scale, in order for the material to be valid. Traditionally, X-ray florescence spectroscopy (XRF) has been used for the direct elemental analysis and evaluation of homogeneity of solid samples, such as glass, ceramics, and soils. However, XRF does not provide sufficient sensitivity to detect heterogeneity in all the elements of interest; it is also unable to measure beryllium, an element of interest in many materials.

A proposed complementary technique to XRF is laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS). The LA-ICP-MS technique uses energy from a laser to directly interrogate a solid surface and create a plume of gas-phase particles that has the same composition as the bulk material. The gas-phase particles can then be transported to an ICP-MS for detection and quantification. The primary advantage of ICP-MS compared to XRF detection is sensitivity, which is on the order of 100 µg kg^{-1} or better for the majority of elements accessible to ICP-MS. The present SURF project explored the effects of different experimental parameters, both within the laser and in the ICP-MS, on micro-homogeneity measurements made by LA-ICP-MS. Parameters of interest included laser beam spot size, repetition rate, and ablation cell dimensions. The results indicated that optimization of experimental parameters is crucial for the successful assessment of micro-homogeneity in solid samples by LA-ICP-MS.

The Dispersion of Single-Wall Carbon Nanotubes
Amber Bokhari

A primary barrier to the use of single-wall carbon nanotubes (SWCNTS) in materials is that the nanotubes, as synthesized, form agglomerates that are not readily individualized and that often contain significant levels of impurities. To isolate the nanotubes as individuals and allow purification and processing, the nanotube powder is thus typically dispersed into a liquid phase through ultrasonic treatment in the presence of a dispersing agent. However, ultrasonic processing is thought to damage the nanotubes, and thus gentler methods for dispersing the nanotubes have been sought. The objective of this project is to test the effectiveness of one of these methods, shear homogenization, to disperse the nanotubes as individuals in aqueous solution.

Ultraviolet-visible-near infrared spectroscopy and other optical techniques were used to monitor both the total quantity of nanotubes dispersed and the effectiveness of the processing in individualizing the nanotubes. A comparison of the effects of shear homogenization versus ultrasonic processing for different nanotube diameters, dispersant concentrations, and processing times will be presented in this talk.

Terahertz Investigation of Dipeptide Nanotubes
Benjamin Ecker

Water affects and is often vital to many biological processes including protein conformational changes. Conformational changes are usually associated with the large, collective motion of atoms or molecules in the system, and many of these motions are highly sensitive to the balance of hydrophobic and hydrophilic interactions with water. Terahertz radiation (one to one hundred cm^{-1}), whose energy is on the order of vibrational modes of non-local, collective motion that are sensitive to hydrogen bonding, provides an excellent means to probe the dynamics of such biologically important processes.

Here, we present a further investigation of the retroanalogue pair of di-aminoacid-peptides, L-alanyl-L-isoleucine (AI) and L-isoleucyl-L-alanine (IA). Both biomolecules form crystalline structures with hydrophobic nanotubes with hexagonal symmetry. Despite being a mere chemical “reversal” of the functional groups, they act vastly differently, including water permeability, pore size, and solvation characteristics. Previous work has been done on structural modeling at the quantum chemical and empirical force field levels to better understand the mechanism behind the transport of water through the nanopores.

Current work involves developing crystallization procedures for deuterated versions. Terahertz absorption spectroscopy measurements of the dipeptide crystals will be taken and will be compared to previous work. The substitution of a hydrogen atom with a heavy hydrogen atom may change or possibly shift the spectral features. Accurate measurements would be useful to check theories, and potentially, give biologist a better understanding of water transport through nanopores.

Detection and Differentiation of Bacillus Endospores
Using Fluorescence Spectroscopy
Neeti Goel

The threat of bacterial pathogens, such as the anthrax- causing Bacillus anthracis, as biological weapons has made it more urgent to understand the mechanism and properties of bacterial endospores. In harsh conditions the bacterium transforms into endospores which can remain dormant for many years and then germinate in favorable conditions, such as a human host. A detailed understanding of certain spore characteristics can help improve the methodology and instruments used by first responders in a biohazard emergency to ensure rapid, accurate, and non-invasive detection. This study attempts to use the characteristic of intrinsic fluorescence to differentiate molecular species by their unique spectra. The effects of certain germinant nutrients and temperature on the growth and germination of the Bacillus spores were also characterized. A comparative analysis was done of the spectra of different strains of Bacillus thuringiensis and Bacillus cereus (both simulants for Bacillus anthracis) grown in three different growth media. After several calibration curves of Dipicolinic acid (DPA) and DPA complexes were created, the samples were scanned for these endogenous fluorescent molecules. Measurements of the concentration of the fluorescent DPA complexes were used to follow the germination of the spores.

Pyrometer Calibration of Nanocalorimeters
Alex Holness

Nanocalorimeters are used to measure heat quantities on nanometer scale samples using microfabricated chips at high heating rates. They are calibrated by determining the sensor temperature-resistance relationship. Previous calibration methods utilized furnace heating of the entire nanocalorimeter chip. Unfortunately, defects form unpredictably in the support material that allows electrical shorting above 350 °C, which makes the resistance determination uncertain and unreliable. To solve this problem, the chip was heated locally by Joule heating and temperature measured by an optical pyrometer. Heater resistance was recorded as a function of temperature. Thus, more accurate calibration can be achieved at temperatures above 350 °C. A virtual instrument with digital data acquisition was used with a pyrometer and a source measure unit to control the test, to acquire data, and to process raw data into calibration parameters. The goal was to create user friendly, accurate, and consistent LabVIEW programs to control and automate the calibration process.

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.

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Optimization Algorithms for Fitting Fundamental Parameters Models for X-Ray Powder Diffraction Line Profiles

Morgan Madeira

Many different algorithms are possible to use to fit models for X-ray powder diffraction line profiles, where the best fit is defined to be at those parameter values that minimize the sum squared differences between the model and measured data. We have examined the results of fitting models using two algorithms: the differential evolution algorithm, which is a global optimization technique, and the Levenberg-Marquardt algorithm for nonlinear regression, a local optimization method. Simulation studies show that the less-powerful Levenberg-Marquardt method was sufficient to estimate the parameter values associated with the best fit of simulated datasets. The simulation studies examined many datasets differing in the random effects (noise), with the random effects inspired by noise due to counting statistics found in measured data associated with NIST Standard Reference Material (SRM) 640b. In addition to performing simulation studies using Levenberg-Marquardt, we applied the commercial software program Topas to estimating parameters. Our results showed that Topas performs similarly to the Levenberg-Marquardt algorithm. This study helps validate the performance of Topas, which is an important tool used extensively in the development of powder diffraction SRMs.

Working Towards a NIST-Certified Phantom for Computed Tomography

David Mason

The usefulness of Computed Tomography (CT) systems in diagnosing and tracking changes of lung disease is dependent on their ability to provide precise, quantitative information regarding the radiodensity of tissue regions. However, the results of a CT scan can vary between systems, affecting both diagnosis and treatment. In order to calibrate CT machines for diagnosing lung disease, it is necessary to have a precise reference standard that mimics appropriate tissue densities. NIST researchers have previously identified a set of commercially available foams that have radiodensities in the appropriate range. As a step towards creating a certified standard, we have measured the x-ray absorption and scattering characteristics of these foams using a high-resolution x-ray imager. For comparison with our in-house data, we have also collected actual CT images of these foams at a local hospital. This comparison offers insight into the precision and accuracy that can be expected in clinical systems.

In our work, we have also considered the limitations and assumptions inherent to the Hounsfield Unit (HU), which is a relative scale for reporting CT measurements of radiodensity. The Hounsfield scale relates all measurements to the radiodensity of water, in an attempt to standardize results across different scanners with different x-ray spectra. However, varying degrees of spectral hardening can have a significant impact on the measured attenuation of a material. Since we have the advantage of working with a well-calibrated source with a known spectrum, we have been able to carefully account for spectral hardening as best as possible. We have also sought to understand the impact of scattering on our measurements and how best to account for it. Ultimately, having such a precise understanding of the attenuation characteristics of these foams will allow for the creation of a NIST-traceable reference material which can be adapted for clinical use.

Visual Similarity Based 3D Model Retrieval Through Multiview Matching
Nadezhda Serova

Three-dimensional (3D) shape retrieval has become an important problem in various fields such as computer graphics, computer vision, and CAD model matching. The problem consists of accurately identifying shapes which are similar to any given model from a certain database and ranking them in order of similarity. Numerous techniques have recently been developed, each with their own strengths and weaknesses. One of the most successful methods to date has been designed by Zhouhui Lian of NIST. After normalizing the model orientation, Lian uses multiple views of the model; depth-image snapshots taken from different perspectives of a geodesic sphere. He uses the popular 2D shape feature extractor SIFT, followed by a Bag of Words, approach to compare the multiple views of the model. This technique proved to be effective on both rigid and articulated model databases.

The goal of the project is to attempt to improve on Lian's techniques by altering different sections of his method. Mainly, various feature extraction algorithms have been tested instead of SIFT. In addition, we tried pre-processing of the 2D depth image views. We also tried combining the views into one image as well as just using a single feature vector per model instead of per view. Finally, certain methods allowed for direct location-based feature comparison of the views instead of using the Bag of Words approach.

University of Maryland College Park

Automated Guided Vehicle Testing in Virtual Environments
Ryan Atkinson

AGVs (Automated Guided Vehicles) utilize a variety of sensors to collect data describing their surrounding world. PRIDE (Prediction in Dynamic Environments) is the framework for on-board data analysis permitting AGVs to navigate their environments with the least threat to hazards. PRIDE, developed by NIST, unifies a series of prediction-based algorithms into a logical hierarchy aiding vehicles in navigation. The framework's innovation lies in its ability to allow an AGV to navigate in truly dynamic environments typical of real world situations.

Epic Games' Unreal Game Engine provides the tools necessary to create the desired structure and attributes of a real world manufacturing environment in a purely virtual setting. The latest Unreal Engine is a vast improvement in realistic gaming, and offers a more accurate testing bed for AGVs utilizing the PRIDE framework. Therefore, a new virtual environment was created to push PRIDE to a new level. The environment, a futuristic manufacturing plant, employs a series of tests to which AGVs may need to respond. Most importantly, dynamic aspects such as vehicles at roadway intersections, traffic control mechanisms, automated plant workers, and other automated vehicles are included in the environment to further test and improve upon the underlying algorithms.

PRIDE functions with the assistance of the NIST developed RND (Road Network Database). Within every AGV environment there is an intended course for vehicles, whether the environment is a highway, office building, or the newly created virtual manufacturing plant. The AGV must be aware of, with sufficient precision and accuracy, a number of road characteristics as defined by the RND. After organizing all pertinent information, the RND is written in XML (Extensible Markup Language) format for AGV interpretation and utilization as the vehicle plans routes along the roadway.

Assessment of Pronase Digestion and Mass Spectrometry-Based Characterization of Biopharmaceutical Glycosylation
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 size 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.

Previous methods of glycoprotein analysis involved numerous mass spectrometry-based techniques, each of which provides various aspects of characterization. The current project involved the assessment of a novel workflow that utilizes pronase, a mixture of proteases capable of cleaving any peptide bond. The resulting glycopeptides allow for glycosylation site identification via solid phase extraction and MALDI-TOF MS, as well as glycan characterization via graphitized carbon LC-MS/MS. This method was applied to Ribonuclease B, a well characterized protein that was used to verify the efficacy of the new protocol. The same method was then applied to Rituxan, an arthritis and cancer drug that holds many similarities to other biopharmaceuticals. The glycosylation site and glycan types of both analytes were identified. Initial results also indicate that with digest optimization, this sample treatment protocol is sufficient for further characterization of any glycoprotein, including glycan linkage analysis and absolute quantitation.

Computing Respirator Fit and Effectiveness
Andrew Bernstein

For an emergency responder, a properly fitted respirator can mean the difference between life and death. A respirator that fits perfectly is one that when pulled onto a responder's face produces a uniform seal with no areas of low or high contact pressure. This is critical because an area of low contact pressure may allow hazardous materials to seep into the mask; while an area of high contact pressure can result in discomfort, leading responders to discard their mask and the protection it offers. The big question is whether we can accurately determine where these low and high pressure areas occur. Current respirator sizing and fitting does not take into account the many variations in facial geometry and skin properties and how these affect the ability of the mask to conform to the responder's face, thereby forming a comfortable impermeable seal. Thus the goal of this project is to use computational modeling to investigate how varying mechanical properties of a modeled face, such as skin elasticity, thickness, and compressibility, can increase accuracy of a model allowing researchers to identify areas of low and high contact pressure.

The first step in creating this model is to use a 3D laser scanner to capture the complex contours of the respirator and a human face. This laser scan is then brought into Raindrop Geomagic, a three-dimensional modeling software tool to create digital models of physical objects. Here the resulting scan is combined with thickness measurements from around the respirator, ultimately generating an accurate digital model of its surface. Once completed, a face is constructed similarly, and both surfaces are meshed into discrete spatial cells. LS-DYNA, an advanced general-purpose multiphysics simulation software package, is then used to perform an FEA (finite element analysis) contact analysis of the respirator seal when pulled onto a person's face. This analysis will account for three varying boundary conditions, a face that has rigid skin, skin with properties defined in literature, and soft skin; in order to determine both the quality of the seal formed and the potential for areas of high and low contact.

Neutron Diffraction Studies on the Structure and Chemical Composition of Superconducting Phases of $Fe_{1+Y}Te_{1-x}Se_x$
Vikas Bhatia

Iron based superconductors, like high temperature superconductors, do not conform to BCS theory (unconventional)[1], and offer the opportunity to study the effects of chemical composition, magnetism, and superconductivity. Iron based superductors are layered, and have a tetragonal crystal lattice at room temperature[2]. FeTe becomes superconducting at ~ 14K upon doping of Se at certain stoichiometric ratios. $Fe_{1+Y}Te$ has two iron sites, one of which is partially occupied, while the Te site is fully occupied.

In order to synthesize the desired compounds, the general formula of $Fe_{1+y}Te_xSe_{1-x}$ was devised. Different values for x and y were chosen in order to study different chemical compositions. In order to control the amount of excess Fe, stoichiometric amounts of I_2 were allowed to react with the compounds forming FeI_2 with the excess Fe[3]. The compounds were synthesized with solid state reactions, and then reacted with I_2 at 473 K or by deintercalation in a solution of acetonitrile at room temperature. The stoichiometry and crystal structures of the compounds were characterized with X-ray and neutron diffraction. The results will be presented.

(1) Zhang A.; Xia T.; Kong L.; Xiao J.; Zhang Q., *J. Phys.: Condens. Matter.* **2010**. 22
(2) Lynn, J.; Dai, P., *J. Physica C.***2009**.*03*.046
(3) Rodriguez, E.; Zavalij, P.; Hsieh, P.; Green, M., *J. Am. Chem. Soc. (in press).*

Logic Synthesis of Functions for Cryptographic Applications
Holman Gao

Circuits that have binary input and output are frequently used in cryptology. For this project, we worked with two different types of circuits: addition circuits used in cryptanalysis of hash functions and multiplication circuits used in error correction. These circuits consist of AND gates and XOR gates, with the XOR gates considered as linear components since XOR is equivalent to addition modulo 2.

Hash functions must contain nonlinear components in order to be pre-image resistant and collision-free. Several hash functions use binary addition circuits as their only non linear component. A possible cryptanalytic attack on such hash functions uses a linear approximation of the addition circuits. This makes it simple to generate multiple inputs given an output, although there does not necessarily exist a collision among the generated inputs. For the best probability of producing a collision, the linear approximation should be as close as possible. Currently, the most popular approximation disregards the carry bit in the addition process. We show that there are other approximation methods that are just as close as, or even better than, the popular method, depending on the metrics used to judge the approximation.

A number of error correction techniques work in the finite field of 2^n elements. One way to do arithmetic in this field is modulo an irreducible degree-n polynomial, in which the elements of the field look like degree-n-1 polynomials with binary coefficients. Due to the nature of this field, unique multiplicative inverses exist for each nonzero element, which is useful in error correction. Since error correction must be fast in order to be of practical use (i.e. consumer electronics), it is important to research efficient representations of the multiplication circuits. Generally, the two most important measures of circuit efficiency are size and depth. While it is unknown whether circuits are optimal in terms of these metrics, we propose a circuit-constructing algorithm that has produced better results than all published circuits.

Testing the Security of Android Applications
William Goh

Applications for the Android platform, an OS created by Google for smart phones, may contain security vulnerabilities that need to be discovered and fixed before they are distributed for use. This is of particular importance if the US government and military choose to have them as a resource. Problems arise if the phone is somehow compromised, whether the phone is damaged, lost, stolen, or hacked. Methods need to be created to deal with these circumstances and safeguards preventing attacks must be put in place.

This project aimed to develop a testing lab to apply combinatorial testing techniques and to automate the testing process to efficiently assess the stability and security of Android applications despite any changes in the configuration of the phone itself. Software was used to generate test case data, convert the data into a series of files for the applications, and then execute tests via an automated testing tool for a virtual Android phone.

Measuring Cell Response to Polymeric Scaffolds in 3-D Culture for Tissue Engineering of Bone
Stevephen Hung

The success of tissue engineering scaffolds is largely determined by the optimal selection of biomaterial properties. Much of the previous work in characterizing cellular response has been performed on planar 2-D biomaterial surfaces. However, cell response in 3-D tissue scaffolds is more representative of their behavior in the 3-D tissue environment in vivo. Scaffold properties such as topography, pore size, hydrophilicity, and protein adsorption play a critical role in directing cell behavior. To investigate the cell response to scaffold properties, 3-D porous scaffolds of two biomedically-relevant polymers poly(ε-caprolactone) (PCL) and poly(D,L-lactic acid) (PDLLA) were fabricated via the salt-leaching technique. Towards tissue engineering of bone, adhesion and proliferation of mouse osteoblasts to changes in scaffold properties were measured. Specifically, the effect of polymer concentration, size of the salt crystal, annealing treatment and the length of pre-incubation in media were investigated in this study. This work provides a systematic understanding of the role of different biomaterial properties on osteoblast response in 3-D culture format.

Evaluation of Systematic Errors in Johnson Noise Thermometry
Kevin Krueger

Johnson Noise Thermometry is the one the most accurate method measuring thermodynamic temperature in the range 600 K to 900 K. In this method, a resistor probe is placed inside a furnace thermowell, and its electrical resistance properties are used to determine temperature. Special design constraints exist, however, on the resistor probes which introduce several systematic errors in the measured temperature. One such effect is the probe immersion error which occurs when the heat transfer between a comparison furnace and the probe is imperfect. Immersion error can be evaluated by comparing resistances of two similar probes while one is fully immersed, and the other is displaced vertically within a furnace thermowell. Another source of error is due to the leakage current through the electrical insulators, which make up the probe. This can be evaluated by deconstructing the probe, and measuring the insulation resistance under open circuit conditions.

Exploring the Surface Chemistry of Engineered Nanoparticles Using Time-of-Flight Secondry Ion Mass Spectrometry

James McCarthy

The unusual properties of engineered nanoparticles (ENPs), as compared to their bulk material counterparts, have sparked concern among members of the scientific community, particularly within the environmental and health sectors. Employed as antimicrobial agents, sunblock additives, or medical imaging contrast enhancers, ENPs play an increasingly active role in everyday life, but their interactions in different surroundings are poorly understood, and may prove hazardous. The large surface area-to-volume ratios of these particles are responsible for their abnormal reactivity, and therefore the key to understanding ENP behavior is to examine their surface chemistry. The surface modification of ENPs is inevitable and will vary from one ambient environment to the next, so it is crucial to study how different surroundings influence particle surfaces, and how variables such as the size of the particles may contribute to the degree of modification.

Past research of ENP surfaces has been limited in that it supplies only bulk chemical information or possibly no chemical information at all. In this research however, the surface chemistries of ENPs exposed to different solvents are studied using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). In ToF-SIMS, a solid surface is bombarded with a high-energy beam of ions, the ejected (secondary) ions from the surface are collected and analyzed, and an interpretable mass spectrum is generated. The existence of peaks for certain masses may indicate the presence of specific functional groups on the ENP surface or contaminants associated with ENP fabrication or sample preparation.

Preliminary results demonstrate the difficulty of studying nanomaterials and highlight the need for methodological evaluation. Briefly, new sample preparation paradigms (that include the use of precision inkjet printer systems and ultraviolet-visible absorbance measurements) are being developed in order to controllably produce deposits of nanoparticles in a manner suitable for proper surface analysis. Detailed analysis of the nanoparticle mass spectra has not shown appreciably different peak signatures in many of the solvent-exposed metal oxide systems being studied. However, ratios of mass spectral signatures may indicate small changes in relative surface compositions. Ultimately, this research seeks to 1) establish reliable protocols for nanoparticle sample preparation, 2) acquire a mass spectral database from ENP surfaces using ToF-SIMS, and 3) use the developed tools to facilitate future investigations of ENP surface chemistry, enabling a better understanding of ENP behavior in the natural environment and various other systems.

Discrete Event Simulation for Sustainable Manufacturing of Golf Ballls

Alexander Muroyama

Sustainability has become a ubiquitous term in almost every field, especially in engineering design and manufacturing. Recently, an increased awareness of environmental problems and resource depletion has lead to an emphasis on environmentally friendly practices. This is especially true in the manufacturing industry where energy consumption and the amount of waste materials can be high. One approach to sustainable manufacturing is the use of Discrete Event Simulation (DES) and Life Cycle Assessment (LCA) to analyze the utilization and processing of resources in a factory setting. Such methods can reduce the financial and environmental costs by evaluating the system performance before its construction or use. Three what-if scenarios in a simplified golf ball factory using as close to real-world data as possible demonstrate DES and LCA's ability to facilitate decision-making and optimize the manufacturing process. Plastic injection molding, an energy-intensive step in the golf ball manufacturing process, is the focus of the model. The flexible 3-D modeling software, AutoMod, was used to build the model and AutoStat was used to run the trials and analyze the data. By varying the input parameters such as type and number of injection molding machines and material used, the simulation model can output data indicating the most productive and energy efficient methods. On a more detailed level, the simulations can provide valuable information on bottlenecks or imbalances in the system. Correcting these can allow the factory to be both “greener” and more cost-effective. This study illustrates a small but important aspect of the supply chain thus demonstrating the systems approach to sustainability.

Validation of the Fire Dynamics Simulator
Taylor Myers

To quantify the accuracy of the Fire Dynamics Simulator (FDS), model simulations were compared with measurements from large scale fire experiments. This testing of FDS is considered to be model validation, as opposed to verification. Verification entails determining that the implementation of a calculation method is done properly, i.e. that the math is right. Validation entails determining if the model is a viable representation of the real world, i.e. that the physics are right.

Several experiments involving obstructed ceilings, sprinkler activation, and smoke movement in a multi-leveled corridor were analyzed and added to the FDS Validation Guide. In addition, the uncertainty of the experiments was estimated by studying the key parameters and combining their relative uncertainties. It is necessary to know the uncertainty of the experimental data to determine the accuracy of the model.

Amplification of mRNA at the Single Cell Level using Microfluidic Devices
Alex Peters

Accurate measurement of gene expression in biological samples has many applications including detection of genetic disease and understanding developmental processes. Microarrays measure the expression of thousands of genes based on relative levels of mRNA species. However, large samples (more than 1 μg) are required. This corresponds to millions of cells worth of mRNA (individual cells contain approximately 10 pg of total RNA, 1-5% of which is mRNA). Hence, unbiased amplification of small sample mRNA is required. The Eberwine process is a commonly used method for mRNA amplification, which consists of reverse transcription of mRNA into complementary DNA (cDNA), and in vitro transcription (IVT) of the cDNA to antisense RNA (aRNA). Commercially available kits that utilize this process typically give a 10^3-10^4 fold amplification without length or sequence bias. Still, these kits require a minimum of 10-100 ng of total RNA (thousands of cells), which inhibits research that requires characterization of a few or individual cells.

To address this limitation, we investigated two modifications to the existing kits. First, polystyrene beads were added to the benchtop kit reactions. T7-oligo$(dT)_{24}$ primers attached to the bead surface hybridize to the poly(A) tails of the mRNA in the samples, concentrating them on the surface of the beads. The second modification utilized microfluidic devices to generate a 1-2 nL bead column and perform reactions under continuous flow. This system incorporates the benefits of concentrating the mRNA—by using nL volumes and beads—and having a continuous stream of fresh reagents and enzymes to reduce any potential phosphate enzyme poisoning. Furthermore, we incorporated pseudo-mRNA standards into the RNA pool to allow for quantitative analysis of amplification.

Both methods exhibited comparable results and amplified initial samples ranging from 10 ng down to 10 pg (single cell level) of total RNA, which is a significant improvement over unmodified IVT kit results (poor results below 10 ng). No significant difference between the benchtop bead and device reactions was observed, suggesting that the reaction is cDNA template limited. We suspect that the higher effective concentration at the surface of the beads allows for the reactions to run more efficiently. This will allow improved quantitation of gene expression in small samples, well below those of the existing techniques.

Automating Measurements for High Voltage, High-Frequency Silicon-Carbide Power Diodes Parameter Extraction Software Tools
Cameron Rose

The emergence of High-Voltage, High-Frequency (HV-HF) Silicon- Carbide (SiC) power devices is expected to revolutionize industrial and military power generation, transmission, and distribution systems. Progress has been made in developing 10 kV SiC PiN and Junction Barrier Schottky (JBS) power diodes. Characterization, parameter extraction, modeling, and simulation of these kinds of SiC diodes are necessary for supporting several research programs designing and developing power electronics systems such as Solid State Power Substations (SSPS) and plug-in Hybrid Electric Vehicles (HEV). NIST is playing a critically important role in enabling the development of SiC devices by providing electrical and thermal measurements, as well as developing and delivering electro-thermal models for circuit simulations to industry and other government agencies.

The goal of this project is enable digital remote control capability on a fast-switching, high-power NIST custom-made current source that is currently used in high-power device characterization. To achieve this goal, the hardware of the current source was modified to allow computer control of the output through a General Purpose Interface Bus (GPIB) port. The GPIB card was first tested and configured independently for proper outputs and was then incorporated into the current source circuitry. National Instrument's LabWindows/CVI was used to design a driver specifically for the current source operation to test the interaction between the card and the current source. The final step was to modify the software of the device test system that uses the current source to include control for the current output level during testing. As a final result, the current source, together with several laboratory instruments such as high-power curve tracers; pulse generators; and digital oscilloscopes, are able to conduct fully automated experimental measurements directly from the computer interface.

The Effects of Surface Methacrylates on Biofilm Growth
Kathy Tang

Many dental composite restorations fail due to secondary caries, or recurrent tooth decay. Bacterial biofilm formation at the interface between tooth and composite is a critical component for the formation of secondary caries, yet the effects of composite properties on biofilm formation are unknown. Degree of conversion (DC) is a critical material property of dimethacrylate-based polymers and composites, because DC affects many mechanical, chemical, and biological properties of the material. In particular, dental polymers with a low DC typically have reduced mechanical properties, increased leachables, increased surface methacrylate groups, and higher toxicity to mammalian cells. Recent studies have shown that low DC reduces metabolic activity of bacterial biofilms consisting of the common oral pathogen, *Streptococcus mutans (S. mutans)*. A combination of leachable products and surface chemistry is hypothesized to be responsible for the decrease in biofilm growth. The objective of this study is to determine the effect of surface methacrylate groups on biofilm metabolic activity to understand the contribution of surface chemistry to the previously observed biofilm effects.

A series of well-controlled, self-assembled monolayers (SAMs) were fabricated on clean glass coverslips, characterized, and used for biofilm studies. SAMs with different concentrations of surface methacrylate groups were prepared by silanizing overnight with varying molar ratios of 3-methacryloxypropyldimethylchlorosilane and n-propyldimethylchlorosilane. SAMs were characterized by X-ray photoelectron spectroscopy (XPS) to assess the elemental composition of the surface and by goniometry to quantify surface hydrophobicity. After sterilizing the SAMs, *S. mutans* UA159 were inoculated on the SAMs for 4 h and 24 h. Biofilms were evaluated using 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) and crystal violet to quantify metabolic activity and biomass, respectively.

Results indicate that metabolic activity was not significantly affected by the varying compositions of surface methacrylates at both 4 h and 24 h. Preliminary results also show that biomass was not significantly affected at 24 h. These results suggest that surface methacrylate groups contribute minimally to reduced biofilm metabolism seen on low DC polymers. Therefore, leachable products may be primarily responsible for the effects of low DC on biofilm metabolism. An improved understanding of the mechanisms responsible for the effects of dental polymers on biofilm growth will enable the design of new materials to reduce the occurrence of secondary caries.

Design of a Rotary Actuator with an Integrated Angle Sensor

Andrew Trettel

Everything is shrinking—computers, music players, cell phones—and many products need ever smaller sensors, either for user input or for measurements. Microelectromechanical systems (MEMS) sensors have advanced far and may soon replace standard sensors.

These new sensors fit into smaller places, like a scanning electron-microscope, where objects must be positioned and manipulated precisely. At this scale, even small errors are comparably large, obligating high precision; and any vibration, large or small, could displace the object severely. These two criteria—high precision and low vibration—prompt the design of a rotary actuator with an integrated angle sensor to position micro-objects.

A study of previous scientific work supported the choice of an electrostatic micromotor for the actuator and a capacitive sensor for the angle sensor. Fabricated from silicon with photolithography, electrostatic micromotors need few parts and generate torque from a capacitance change. For maximum precision, the motor was designed to allow rotation in either direction and at any angle. The capacitive sensor exploits a change in area between the motor's rotor and a plate below the rotor. This area increases as the motor rotates, raising the sensor's capacitance. With the design complete, two SolidWorks CAD models were made: a micro-scale model and a meso-scale model.

The Production of Nanoparticle Arrays with Nanosphere Lithography

Martin Vilarino

Nanosphere self-assembly is a 'bottom-up' nanofabrication technique for creating a variety of simple patterns with nanoscale dimension over relatively large areas. The method is based on depositing polystyrene or silica nanospheres with diameters that range from ~50 nm to over 1 μm onto a given surface. The nanospheres pack in a close-packed pattern and define a 'mask' which is used to either pattern an underlying film using plasma etching, or used as a lift-off layer to pattern a film which is deposited over the nanospheres. The lift-off approach has been widely used to create Au and Ag nanostructures with interesting and useful plasmonic properties. The focus of my research project has been to use nanosphere assembly to fabricate Au plasmonic substrates for application in spectro-electrochemistry. One of my key goals was to develop a protocol for large area assembly of nanospheres on ITO and glass substrates.

Polystyrene nanospheres were employed to create two patterned surfaces: a periodic array of gold pyramids and a nanohole gold array. These were produced through self assembly of a closely packed monolayer of spheres onto substrates. Parameters that determined the extent of monolayer regions included dipping speed, evaporation rate of solution, concentration of spheres in solution, sphere diameter and proximity of substrate to container walls. Once the ideal combination of parameters yielded large monolayer regions, the spheres were used as a mask through which gold could be evaporated onto the substrate. Removal of the mask through sonication in ethanol left the desired array on the substrate.

These arrays could then be tested optical and chemically based on extinction spectra, surface enhanced Raman spectroscopy (SERS) and UV-visible spectroscopy.

Production of these periodic arrays not only promotes the development of enhanced techniques in nanosphere lithography, but also enables further research to be conducted on Plasmonic surfaces, including chemical and biosensing based on extinction spectroscopy and SERS. Further research in the development and use of Plasmonic electrodes is key in providing the most sensitive biological and chemical sensors known to mankind.

A Framework for Emergency Response Official Authentication and Authorization
Pragun Vohra

Many emergency incidents (such as natural disasters and terrorist attacks) in the U.S are often handled on a local level, though some of them may be of a magnitude that requires help across jurisdictions (from a neighboring county or another state) and even from the federal government. To facilitate the call-up and utilization of such mutual aid, it is necessary that the resources (both human and equipment) needed for responding and recovering from such incidents are accessible through well-defined descriptions (data schemas) and that a procedure exists for properly identifying the personnel at incident sites and providing the necessary authorizations for carrying out vital tasks.

The goal of the research project is to develop a framework for the authorization and authentication of emergency response officials at various incident sites. The overarching problem can be divided into various subproblems: designing platform-neutral XML schemas for capturing and storing information about the domain expertise of various types of emergency response officials (e.g. emergency medical service, firefighters, etc.), implementing access control policies for storage repositories containing this data using XACML, creating XML schemas for the exchange of such information between jurisdictions, dynamically transforming data under storage schemas to data exchange schemas using XSLT transforms, and developing protocols (e.g. SAML queries and responses) for the cross-jurisdictional retrieval of attributes (expertise, training, qualification etc) of first responders.

Obtaining Sensitive Electro Reflectance Spectra for High K Dielectrics
Sean Weerakkody

Electro Reflectance Spectroscopy, a method that which utilizes the change in reflectance of a sample as a response to periodic electrical perturbations, is a useful technique that allows us to better understand the physical properties of a material under observation. The goal of our project is to obtain highly sensitive electro reflectance spectra for high K dielectrics as we modulate electric field. This will allow us to analyze defects that may exist in these dielectrics. When a spectrum has large peaks, the sensitivity of a detector must be reduced to prevent saturation. In order to maximize the sensitivity of our detector, it is desirable for light intensity to be nearly uniform as a function of wavelength. As such, a large focus of the project is implementing an attenuator attached to a servo motor that will respond to the light intensity as we vary wavelength. To do so, a feedback circuit to the servo was constructed which allows the servo to rotate clockwise or counterclockwise in response to two digital input/output bits of a data acquisition module. Moreover a Labview program has been written to determine the direction and degree of rotation of the servo as a function of the reflectance data being gathered. By maximizing the sensitivity of our detector, we hope to obtain a large amount of useful data that will allow for better understanding of high K dielectrics and their new potential applications.

The Methodology of Assessing Robot Generated Maps
John Welsh

Advances in computing, sensing and actuator technologies have equipped mobile robots with the ability to sense and navigate their immediate surroundings. For mobile robots to perform tasks that require information beyond their field of view, they require not only high performance hardware, but also an accurate internal representation of their environment. Researchers continue to develop algorithms aimed at incrementally building a map of the environment, and localizing a robot within that map. However, the advancement and future use of emerging mapping algorithms is halted by the lack of a standardized method for evaluating their performance.

To address the issue of quantitatively assessing robot generated maps, this presentation reviews the methodology of implementing and testing mapping algorithms. While any mapping algorithm is at the mercy of the robot's hardware accuracy, an effective evaluation of a given mapping algorithm can be achieved by comparing the results to a map generated where the robot's position and orientation are necessarily accurate, but not perfectly precise.

IEEE 1451.4 Sandard: A Smart Transducer Interface for Mixed-Mode Communications
David Westbrook

The increasing power of electronics and computers in addition to the widespread availability of networks has made possible the use of transducers (sensors and actuators) to measure, characterize, and model many structures and environments. With the potential to use hundreds of transducer in a system, transducers must have built-in identification data. IEEE developed the 1451.4 standard, where a 1451.4 transducer has a unique registration number (URN), a transducer electronic data sheet (TEDS), and a mixed-mode interface (MMI) to communicate information to a user.

This project concentrates on the Class 1 MMI, (i.e., the transmission of a transducer's analog signal or digital TEDS data is done on a single wire). Incoming voltage polarity controls the mode: positive voltages represent analog mode and negative voltages represent digital mode. The digital data transmission protocol is a master-slave relationship, where a single master device initiates each transaction with the transducer nodes (slave devices) by supplying a defined sequence of pulses on a single wire. Each transaction consists of an initialization sequence, command to read the URN, and a command to read the TEDS. Transducers will automatically be detected when they connect to the circuit and the master will then initiate data transmission (i.e., plug-and-play sensor).

The Basic TEDS includes the manufacturer ID, model, version, and serial number. Additionally, most transducers make use of a 256-bit data memory to store optional data, such as calibration constants, board identification, and product revision status. The master device can read from and write to the data memory by using a built-in buffer, (i.e.,a scratchpad). The ability to view and change data memory has many practical uses; for example, pulse analyzers have been created to automatically detect connected transducers and set the sensitivities before making measurements. The 1451.4 interface will allow sensors to be used in diverse environments and to be configured into the system automatically upon connection (hence it is called self-configuration).

This project will provide a functional 1451.4 interface that gives transducers "plug and play" compatibility very similar to that between a computer mouse and any desktop. This interface will also allow for future interactions with other members of the 1451 family of standards giving 1451.4 transducers network and web access.

Direct Tension Cyclic Fatigue Test on Asphalt Concrete Material
Joseph Yan

Asphalt concrete mixtures are subject to three potential forms of major distresses: permanent deformation, thermal cracking, and fatigue cracking. Fatigue cracking occurs as a result of the accumulated damage under repeated load applications, caused, for example, by the deflections required of pavement from each passing vehicle. The fatigue performance of different mixtures can be evaluated in the laboratory via the application of a cyclic load to asphalt specimens.

A new test method, proposed by Dr. Richard Kim of North Carolina State University, involves determining the damage characteristic curve of asphalt concrete from a dynamic modulus test and a direct tension cyclic fatigue test. The damage characteristic curve shows how the pseudo secant modulus varies with damage and defines the fundamental relationship between the structural integrity and the amount of damage in a given mixture of asphalt. In combination with the linear viscoelastic properties of asphalt concrete, the curve can be used to analyze fatigue characteristics and potentially assess and predict fatigue behavior of in-service asphalt concrete mixtures. This test protocol may provide a means of allowing the comprehensive characterization of fatigue properties from a simplified viscoelastic continuum damage model.

In order to evaluate the efficacy of the proposed AASHTO standard test method, tests need to be performed to compare data from established fatigue models. The existing hydraulic asphalt testing machine was designed by IPC Global to perform tests developed to find the dynamic modulus, flow number, and flow time of hot-mix asphalt. This machine had to be programmed in order to run the newly developed test method, accepting all of the necessary parameters to control the cyclic loading and displaying real-time sensor readings and calculations as needed. Trial tests were then begun using the developed program in order to determine acceptable and realistic data ranges for various test parameters and measurements. An evaluation of the accuracy and clarity of the procedures and calculations outlined in the draft protocol under review was also made.

University of Michigan

Characterizing the Compositional-Structural Properties of Mixed-Phase Light-Absorbing Carbonaceous Atmospheric Particles: Implications for Climate Change Modeling
Sean Collins

The role of atmospheric aerosols is a critical source of uncertainty in climate change modeling as both the direction and magnitude of the warming/cooling effects of atmospheric aerosols are not fully known. The climate effects of individual particles depend not only on whole-particle characteristics such as size, shape, and overall composition, but depend significantly on the internal structure as well. Light-absorbing carbon is known to have a net atmospheric warming effect, and so the case of mixed carbonaceous particles represents a climatically relevant class for studying mixed particles. In this study, particles from an air sample from Los Angeles, CA were first screened using light microscopy for qualitative assessment of optical properties. Computer controlled scanning electron microscopy (CCSEM) with energy dispersive spectroscopy (EDS) was then used to provide a compositional survey of the particle sample. Individual mixed-phase particles identified in the screen were investigated using high resolution SEM and two-dimensional EDS mapping to assess the spatial distribution of chemical species. Particles with high spatial complexity were further studied using focused ion beam scanning electron microscopy to slice particles for cross-sectional examinations by SEM-EDS. Slices were also removed by micromanipulator lift-out for analytical electron microscopy to examine phase distribution at the highest possible resolution. These combined analyses yield a three-dimensional description of the compositional and structural characteristics of mixed-phase carbonaceous particles present in the atmosphere and demonstrate that light-absorbing carbon occurs in a wide variety of mixing states from simple binary aggregations to complex internal mixtures with hundreds of discrete inclusions in a single particle.

University of Puerto Rico

Investigating the Adsorption Behavior of Thiolated Polyethylene Glycol on Gold Nanoparticles using Infrared Spectroscopy: Applications in Targeted Drug Delivery for Cancer Therapeutics
Melissa Davila Morris

In applications of nanoparticle-based cancer therapeutics, there is a need for measurement tools to quantify and characterize molecules bound to the surface of nanoparticles (e.g., targeting moieties, therapeutic agents). In this study, attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy was utilized to perform a quantitative characterization of thiolated polyethylene glycol (SH-PEG) uptake onto gold nanoparticles (Au-NPs), as a model system for targeted drug delivery. Adsorption isotherm studies were performed using SH-PEGs with different relative molecular masses, M_m, (1 kDa, 5 kDa and 20 kDa), and showed that surface coverage for SH-PEG on Au-NPs is inversely proportional to M_m. Equilibrium binding constants for SH-PEG on Au-NPs were analyzed using a Langmuir adsorption model, and indicated a strong binding affinity towards Au-NPs ($>10^4$ L/mol) via Au-thiol bonds. Moreover, we demonstrate the capability of using the ATR-FTIR method to quantify the competitive adsorption between SH-PEG and bovine serum albumin, as a model serum protein, at the Au-NP/solution interface, providing a prototype approach for understanding possible ligand displacement by molecular species commonly present in biological systems.

Attribute Assurance in Anonymous Transactions
Eliezer Ferra

The increase in identity theft incidents has given rise to new questions about the secure delivery of attributes to parties to a transaction. Sometimes a relying party asks for information that is important to identify the subject. One possible scenario would develop if a framework known by the relying party and trusted by the subject could perform an authentication of the subject. Is it possible to deliver attributes with strong assurance of their subject without identifying the subject? It is possible, if certain conditions exist and certain steps are followed. First, the transaction needs to be among three (or more) parties. In addition, the Subject and the Relying Party, must trust the Attribute Provider, therefore the Attribute Provider can act as an intermediary between the Subject and Relying Party. The goal of the project was to implement a Strong Attribute Assurance using Diffie-Hellman Key Exchange as encryption keys for the transaction. In this presentation I will explain the importance of this implementation and give examples of how can it be useful in our daily practice. I will also talk about the problems I encounter when building the demo and finally I will show an example of a transaction that utilizes the implementation I developed.

Comparison of SiO_2 and SiN Substrates for Graphene Devices
Mairin Nieves-Nevarez

Since its discovery, graphene, a two-dimensional honeycomb lattice of carbon atoms, has drawn a lot of attention in the scientific community as a prospective material for future electronic devices. One of the possible applications of graphene is the development of novel quantum resistance standards based on Quantum Hall effect in graphene.

Silicon dioxide/silicon (SiO_2/Si) substrates have been widely used for gated graphene devices, but it has been proven that any substrate limits the mobility of graphene due to surface roughness and trapped charges in the insulator. The goal of this research project is to explore the effect of two different substrates, SiO_2/Si and silicon nitride/silicon (SiN/Si), on the mobility of graphene devices. This would help to fabricate a high-quality graphene device that can be used as a quantum Hall resistance standard. We first calculated the optimal thickness of SiN that would make single-layer graphene, exfoliated on SiN/Si, visible under optical microscope. Once the proper thickness is calculated, the SiN of certain thickness will be grown on Si substrate. The graphene flakes will be obtained by mechanical exfoliation of natural graphite on SiO_2/Si and SiN/Si substrates. Subsequently, Quantum Hall bar devices will be designed in AutoCAD and fabricated using e-beam lithography. After that a series of transport measurements of graphene Hall bar devices will be performed. The subsequent data analysis will show what type of substrates, SiO_2/Si or SiN/Si, gives a higher mobility.

Analysis of Efficiency of Mapping Distributon Protocols in Scalable Routing and Addressing Architectures

Kevin Rivera Delgado

It is known that in the current Internet architecture there is a routing scalability problem. One way to solve this problem is to separate the routing locators from the End-point Identity (EID). This class of solutions is called map-and-encap, and uses IP-over-IP tunneling. The leading map-and-encap protocol proposal in the Internet Engineering Task Force (IETF) currently is the Locator ID Separation Protocol (LISP). NIST researchers have shown that in the original map-and-encap proposals in the IETF (including LISP), the mapping distribution protocol (MDP) was not designed efficiently. This inefficiency was due to the fact that the presence of what are called “holes” (or exceptions) was not handled efficiently. A hole (or exception) occurs in a map when an aggregate (less prefix) prefix maps to one AS (or routing locator) and a more specific prefix contained in that aggregate maps to a different AS (or routing locator). The presence of so many holes makes the MDP work inefficiently due to significant proliferation of the map entries and map messages. NIST’s proposal is known as Enhanced Efficiency of Mapping Distribution Protocols (EEMDP). My SURF project was to help with the modeling and quantification of the extra map messages that would need to be stored and distributed due to the presence of holes in the prefixes in today’s Internet. I wrote a program to identify and count all the extra map messages that are necessary in map-and-encap proposals due to the presence of holes if NIST’s EEMDP proposal was not used. I also estimate the total number of map messages that would be needed if EEMDP is used with a map-and encap solution (such as LISP). We find that significant savings in the number of maps in the mapping system occurs, and hence significant savings results in the storage and processing of map messages when EEMDP is used together with map-and-encap protocols.

University of Rochester

Modeling of Multiphase Flow with Interfacial Agents

Daniel Reynolds

Multiphase flows which use interfacial agents such as surfactants or compatibilizers are common in many industrially important applications including emulsion technologies, polymer mixing, medical applications, and a number of Polymers Division measurement projects. Surfactants are amphiphilic molecules which possess a hydrophilic head and a hydrophobic tail. The two distinct domains cause the surfactant to accumulate at the interface between immiscible fluid phases. This lowers the surface tension between the phases and leads to more stable emulsions and finer drop size. Compatibilizers are block copolymers that possess alternating domains throughout its structure and serve a similar function as surfactants but in polymer-polymer mixtures. Interfacial agents are used to control surface tension and drop size by enhancing breakup and suppressing coalescence. The ability to control surface tension is important for industrial and scientific applications because of the need to control emulsion stability and the mechanical and optical properties of immiscible polymers generally improve with a decrease in the dispersed droplet size.

In this project we have developed models for multiphase flows involving surfactants and compatibilizers. The models have been implemented in the finite element package COMSOL Multiphysics. In order to model these multiphase systems, we have implemented a number of diffuse-interface models that couples the thermodynamic equations of interfacial agent adsorption with the hydrodynamic equations governing droplet flow and the species balance equations. Experimental evidence has shown that surfactant molecules become redistributed on the droplet interface as a droplet undergoes deformation. One use of our model is to gain a better understanding of how surfactant redistribution affects droplet hydrodynamics. Similarly, the model for compatibilizers is used to study mixing in polymer-polymer systems.

Measuring Silver Nanoparticle Dissolution with the Donnan Membrane Technique

Benjamin Yezer

Silver nanoparticles (Ag NPs) are often used in medical and household equipment as anti-microbial agents. Currently, it is unclear whether Ag NPs are toxic to microorganisms or simply their dissolution product (ionic silver), which is known to be toxic to aquatic organisms. Subsequently, measuring the dissolution rate of Ag NPs under different environmental conditions is a key component to rectifying the growing body of Ag NP toxicological data. Current methods used to distinguish between ionic and NP silver may underestimate silver in the NP form. For example, ultracentrifugation may not fully distinguish between small (<10 nm) NPs and fully dissolved cations. This project explores a new method of separating Ag NPs from ionic silver using a novel procedure called the Donnan Membrane Technique (DMT).

The DMT relies on the diffusion of cation species from a large-volume “donor” solution into a small-volume “acceptor” solution, with the rate of diffusion being controlled by a negatively charged membrane that physically separates the two solutions. Theoretically, only cations should be able to diffuse through the membrane, and therefore the DMT should be able to quantify ionic silver, even in the presence of very small Ag NPs. The purpose of this investigation was to determine whether the DMT was sufficiently robust to quantify ionic silver that had been liberated during photolysis of Ag NPs.

Analysis of donor and acceptor solutions using inductively coupled plasma mass spectrometry (ICP-MS) shows evidence of ionic silver diffusing through the membrane at a rate slower than predicted literature values, likely due to characteristics of the membrane. Collected data displays Ag NPs adhering to the membrane surface, but NPs are not appearing to diffuse into the acceptor solution. The DMT proves to inhibit transfer of Ag NPs and be a viable procedure for the separation of Ag NPs from ionic silver. Future experiments will refine the DMT procedure to quantify Ag NP dissolution in natural water systems.

University of Southern Mississippi

Chromium Single-Photon Emitters in Bulk Diamond

Olivia Hoff

The development of quantum applications such as quantum communications, quantum metrology, and quantum computation is dependent upon single-photon emitters (SPEs). Diamond color centers are a source of SPEs that are usable at room temperatures. This experiment investigates single-photon sources in bulk CVD (chemical vapor deposition) diamond by chromium ion implantation begun by Aharonovich et al (1). The single-photon emitters were created in CVD diamond samples through the co-implantation of chromium, oxygen, and boron atoms at different fluencies and beam energies. Light at 689nm is expected to cause the color centers to fluoresce at 750nm. The color centers were examined by a CCD camera and a spectrometer.

(1) Igor Aharonovich, Stefania Castelleto, Brett C. Johnson, Jeffery C. McCallum, David A Simpson, Andrew D., Greentree, and Steven Prawer. "Chromium Single-Photon Emitters in Diamond Fabricated by Ion Implantation." *Physical Review B 81, 121201(R) (March 2010)*. Available from NIST internal website Gaithersburg E-Journals, American Physical Society, http://prb.aps.org/toc/PRB/v81/i12 accessed May 2010.

Selective Gas Sorption in Metal Organic Frameworks

T. Grant White

Selective gas separation technologies are a critical component of a number of industrial process, including chemical and energy production. Use of hydrocarbon fuel sources constitute approximately 85% of worldwide energy production and result in extensive emissions of carbon dioxide (CO_2), a greenhouse gas. Presently, cost-effective efforts to reduce anthropogenic CO_2 are being explored. Given that that the resulting exhaust is a mixture of gases, it is important to consider the extent of selectivity in CO_2 gas separation. The prevailing methodology is based on aqueous amine absorption, and, though technically effective, these systems are not fiscally prudent due to massive energy consumption, as well as degradation of the amine during the process of CO_2 extraction. Recently, adsorption-based carbon capture technologies have been explored. As adsorption is fundamentally different from absorption, adsorption-based gas separation could result in a more efficient process for capturing CO_2 for eventual sequestration, offering lower regeneration costs and improved sorbent stability.

Some examples of adsorbent materials from daily life include alumina, silica, zeolites, activated carbons, and polymers. A more recent class of porous materials is Metal Organic Frameworks (MOFs), crystalline materials that possess highly tunable organic-inorganic hybrid structural features. The attractive property of MOFs for this effort is their remarkable surface areas, with a recently-reported material possessing a surface area of 6,240 m^2g^{-1}. The combination of these properties makes them particularly amenable to adsorptive processes with a variety of guest molecules, permitting applications in both alternative energy and carbon capture. One subclass of MOFs is that of Zeolitic Imidazolate Frameworks (ZIFs). ZIFs are easily synthesized, chemically and thermally robust materials that have been shown to have an affinity for CO_2.

This talk will cover the synthesis of several porous MOF and ZIF powders and measurements of the adsorption and diffusion of CO_2 and other gases. In addition, attempts have been made to generate MOF membranes via seeded growth of thin films on a macroporous support. As the project is a fresh endeavor, significant efforts have been focused on the construction and calibration of a new measurement system to accurately measure gas permeance through MOF columns and membranes. Gas selectivities in each MOF/ZIF are derived from single-gas measurements using the Ideal Adsorbed Solution Theory and from their relative gas permeances. Additionally, further improvements to the measurement system will be discussed.

University of Texas Austin

A Long Wavelength Photoresist for Plasmonic Field Metrology
Richard Webb

Surface Plasmon Polaritons (SPPs) have gained much research attention in recent years as a method of locally confining light for use in nano-optics, lithography and biosensing. The utility of SPPs in these fields is dependent upon four SPP length scales that are important to device fabrication: the SPP wavelength, the propagation length, the penetration depth into the metal, and the penetration depth into the dielectric. A long propagation length is particularly useful to sensing applications, but long propagation lengths require long wavelength (into the red) incident light. SPPs launched with visible light are also of critical importance for future applications in solar cells and LEDs; however, imaging SPPs as they propagate at visible wavelengths has been a significant metrology challenge. The current best method for imaging plasmons, near-field imaging, is strongly perturbative, sequential, and is resolution-limited by the tip geometry.

Our laboratory is developing photoresists that are optimally designed for imaging plasmons. A photoresist is well-qualified as a plasmon metrology tool because it converts the local plasmon field into a topological relief pattern that can be measured by high resolution AFM. The problem with using current photoresists as metrology tools is their insensitivity to visible light, development issues such as swelling, and that they are typically applied in relatively thick (>50 nm) layers. These issues make current photoresists a poor choice for quantitative plasmon metrology.

Here, we present a new molecular glass photoresist that is broadly sensitive to visible light, can be applied in ~10 nm thin layers over large areas, and develops a light-sensitive pattern with gentle heating. Furthermore, the resist is a single-component system requiring no solvent, is easily modifiable, and is synthesized for under a dollar per gram in material costs. We demonstrate the application of this resist for high resolution imaging of SPPs launched from long wavelength (λ>600 nm) incident light.

University of Texas Dallas

Obtaining Accurate Estimates of the Diffusion Coefficient
Philip Campbell

Camera-based single-particle tracking relies on the analysis of particle position at each time point to determine characteristic properties such as the particle size or shape, as well as the fluid viscosity. This analysis uses images taken of microscopic particles as data from which the positions of particles are estimated. It is important in these measurements to use as accurate a method of estimation as possible in order to achieve the optimal results using this kind of analysis. Difficulties in the estimation arise from localization noise, which is present in all images as a result of the camera, and motion blurring of particles due to the length of camera frames taken.

The most commonly used method of estimation currently is the mean-square displacement method. In this study, we compare the mean-square displacement method with a recently developed maximum likelihood estimator. The two estimators are simultaneously used to estimate both the diffusion coefficient of a particle and the localization noise on the image. We also examine the effects of a motion blur coefficient, determined by varying the illumination within a single frame, on the spread of estimates provided by each estimator. We find that the maximum likelihood estimator provides a much smaller spread of estimates compared to the mean-square displacement for all experimental conditions tested. In addition, we prove that the precision of our estimates increases with the motion blur coefficient, leading to a double-pulse sequence as the optimal frame illumination to provide the best measurement.

TDDB Testing
Scott Carlson

How to ensure that cars will still be functioning reliably after it has been on the road for more than 10 years? To quantitatively predict the probability of failure that far into its usable life, good statistics in accelerated tests is critical. This is something that is easier said than done. While it is well known that large number of devices must be stress tested, the technology to do so is not there. Time-Dependent-Dielectric-Breakdown (TDDB) is one of the potential modes that automobile electronics can fail, leading to catastrophic system failure. Current TDDB testing algorithm at NIST is limited by not being able to test more than 20 devices at a time. My project is to seek a novel testing method that can stress test 1500 SiC devices at a time. The testing method ultimately will involve the relationship between voltage, ambient temperature, and the failure times for each device's dielectric. The scheme that I am developing uses the idea of 24 circuit cards with 64 probes on each one to measure current through the gate stack of each device. Capacitors are stressed at certain voltage at certain temperature. The leakage current for each capacitor is monitored. Normally, the dielectric material has few free electrons, and blocks current. As the voltage is increased, charges can tunnel through the dielectric and create defects over time. As the capacitor degrade, the leakage current increases slowly. This increase carries information about how the dielectric wears out. When breakdown failure occurs, the current will jump up by several orders of magnitude. The initial application of this testing method is on SiC metal-oxide-semiconductor (MOS) capacitors. SiC devices as a whole are superior to purely silicon devices for power electronics applications in that they can handle more power, more heat, and operate at a higher frequency. They are used by NASA, the U.S. military, and other organizations with a high demand for reliability, power, performance, etc. The devices have a higher band-gap than Silicon, which is what allows them to operate at higher temperature. Currently, our parallel testing method is still under development. The circuit card is still not fully functional, due to some components being unavailable.

Sub-Nanometer Metrology with Charged Particle Microscopes
Benjamin Swedlove

Microscopes such as the Scanning Electron Microscope (SEM) or Focused Ion Beam (FIB) are excellent for viewing samples with extreme magnification, yet sub-nanometer resolution remains out of reach for many machines due to vibration and heat from the surroundings and from the instruments themselves. Heat and vibration cause drift and inhibit the microscopes' ability to accurately measure the dimensions of next generation semi-conductors. With accurate measurements, industry can do more than experimentally optimize for higher yield, but can study why certain products fail and what features are the critical weakest links.

We are developing drift correcting software that can mitigate environmental factors. This software must be tested with computer generated images so that the calculated amount of drift in the image can be compared against a known value. This has shown definitive proof that drifting samples can be acquired under noisy conditions. The ability to mitigate drift in noisy images is a great benefit, allowing someone to take pictures of the sample more frequently, which inherently decreases the drift between each picture. I have implemented a frequency filter that has significantly improved results in noisy images. The project's research has progressed to testing and refining the filter to decrease error and to discover under what conditions the program works effectively.

Our software will aid researchers who must delve into the structure of materials, or measure the radii of novel nanotubes, and help the staggering semi-conductor industry see the ever smaller features they are producing. This work opens up the possibilities for what science can be done, and where. Imagine the ability to image samples at sea, or even on buzzing spacecraft. This software will not only extend the range of science into the far reaches of space, but will greatly increase the accuracy of measurements made here on Earth.

University of Wisconsin Stout

Heat Treatment Effects on the Microstructure, Mechanical Properties, and High Strain Rate Deformation of AISI 1075 Steel

Jacob Huber

Steels are ferrous alloys possible of a wide range of highly adaptable mechanical properties. Through the use of various alloying elements, heat treatments, and secondary processes, one can tailor an alloy to achieve certain properties necessary for a specific application. It is important to understand and predict how these materials will react to external forces imposed on them during processing and their useful life.

There are numerous heat treatments available that create drastically different properties for a single alloy. Heat treatment methods include spheriodizing, normalizing, quenching, and many others. Such thermal processes produce a variety of microstructures that result in these changes in mechanical behavior. Each process will have a different affect on the microstructure, which directly influences properties such as the yield strength, ductility, hardness, etc.

There are many tests available to understand the microstructure and mechanical properties present in a material. Our research focused on metallographic work, Vickers hardness testing, and Kolsky Bar testing to analyze the plain carbon steel specimen. Metallographic work was performed to determine the microstructures present in the alloys. Vickers hardness testing was used to determine uniformity in samples and how mechanical properties varied as different thermal processes were done on the specimen. Kolsky bar testing is a high strain rate dynamic testing process where an elastic compression wave deforms a sample. Through the use of an oscilloscope and digital image correlation during a Kolsky Bar test, a stress-strain curve and a strain rate data can be collected for each specimen tested.

Valparaiso University

Measurement of Neutron Reflectivity for a Silicon Crystal: Preparation for an nMDM Measurement

Benjamin Barber

The study of neutron magnetic dipole moment (nMDM) interactions in a perfect silicon crystal is an important check on a novel method to measure the neutron electric dipole moment (nEDM). Physicists from Argonne National Laboratory, Valparaiso University, University of Hawaii, and NIST have designed an experiment to use the known nMDM to measure a phenomenon known as Schwinger scattering in silicon, a process whereby the orientation of the neutron magnetic dipole polarization is altered by interactions with the atomic electric fields in the silicon crystal. This measurement is intended to be a precursor to a search for a neutron electric dipole moment employing a similar spin rotation via a different fundamental interaction. Both measurements depend on neutron Bragg reflections down a slotted silicon crystal. For a successful measurement, the neutron beam has to reflect approximately 150 times down a slotted crystal, without a large loss of beam intensity. This requires a crystal with a high reflectivity, on the order of 99% reflective. In order to make an accurate measurement of the Schwinger scattering, both the incident neutron beam and the crystal's reflectivity need to be well understood. This summer we have characterized the newly commissioned 'nMDM Experiment' neutron beamline at the NIST Center for Neutron Research, and have measured the reflectivity of the slotted silicon single crystal intended for the experiment. These measurements lay the groundwork for the coming nMDM Schwinger scattering measurement.

Virginia Polytechic Institute and State University

A High-Resolution Interferometer for Nanomechanical Measurements
Cadence Martin

A Fabry-Perot interferometer with sub-nanometer resolution and SI-traceability has recently been developed at NIST. A displacement sensor with such high accuracy and resolution has many useful applications in nanomechanical testing. This summer's research focused on improving upon existing systems and adapting them for these various applications. Two interferometers are currently being used in an atomic break-junction experiment; one is for measuring displacement, and the other is for indirectly measuring the force required to break a single-atom chain by determining the deflection of an AFM cantilever. In addition, an interferometer was used to verify the calibration of the displacement sensor in a commercial nanoindenter. Lastly, a precision nanoindenter is currently being developed which will utilize the interferometer.

The interferometer functions by forming a Fabry-Perot (FP) cavity between the end of an optical fiber and a parallel reflective surface. Light from an infrared laser is guided to the FP cavity through an optical fiber. Reflections from the end of the fiber and from the opposing surface interfere due to the difference in path length, which is equal to twice the length of the gap between two surfaces. This reflected light is converted to a voltage by a photodetector and amplifier; changes in voltage can then be correlated to changes in gap length. Additionally, the interferometer can be used in short-range (sub-nanometer to tens of nanometers) or long-range (micrometers or larger) mode, by varying technique but not physical set-up.

Wellesley College

Creating a Scanning Laser System for Manipulating Bose-Einstein Condensates
Yomay Shyur

At temperatures close to absolute zero, the underlying quantum mechanical nature of matter can become apparent, giving rise to interesting phenomena such as Bose-Einstein condensation (BEC) and superfluidity.

Our lab studies metastable superfluid flow in a ring-shaped atomic BEC. One important precision tool for manipulating and stirring the BEC in these experiments is an optical dipole potential formed by a tightly focused laser beam. My contribution to the project has been to develop a system for scanning the position of the laser beam to create a time-averaged optical potential. This potential can, for example, form a movable barrier for obstructing the superfluid flow. The beam scanning is accomplished with an acousto-optic deflector (AOD), which provides high-speed control over the intensity and deflection angle of the transmitted laser beam.

This project demonstrates a working AOD system that will be used to create a movable optical potential for manipulating the BEC in the present experimental system. This system takes advantage of the versatility of the AOD, allowing creation of barriers with different shapes, intensities, speeds, and accelerations. These potentials can be combined in complex sequences. Preliminary tests of the system indicate that the precision and uniformity of the optical potential are very high, and in an operational range that matches the experimental requirements.

West Virginia University

Optimized Thermal Photoresist Processing for Nano-Structured Optics
Jesse Hood

Photolithography is a key technology for the fabrication of structures with micrometer dimensions. Examples are integrated circuits, micro and nano optics, and micro-electro-mechanical-systems. Photolithography is used to remove parts of thin film or the bulk of the substrate. It uses light to transfer a pattern from a photo mask to the light-sensitive photoresist on a substrate. The basic process involves several chemical processes: use photo mask to transfer its very precise pattern, create a substrate made of glass with a layer of chrome and photoresist, spin coat and soft baked the photoresist onto the substrate, exposure and developing, etching, and then photoresist removal.

After the spin coating step, the photoresist can still contain some solvents, and a process called soft baking is used to remove the rest. Soft baking is a vital part of photolithography because if the photoresist is overheated parts of it can be destroyed, but if it is under heated, light will not be able to reach the sensitizer. To get rid of the solvent the photoresist needs to be heated to around 115 °C for one minute. Several challenges exist during this heating process: Substrate thickness can affect the heating pattern, also the infrared heater may cause problems in heating the substrate evenly, thicker substrates take a longer time to heat up and the optimum temperature of 115 °C cannot be reached with using a hotplate. A new thermal treatment technique is needed when heating the thicker substrate.

To make this process faster and more efficient for the large 6 inch substrate, an infrared oven was constructed to determine the effectiveness of heating the photoresist. Many tests were done to see how fast and how uniform this new heating technique could heat the photoresist on the large substrate. A temperature controller and temperature sensors were used to regulate and measure the temperature inside the oven. This talk will discuss the efficiency of the new oven design and the challenges that were encountered. It will also present ideas for future directions on this challenge.

Worcester Polytechnic Institute

Verification of the Fire Dynamic Simulator
Danielle Antonellis

The Fire Dynamic Simulator (FDS) is software used to analyze fire-driven fluid flow using Computational Fluid Dynamics (CFD), originally released in 2000 by the National Institute of Standards and Technology (NIST). FDS is a valuable tool for research, investigation, and design of fire systems and can be used to evaluate many scenarios; it is still in heavy development with Version 6 expected to be released by the end of the summer.

It is important for FDS developers to perform examples of plausible situations to insure that their results are accurate and repeatable. There are two processes, validation and verification, that are used by FDS developers to confirm that the program is coded correctly and running appropriately. For validation, data is compared from FDS output files and experiments; these results are compared quantitatively to determine if FDS is predicting fire dynamics correctly. For verification, numerical solutions are obtained from FDS and compared to analytical solutions to determine if the source code of FDS supports the theory behind it. A specific test for verifying the numerical scheme used to solve the continuity equation in FDS was analyzed and plots of “time vs. density” were created to demonstrate how accurate the FDS solution can be, relative to the analytical solution. There are three schemes: central differencing, CHARM, and Superbee which have flux limiters of zero, on, and two, respectively. Plots have also been created to demonstrate how these schemes converge to second-order accuracy.

Water Calorimetry Using Ultrasonic Interferometry

Long Tong

The possibility of using an ultrasonic interferometry setup for performing water calorimetry is explored. As a primary standards laboratory, NIST holds the primary reference standard for the calibration of instruments used in quality-assurance protocols for radiotherapy beams used in cancer treatment at US hospitals and clinics. The static, uniform standard-reference beams used with the primary-standard water calorimeter differ markedly from those defining state-of-the-art beam therapies actually used in cancer treatment, which may employ highly non-uniform, time-varying fields. Thus, calibration conditions for clinical dosimeters bear little resemblance to the treatment conditions, which might introduce errors into treatment plans. Moreover, with the increasing use of smaller and more complex beam configurations in radiation treatment plans, such as those used in intensity-modulated radiation therapy (IMRT), the use of an ionization chamber for the calibration of these smaller beams become problematic. This creates a need for a primary reference standard instrument that is capable of providing absolute dose measurements in non-standard-reference beams.

The Radiation Interactions and Dosimetry Group at NIST has been investigating the feasibility of using time-of-flight ultrasonic techniques for purposes of mapping absorbed dose in dynamically changing, non-uniform beams. My work this summer has focused on developing a pulsed interferometer for thermometry that would measure absorbed dose. Using an ultrasonic interferometry configuration in a water phantom may allow some of the issues associated with using an ionization chamber when assessing the strength of smaller radiation fields to be avoided. My talk will go into the different setups built for testing the feasibility of such a method for performing water calorimetry as well as some of the issues with such an approach.

APPENDIX A. QUICK CROSS-REFERENCE – SURF 2010

2010

SURF STUDENTS

BY UNIVERSITY

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STUDENT	UNIVERSITY	TITLE OF TALK	OU
Geraghty, John	American University	Transverse Motion of the Main Induction Coil in the Electronic Kilogram Experiment	EEEL
Nadeau, Michelle	American University	Calibration of Transition-Edge Sensor (TES) for Applications in Testing Bell's Test of Nonlocal Realism	PL
Perkey, Virginia	American University	Development of a Point Sensor to Measure Greenhouse Gases Using Novel THz Spectroscopic Techniques	PL
Bougher, Cortney	Appalachian State University	Calibrating Spectrophotometric Standard Stars	PL
Robertson, Luke	Appalachian State University	Simulation of High Reflectivity Photonic Crystal Mechanical Resonators	PL
Riedel, William	Brown University	Data Acquisition and Analysis of Shim Arm Position During a 5 Degree Rod Drop Test	MSEL/NCNR
Truong, Jonathan	Brown University	Off-Line Two-Dimensional Separation of Proanthocyanidins in Botanical Standard Reference Materials	CSTL
Markwalter, Daniel	Bucknell University	Engineered Titania Nanoparticle Dispersions for Environmental Health and Safety (EHS) Applications	MSEL/NCNR
Terrell, Elise	Bucknell University	Creating a Graphical User Interface (GUI): Comparing Technical Performance and End-User Utility	MEL
Noah, Ramsey	California State University Long Beach	Growth of Diamond Thin Films for Use in Investigation of Nanoscale Friction	CNST
Gehrels, Emily	Carnegie Mellon University	Raman Spectroscopy of Graphene Decorated with Copper Nanoparticles	PL
Jia, David	Carnegie Mellon University	Controlling GPIB-Compliant Instruments Using a JAVA-Implemented Interface	EEEL
Keller, Joshua	Carnegie Mellon University	Neutron Imaging of Rechargeable Lithium-Ion Batteries	PL
Swisher, Matthew	Carnegie Mellon University	Characterization of Micro Electro Mechanical Sensors	CNST
Chhabra, Amandeep	City College of New York	Quartz Tuning Fork Kelvin Force Microscope	EEEL
Kaur, Navjot	City College of New York	Studying Protein Clusters in Solution Using SANS and Rheometry	MSEL/NCNR
Callo, Catherine	City University of New York Hunter College	Temperature-Dependent Optical Properties of Semiconductor Colloidal Quantum Dots	PL
Patel, Dixitchandra	City University of New York, City College	Evaluating Changes in Physical and Mechanical Properties of Asphalt Binder with Short-Term and Long-Term Aging	BFRL
Need, Ryan	Clemson University	Electrodeposition of CdS-CdTe Photovoltaic Devices on Interdigitated Back-Contacts	MSEL/NCNR
O'Brien-Applegate, Kimberly	College of William and Mary	Testing the Security of Android Applications	ITL

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Richards, Brian	College of William and Mary	Precision Resistance Measurement Methods Applied to Magnetic Tunnel Junctions	PL
Valentin, Luis	College of William and Mary	On Estimating the Number of Leaf Nodes on Trees	ITL
Galloway, Benjamin	Colorado School of Mines	Theoretical Limits of RECIST in Medical CT as a Measure of Tumor Volume	PL
Robbins, Bryce	Colorado School of Mines	Stability of Novel Solitons on a Bosonic Lattice	PL
Casil, Julianne	Converse College	The Effect of Electrolyte Concentration on Poly(ethylene glycol) in a Nanopore-Based Single-Molecule Mass Spectrometry	EEEL
Schmidt, Colin	Cornell University	Optimizing Performance in NGF Equipment Metadata Quality Assurance Tool	EEEL
Wang, Alexander	Cornell University	Developing an R Package for Reading and Analyzing Medical Hyperspectral Images	ITL
Chowdhury, Shwetadwip	Duke University	Automated Extraction of Cellular Features for Potential Robust Classification Scheme	ITL
Rohlfing, Anne	Duke University	Cytotoxicity Study of Carbon Nanotube Treated Primary Normal Breast Cells, Normal Breast Cell Line, and Breast Cancer Cell Line	CSTL
Strom, Mark	Duke University	Increasing Precision of a Small Mass Balance	MEL
Nowak, Stephen	Franciscan University of Steubenville	Calibration and Evaluation of a Computer Vision System	MEL
Singal, Poorva	Franklin Olin College of Engineering	Creating Patterns of Glass Breakage Automatically	ITL
O'Beirne, James	George Mason University	Improving Performance in FiPy with Mesh Partitioning	MSEL/NCNR
Messier, Nicole	George Washington University	Digital Image Correlation and the Influence of Speckle Pattern Characteristics	MSEL/NCNR
Myung, Soohyun	George Washington University	Optical Phantoms for Oximetry Studies	PL
Soares, Nathaniel	George Washington University	Economic and Environmental Impacts of Building Energy Efficiency	BFRL
Portuguese, Andrew	Hamilton College	Filtering, Processing, and Analysis of aCORN Project Data	PL
Hoyt, Robert	Harvey Mudd College	Characterizing Quantum Dots in Fiber-Coupled Nanofabricated Waveguides	CNST
Soe, Brian	Harvey Mudd College	Spintronic Effects in Nanomagnet Dynamics	CNST
Schneider, Jeff	Haverford College	The Effect of Manganese Particles on SH-SY5Y Neuroblastoma Cells: Oxidatively Induced DNA Damage	CSTL
Henry, Jessica	Hood College	Effects of Sidechain and Backbone Structure on Semiconducting Polymers	MSEL/NCNR
Jacobson, Nathan	Hood College	OMCE Merging	ITL

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Williams, Kandice	Jackson State University	Smart Polymer Surfaces for Controlling Interfacial Adhesion	MSEL/NCNR
Joress, Howard	Johns Hopkins University	Combinatorial Methodologies Applied to Thermoelectric Materials Development	MSEL/NCNR
Ginley, Theresa	Juniata College	Neutron Reflectivity and Magnetization Reversal in Heusler Alloy Spin Valves	MSEL/NCNR
Thiesse, Matthew	Lebanon Valley College	Characterizing Anomalies in Retroreflective Sheeting Material Using Goniometric Scanning Techniques	PL
Goleb, Melissa	Lehigh University	Interaction of Single-Wall Carbon Nanotubes with Biomolecules in Aqueous Solutions	MSEL/NCNR
Janicki, Charles	Marquette University	Topography Measurements and Correlations for NIST SRM 2461 Standard Casings	MEL
Lemanski, Bethany	Massachusetts Institute of Technology	Mechanical Properties of the Active Layer in Organic Solar Cells	MSEL/NCNR
Silva, Thomas	Miami Dade College	Software Validation and Verification	TS
Denton, Alexis	Miami University of Ohio	Measuring Optical Detector Linearity	PL
Helmuth, Nicholas	Miami University of Ohio	Understanding Kinematic Positioning of an X-Ray Optic Using 3-Dimensional CAD Modeling	MSEL/NCNR
Campbell, Derek	Middlebury College	Automated Logical Inference and Reasoning	MEL
Redmon, Joseph	Middlebury College	WRed: Data Reduction in a Web-Based Environment	MSEL/NCNR
Westling, William	Middlebury College	Real-Time Person Tracking in Video Streams for the Smart Space Project	ITL
Killian, William	Millersville University of Pennsylvania	Developing a Real-Time Face Identifier for the Smart Space Project	ITL
Knierim, Cassandra	Montana State University	Research for the Revision of National Fire Protection Association 1982 Standard on Personal Alert Safety Systems	BFRL
Geronimo, Carly	Mount Saint Mary’s University	Analysis of the Nanomechanical Properties of Biocompatible Coatings on Gold and Silver Nanoparticle Surfaces	MSEL/NCNR
Halter, Melissa	Mount Saint Mary’s University	Controlling Agglomeration Sizes of Silver Nanoparticles with Different Polymer Coatings: Effect of Coating on Agglomeration and Cytotoxicity	CSTL
Herb, Jake	Muhlenberg College	Accurate Optical Models for OPV Device Performance	CSTL
Hewitt, Andrew	North Carolina State University	Electrical Characterization of Soluble Organic Materials	EEEL
Marley, Daniel	North Carolina State University	Analysis of Marginally Trapped Ultra-Cold Neutrons for a Neutron Lifetime Experiment	PL
Sudbrink, Bryan	Oklahoma State University	Three-Dimensional Phase Reconstructed Data Cube	CSTL
Blumenfeld, David	Pennsylvania College of Technology	Production and Evaluation of a 5-Axis Test Artifact	MEL

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Cox, Matthew	Pennsylvania College of Technology	Initial Research Towards the Development of a Uranium Glass Analogue	MEL
McCormick, Patrick	Pennsylvania College of Technology	Using Machine Vision Systems to Improve Part Quality in Additive Manufacturing	MEL
Vandervort, Michael	Pennsylvania College of Technology	Aspects of Micro Manufacturing	MEL
Brennan, Tegan	Princeton University	Using Mathematica to Compute the Geodesic Path Between Cell Shapes	ITL
Kutten, Johannes	Rensselaer Polytechnic Institute	Development of a Feedback Controller for a Droplet-Forming Microfluidic Device	MSEL/NCNR
Nunnally, Steven	Roanoke College	The Human and Robotic Team: Adding Humans to USARSim to Aide Research	MEL
O'Neil, Colleen	Saint Mary's College of Maryland	Determining the Differences in the First Steps of Hyaluronan Mediated Cell Adhesion Under DEP Conditions	EEEL
Randazzo, Lucia	Saint Mary's College of Maryland	Human-Computer Interaction Performance Testing on Medical Interfaces	ITL
Lovell, Magdalen	State University of New York Albany	Synthesis, Characterization and Neutron Studies of a Spin-1 Frustrated Kagome Lattice	MSEL/NCNR
Chernow, Eric	State University of New York Binghamton	Modeling and Simulation for Sustainable Machining	MEL
Chiu, Wesley	State University of New York Binghamton	Development of Resistance Standards in the 1 MΩ to 1GΩ Range Using Hamon Transfer Methods	EEEL
Imburgia, Michael	State University of New York Binghamton	Durability of Adhesives in Salty Environments	BFRL
Shamah, Joseph	State University of New York Binghamton	Residential Appliance Energy Research	BFRL
Hwang, Steven	Swarthmore College	DMIS Test File Reducer	MEL
Leland, Julian	Swarthmore College	Characterization and Compensation of Micro-Scale 3-Axis Milling Machine	MEL
Giltinan, Joshua	Towson University	Design and Control of a Bi-Directional Microscopic Robot	EEEL
Hariri, Sara	University of California Irvine	Absorption Coefficient Measurements of Aerosolized Nigrosin Particles Using Laser Heating	CSTL
Crawford, Amanda	University of Colorado Boulder	Approximating the Number of Topological Sorts	ITL
Leibowitz, Joshua	University of Connecticut	The Effect of Temperature Change on Plasma Etching Processes	CNST
Baker, Andrew	University of Delaware	Investigating Lamellar Structures in Hydrated Nafion Thin Films	MSEL/NCNR
Anzaldi, Laura	University of Maryland Baltimore	Developing a Root-Based Semantic Vocabulary	CSTL

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Bier, Naomi	University of Maryland Baltimore	Homogeneity Analysis by Way of Laser Ablation Solid Sampling Coupled with Inductively Coupled Plasma Mass Spectrometry for the Assessment of Micro-Scale Sample Homogeneity	CSTL
Bokhari, Amber	University of Maryland Baltimore	The Dispersion of Single-Wall Carbon Nanotubes	MSEL/NCNR
Ecker, Benjamin	University of Maryland Baltimore	Terahertz Investigation of Dipeptide Nanotubes	PL
Goel, Neeti	University of Maryland Baltimore	Detection and Differentiation of Bacillus Endospores Using Fluorescence Spectroscopy	CSTL
Holness, Alex	University of Maryland Baltimore	Pyrometer Calibration of Nanocalorimeters	MSEL/NCNR
Iglehart, Christopher	University of Maryland Baltimore	Residential Appliance Energy Research	BFRL
Madeira, Morgan	University of Maryland Baltimore	Optimization Algorithms for Fitting Fundamental Parameters Models for X-Ray Powder Diffraction Line Profiles	MSEL/NCNR
Mason, David	University of Maryland Baltimore	Working Towards a NIST-Certified Phantom for Computed Tomography	PL
Serova, Nadezhda	University of Maryland Baltimore	Visual Similarity Based 3D Model Retrieval Through Multiview Matching	ITL
Atkinson, Ryan	University of Maryland College Park	Automated Guided Vehicle Testing in Virtual Environments	MEL
Au, Jennifer	University of Maryland College Park	Assessment of Pronase Digestion and Mass Spectrometry-Based Characterization of Biopharmaceutical Glycosylation	CSTL
Bernstein, Andrew	University of Maryland College Park	Computing Respirator Fit and Effectiveness	BFRL
Bhatia, Vikas	University of Maryland College Park	Neutron Diffraction Studies on the Structure and Chemical Composition of Superconducting Phases of $Fe_{1+y}Te_{1-x}Se_x$	MSEL/NCNR
Gao, Holman	University of Maryland College Park	Logic Synthesis of Functions for Cryptographic Applications	ITL
Goh, William	University of Maryland College Park	Testing the Security of Android Applications	ITL
Hung, Stevephen	University of Maryland College Park	Measuring Cell Response to Polymeric Scaffolds in 3-D Culture for Tissue Engineering of Bone	MSEL/NCNR
Krueger, Kevin	University of Maryland College Park	Evaluation of Systematic Errors in Johnson Noise Thermometry	CSTL
McCarthy, James	University of Maryland College Park	Exploring the Surface Chemistry of Engineered Nanoparticles Using Time-of-Flight Secondary Ion Mass Spectrometry	CSTL
Muroyama, Alexander	University of Maryland College Park	Discrete Event Simulation for Sustainable Manufacturing of Golf Balls	MEL
Myers, Taylor	University of Maryland College Park	Validation of the Fire Dynamics Simulator	BFRL
Peters, Alex	University of Maryland College Park	Amplification of mRNA at the Single Cell Level Using Microfluidic Devices	CSTL

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Rose, Cameron	University of Maryland College Park	Automating Measurements for High-Voltage, High-Frequency Silicon-Carbide Power Diodes Parameter Extraction Software Tools	EEEL
Tang, Kathy	University of Maryland College Park	The Effects of Surface Methacrylates on Biofilm Growth	MSEL/NCNR
Trettel, Andrew	University of Maryland College Park	Design of a Rotary Actuator with an Integrated Angle Sensor	MEL
Vilarino, Martin	University of Maryland College Park	The Production of Nanoparticle Arrays with Nanosphere Lithography	CNST
Vohra, Pragun	University of Maryland College Park	A Framework for Emergency Response Official Authentication and Authorization	ITL
Weerakkody, Sean	University of Maryland College Park	Obtaining Sensitive Electro Reflectance Spectra for High K Dielectrics	EEEL
Welsh, John	University of Maryland College Park	The Methodology of Assessing Robot Generated Maps	MEL
Westbrook, David	University of Maryland College Park	IEEE 1451.4 Standard: A Smart Transducer Interface for Mixed-Mode Communication	MEL
Yan, Joseph	University of Maryland College Park	Direct Tension Cyclic Fatigue Test on Asphalt Concrete Material	BFRL
Collins, Sean	University of Michigan	Characterizing the Compositional-Structural Properties of Mixed-Phase Light-Absorbing Carbonaceous Atmospheric Particles: Implications for Climate Change Modeling	CSTL
Davila Morris, Melissa	University of Puerto Rico	Investigating the Adsorption Behavior of Thiolated Polyethylene Glycol on Gold Nanoparticles Using Infrared Spectroscopy: Applications in Targeted Drug Delivery for Cancer Therapeutics	MSEL/NCNR
Ferra, Eliezer	University of Puerto Rico	Attribute Assurance in Anonymous Transactions	ITL
Nieves-Nevarez, Mairim	University of Puerto Rico (InterAmerican University of Puerto Rico)	Comparison of SiO_2 and SiN Substrates for Graphene Devices	EEEL
Rivera Delgado, Kevin	University of Puerto Rico (InterAmerican University of Puerto Rico, Bayamon Campus)	Analysis of Efficiency of Mapping Distribution Protocols in Scalable Routing and Addressing Architectures	ITL
Reynolds, Daniel	University of Rochester	Modeling of Multiphase Flow with Interfacial Agents	MSEL/NCNR
Yezer, Benjamin	University of Rochester	Measuring Silver Nanoparticle Dissolution with the Donnan Membrane Technique	CSTL
Hoff, Olivia	University of Southern Mississippi	Chromium Single-Photon Emitters in Bulk Diamond	CNST
White, T. Grant	University of Southern Mississippi	Selective Gas Sorption in Metal Organic Frameworks	MSEL/NCNR
Webb, Richard	University of Texas Austin	A Long Wavelength Photoresist for Plasmonic Field Metrology	CNST
Campbell, Philip	University of Texas Dallas	Obtaining Accurate Estimates of the Diffusion Coefficient	CNST

STUDENT	UNIVERSITY	TITLE OF TALK	OU
Carlson, Scott	University of Texas Dallas	TDDB Testing	EEEL
Swedlove, Benjamin	University of Texas Dallas	Sub-Nanometer Metrology with Charged Particle Microscopes	MEL
Huber, Jacob	University of Wisconsin Stout	Heat Treatment Effects on the Microstructure, Mechanical Properties, and High Strain Rate Deformation of AISI 1075 Steel	MSEL/NCNR
Barber, Benjamin	Valparaiso University (Lutheran)	Measurement of Neutron Reflectivity from a Silicon Crystal: Preparation for an nMDM Measurement	PL
Martin, Cadence	Virginia Polytechnic Institute and State University	A High-Resolution Interferometer for Nanomechanical Measurements	MSEL/NCNR
Shyur, Yomay	Wellesley College	Creating a Scanning Laser System for Manipulating Bose-Einstein Condensates	PL
Hood, Jesse	West Virginia University	Optimized Thermal Photoresist Processing for Nano-Structured Optics	MEL
Antonellis, Danielle	Worcester Polytechnic Institute	Verification of the Fire Dynamic Simulator	BFRL
Tong, Long	Worcester Polytechnic Institute	Water Calorimetry Using Ultrasonic Interferometry	PL

- THE END -

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