2012 SURF

summer undergraduate research fellowship

ABSTRACTS

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Alabama Agricultural and Mechanical University

Fire Resistant Foam
Shannon Hines

In the United States alone, fires are responsible for roughly 3,000 fatalities annually, 17,720 fire injuries and an estimated 11 million in direct property loss. In 2010, there was a fire death every 169 minutes and fire injury every 30 minutes. Home fires usually cause 85%-90% of those deaths. Polyurethane foams are typically contained in many areas of a home; existing in furnishing, bedding, appliances and insulation. Polyurethane foam is one of the numerous ways fires persist when met in contact.

To help suppress fires, we are using the layer-by-layer assembly technique to cover polyurethane foam in fire retardants. Our goal is to create a coating that contains bilayer systems of polyacrylic acid (PAA), polyethylenimine (PEI), layered double hydroxides (LDH), and Cloisite (MMT) which create low heat release rates, environmentally safe conditions, and minimize fires in comparison to our control foam. Our control, standard polyurethane foam, in contrast created a toxic atmosphere, high heat release rates, and dangerous flames.

Cone colorimeter and open flame tests were completed to show comparisons between flame retardant coated foam and control foam. The coated foam with LDH and MMT incorporated in the system resulted in low heat release rates and a high percentage of remaining foam after testing.

Molecular Modeling Tools for Advanced Materials
Justin Lewis

As part of Polymers Division activity for the Materials Genome Initiative (MGI), we are developing a computational toolbox for calculating the properties of Advanced Composite materials. This endeavor involves the development of modeling tools with verified source code, associated standard procedures and rules for usage, and eventually a knowledge base. The objective of MGI is to "advance materials development and time to market by 50%". Using the language Python, I helped to develop a class library for building coarse-grained molecular structures. These structures can be read into the molecular modeling package MAPS® (Scienomics, Inc.) in order to build complex systems, and then simulated using the molecular dynamics program LAMMPS. We show how the new tools can be used in series of demonstration simulations relevant to ongoing projects. For example, Microrheology is a specific computational application that is being used. In order to develop standard procedures and rules for its use in our toolbox, we are studying the effect of particle properties, force fields and system parameters on the Microrheology calculation.

Measurements of Vitamin A in Northern Fur Seals
Tamika Ragland

Northern fur seals (*Callorhinus ursinus*) have a breeding range throughout the Pacific perimeter from Japan to the Channel Islands of California with the main breeding colonies in the Pribilof and Commander Islands in the Bering Sea. The Pribilof Islands (Alaska) are a chain of five islands with the largest northern fur seal population on St. Paul Island. For many years, the northern fur seal population remained stable on the St. Paul Island, but the population has been declining since the 1990s. In order to elucidate possible factors contributing to the declining population, the concentrations of legacy and emerging chemical contaminants have been measured in northern fur seal liver and blubber samples collected on St. Paul Island from 1987-2007. Other important factors potentially contributing to the declining populations may be related to changes in diet. This can be determined through the measurement of health status markers such as vitamins. In this study the concentration of vitamin A has been determined in sub-adult males collected from 1987-2007 and banked by the National Institute of Standards and Technology's National Marine Mammal Tissue Bank.

Northern fur seal livers were screened for fat-soluble vitamins (FSV) A, E, D, and K by reversed-phase liquid chromatography (RPLC) with absorbance and fluorescence detection. For the qualitative and quantitative identification and measurement of FSVs, liver samples were saponified and the FSVs were extracted into hexane/petroleum ether. The chromatographic column, mobile phase solvents, and temperature conditions were optimized for the separation of standard solutions of vitamins. Sample size, concentration of hydroxide ion for saponification, and number of extraction cycles to maximize the amount of retinol extracted from the samples were also optimized. This talk will emphasize the analytical procedure for the separation and determination of FSVs in marine mammal liver samples, and provide preliminary data for vitamin A in northern fur seal samples. Northern fur seal livers were screened for fat-soluble vitamins (FSV) A, E, D, and K by reversed-phase liquid chromatography (RPLC) with absorbance and fluorescence detection. For the qualitative and quantitative identification and measurement of FSVs, liver samples were saponified and the FSVs were extracted into hexane/petroleum ether. The chromatographic column, mobile phase solvents, and temperature conditions were optimized for the separation of standard solutions of vitamins. Sample size, concentration of hydroxide ion for saponification, and number of extraction cycles to maximize the amount of retinol extracted from the samples were also optimized. This talk will emphasize the analytical procedure for the separation and determination of FSVs in marine mammal liver samples, and provide preliminary data for vitamin A in northern fur seal samples.

American University

Synthesis of PEG Compounds for CB2 Structure Characterization With Neutron Scattering and Reflectivity Techniques

Elizabeth Ghias

G-protein coupled receptors (GPCRs) are a large family of membrane proteins that are involved in signal transduction in cells. To characterize the structure and function of GPCRs, in particular the human peripheral cannabinoid receptor (CB2), neutron reflectivity techniques and other methods can be used. To use these methods, proteins must be immobilized on a surface that mimics the protein's natural environment. Histidine tagged proteins can be tethered to a self-assembled monolayer (SAM) that contains terminal nitrilotriacetic acid (NTA) groups constructed on a gold surface. The NTA groups are activated with nickel chloride to link the tether to the histidine tag of the protein. Attachment of the NTA groups ensured that the proteins have a uniform orientation, which is essential for neutron analysis.

Thiol terminated polyethylene glycol (PEG) compounds were developed through organic synthesis to tether the protein to the SAM. The reaction was a NHS ester crosslinking reaction, in which the N-Hydroxysuccinimide (NHS) ester group on the PEG reacted with the terminal amine group of the NTA. The water-soluble NTA terminated PEG thiols were synthesized with eight and twelve ethylene oxide groups. The NTA groups were attached to ensure that the proteins have a uniform orientation with specific binding, which is essential for neutron analysis. PEG compounds were synthesized on a 100 mg scale and were reduced using Tris(2-carboylethyl) phosphine hydrochloride (TCEP ● HCl). High Performance Liquid Chromatography (HPLC) was used to purify the synthesized compounds and MALDI TOF Mass Spectrometry was used to ensure purity. Once synthesis of the PEG compounds has been completed, surface plasmon resonance will be used to determine if protein binding is specific or nonspecific adsorption.

Creating Thermometers of the Future: Imaging Temperature Gradients Using Ultrasonic Transducers

Matthew Tweardy

Ultrasonic speed-of-sound imaging for thermometry, in which time-of-flight (TOF) measurements done with an ultrasonic transducer array are used to map temperature distributions inside a medium, is a developing technology for the dosimetry of clinical radiotherapy beams, where it has the potential to improve precision, safety, and costs in future IMRT systems. My research focuses specifically on determining temperature, spatial, and time resolutions and limitations of an ultrasonic TOF array system recently acquired by NIST.

This involves design/construction of controlled heat delivery methods that mimic clinical radiotherapy systems, to compare output from the transducer array to that of a calibrated thermistor probe. Finite element modeling is used to quantify and correct for errors attributed to heat transfer effects. Subsequent testing in clinical radiotherapy beams is planned.

These results are expected to improve the accuracy of the NIST thermal imaging system and move it one step closer to implementation in radiotherapy beams. My results also serve as a good proof-of-principle, demonstrating that this technology has real potential to improve clinical radiotherapy.

Temperature Monitoring and Control in Laser Cooling Laboratories

Brian Weinstein

In laser cooling labs, precision temperature control of different components of the apparatus is essential. This is true not only for the sake of the experiments being performed, but also for the protection of the million-dollar laboratory equipment. Overheating of magnetic coils or ovens can be disastrous, setting experiments back by months.

To monitor magnetic coil and oven temperatures, I constructed a versatile laboratory protection and control system using the Arduino microcontroller. The assembled system acts as a standalone device in the laboratory and is fully reconfigurable via USB.

The first of these devices has already been implemented and is in service in the lab. Integrated into the laboratory's error control circuit, the microcontroller uses eight thermocouples to monitor the temperatures of various magnetic coils. If the coil temperatures become too high, the instrument outputs an alert signal to cut off electrical current to the coils. The second device will control the temperatures, both for creating Rubidium vapor in an oven and also for general vacuum bake-outs.

Andrews University

Magnetic Field and Position Probe

Thomas Zirkle

The kilogram is the last SI unit whose definition still relies on an artifact. In a redefined SI, where all units are traceable to fundamental constants, the watt balance is one of the ways to realize mass. A watt balance is a device that relates electrical power to mechanical power. This relationship between mass and electrical units allows for extremely precise measurements and since electrical power can be related to Planck's constant, h; the watt balance effectively links the kilogram to h.

NIST is currently in the process of designing and building a new watt balance. The new design incorporates a large permanent magnet to generate the necessary magnetic field. In order to validate the magnet and ensure that it has the necessary precision, a custom made magnetic field probe is needed. The probe will combine both a position and field measurement in one instrument. The field measurement is done by measuring the voltage from a rotating coil. The position measurement is accomplished using the capacitive effect between the probe head and the magnet. In the summer of 2012, a wireless transmission from the rotating probe head to the lab computer was developed. The data transmission and the probe were successfully tested on a test magnet.

Appalachian State University

The Brightness of the Moon: Lunar Spectral Irradiance

Zachary Pruett

The goal of this project is to determine the spectral irradiance of the moon. As of yet, astronomical standards for spectral irradiance have been relegated to objects such as the sun and standard stars, leaving a gap where standard stars do not suffice and the sun is not available for use. The spectral irradiance of the moon near the visible spectrum (345-875 nm) has the potential to fill this gap in astronomical standards. The light reflected off of the moon is very stable when parameters such as phase, libration, and atmosphere are accounted for. Although the irradiance of the moon has been studied before, it was studied photometrically with larger than desired error bars and at specific wavelengths. For this project a method using spectrometers, which have a much better ability to characterize spectra for a wide range of individual wavelengths, is shown. A precision of within 1-2% can be obtained for the spectral irradiance of the moon to use as a standard. A better determination of the irradiance at each part of the visible spectrum will aid programs such as satellite spectral observations and nocturnal aerosol measurements.

Observations of the moon occurred on several nights at an outdoor deck on the National Institute of Standards and Technology (NIST) campus in Gaithersburg Maryland. Data was collected by a spectrometer that was connected to a small integrating sphere on the end of a telescope. The telescope was mounted on a computerized mount. The telescope pointed to and took spectra of the moon, a background 5° off of the moon, and a comparison lamp in a larger integrating sphere some distance sufficiently far away for all the light to be focused at the small integrating sphere on the end of the telescope. This larger sphere was monitored by a different spectrometer to calibrate the telescope-integrating sphere-spectrometer setup. It also served as a check to see that the setup was not drifting in calibration throughout the observation. This entire setup was controlled by a computer. Special care must be taken to see that observations have a sufficiently large range in air mass (optical depth) for a proper Langley analysis.

Analysis of Toolmark Topographies from Ten Consecutively Manufactured Chisels

John Villanova

Whenever a tool contacts an impressionable material with sufficient force, a toolmark can be made. These marks and impressions are unique to individual tools, and firearms examiners and forensics experts have taken advantage of this fact to identify firearms by toolmarks left on bullets and cartridge casings. When identifying toolmarks, the most challenging scenario involves comparing toolmarks produced by consecutively manufactured tools. These have the highest chance of having similar surface topographies and leading examiners to possible erroneous identifications. In the past, many consecutively manufactured studies have utilized comparison microscopy and relied on the experience of toolmark examiners rather than quantitative, objective measures. The aim of this study is to use the Cross Correlation Function (CCF) to establish a quantitative value for identification. This is the same correlation method that the National Institute of Standards and Technology (NIST) used to quantify similarity among the certified standard bullets (SRM 2460). Ten consecutively manufactured chisels were obtained from Western Forge (a supplier of craftsman tools) during witnessed manufacture. Each chisel was used to make known and labeled toolmarks. The topographies of the toolmarks were measured using a profilometer, and all were correlated against each other using the CCF to establish a statistical distribution of known-match and known-non-match comparison results. The distributions establish a minimum CCF score control limit for matching or non-matching identification. Each chisel's identity is then coded and used to make unknown toolmarks, which are correlated against all of the known and unknown toolmarks to determine which tool caused which mark. The study provides a mathematical and statistical validation of the methods utilized by toolmarks examiners and provides support for the validity of their science in a court of law.

Arizona State University

Parsing COLLADA: A Robust Method for Inputting Geometry Into FDS
Abbas Jaber

The Fire Dynamics Simulator (FDS) is a computational fluid dynamics model focused on simulating smoke and heat transports in fire-driven flows. Objects, such as furniture, in the FDS domain are treated as obstacles to the flow. However, objects in FDS are currently limited to block Cartesian geometries, with no direct way for handling smooth and round surfaces. In addition, when the geometries become complex where they don't conform to the mesh, FDS lacks accuracy when computing wall shear stresses. In this presentation, I will discuss how the limitation of block geometries can be addressed by parsing COLLADA files. COLLADA files define an open standard XML schema used for transferring information between different CAD packages, Computer Aided Drafting software. These files define geometry as sets of vertices and faces, and contain other useful information such as material types and colors. Using free CAD packages, like Google SketchUp, any drafted geometry can be exported as a COLLADA (.dae) file. In addition, the online Google 3D Warehouse holds tens of thousands of projects ranging from Hockey arenas to castles and palaces that can be downloaded in the COLLADA format. In order to extract geometry information, MATLAB is used to parse COLLADA files by converting the XML schema into MATLAB structures. In this presentation, I will also discuss a verification case I set up to investigate the FDS outputs of YPLUS, distance from wall measured in viscous lengths. Once the model used to calculate YPLUS is verified, YPLUS can then be used as a physical parameter that determines if the grid resolution requires more refinement. This is done by assigning a critical value for YPLUS for a given FDS case; if the calculated YPLUS is less than the critical value, the resolution is deemed acceptable.

Evironmentally-Friendly Flame Retardant Coating for Polyurethane Foam
Kathelyn Keberle

Polyurethane Foam is a common material in upholstered furniture and mattresses. Its high energy density and tendency to liquefy when exposed to a fire makes it one of the deadliest ingredients in any household fire. Current flame retardant coatings are effective at minimizing the heat release rate and preventing dripping of the foam but give off toxic fumes when burned. This research works to further explore the use of layer-by-layer deposition as an effective fire retardant coating for polyurethane foams. The effects of pH value, number of layers, choice of polymers, and concentration of solutions are tested to optimize a more sustainable, safe, and effective flame-retardant coating.

Characterization and Preparation of Actin Surfaces and Tethered Bilayer Membranes
Arad Lajevardi-Khosh

Biomimetic structures are necessary as a tool to perform a wide variety of biophysical experiments such as protein/membrane interactions and protein/protein interactions. This allows phenomena like protein adsorption, ion transport, and membrane mechanical properties to be studied. Additionally these structures provide the measurement platform for many biotechnological applications such as drug delivery, biosensing, and biocatalysis. In this talk, I will discuss the preparation, and characterization of two biomimetic interfaces: actin surfaces to study muscle proteins and a tethered bilayer lipid membranes (tBLMs) to simultaneously study structure and function of membrane proteins. These surfaces along with electrochemical, optical, and imaging tools allow us to better understand the function of biological molecules.

Enhancing the NIST Chemistry Webbook with Optimized 3D Structures – Part 1
Stuart Ness

The NIST Chemistry Web Book is an online database containing various physical and chemical data on over 100,000 chemical compounds. Currently, all information on the site is experimental data culled from chemical literature and collaborating authors. In the future, NIST could provide high quality theoretical data, oftentimes difficult or impossible to experimentally measure, through the use of computational chemistry. The first step to providing such data is to generate optimized 3-dimensional structures for all relevant compounds. For any computed data to be meaningful, these structures must be highly accurate in regards to bond angle and length, and thus must be calculated with quantum mechanics. This summer, will calculate 20,000 such structures using a two-step method. Our first step was to run every structure through a PM6 optimization, a semi-empirical method that uses both quantum chemistry and empirical parameters to calculate a molecules minimum energy state. PM6 calculations provide a good starting point for acquiring optimized structures, but PM6 is not the standard procedure for molecular geometry. Thus, we then fed these structures into B3LYP, a hybrid functional that employs Density Functional Theory, DFT, with only 3 empirical parameters, providing structures that more closely match theory. In addition to generating optimized 3 dimensional structures, we also calculated vibrational frequency data for every molecule. These two sets of data provide a strong starting point for all future calculated data to be included in the Web Book.

Beginning Standardization of Condition Monitoring Tests for Cables in Nuclear Power Plants
Daniel Stehlik

In nuclear power plants (NPPs), electrical cables can be considered the plant's nerve center due to their wide use in feedback and control tasks as well as communication functions. Recently, a number of premature electrical cable failures in active NPPs have prompted investigation into the long-term performance of electrical cables. While industry and government have been researching NPP electrical cable life prediction and degradation for decades, standardization and consistent methodology are scarce. The project with which I am working will seek to establish acceptance criteria for condition monitoring tests (CMTs), which are any of a number of mechanical and chemical-physical tests for cable aging and which perform a critical role in understanding and monitoring aging in NPP electrical cables.

My work this summer focused on beginning the physical set up for accelerated cable aging and developing methodologies for mechanical and chemical analysis of electrical cable insulation. Apparatus for accelerated cable aging in submerged and controlled relative humidity (RH) and temperature conditions were designed, and submerged degradation begun. It is anticipated that the non-submerged apparatus will be constructed and in use by the end of July. Method development experiments were performed to find an affordable, reliable, and reproducible method for mechanical testing, with much progress but as-yet uncertain results. A primary chemical analysis method is microscopic Fourier Transform Infrared Spectroscopy (FT-IR), in both reflectance and Attenuated Total Reflectance (ATR) configurations. Parameter optimization experiments were performed and standard operating procedures were developed for both configurations of FT-IR, and ATR was performed on new and aged cables. Spectroscopic data of cables aged for various time periods will be qualitatively and quantitatively compared to data from new cables, examined to identify chemical aging mechanisms, and correlated with mechanical testing results. The mechanical and chemical testing methodologies developed at this early stage will prepare for coming years of accelerated aging and resulting characterization, which will be compared to data from other CMTs to establish accepted and reliable CMTs.

Augsburg College

Uncertainty in Live Cell Fluorescence Intensity Measurements Estimated with a Mean Squared Displacement Analysis

Nathaniel Ly

Quantitative measurements of dynamic processes in single cells by live cell imaging present the opportunity to monitor temporal patterns in gene regulation, to identify correlations between gene expression and cell behavior, and to model the mechanisms that give rise to biological variability. These measurements require engineering cells to express fluorescent proteins, then imaging large numbers of these engineered cells by optical microscopy over several days. To obtain data describing the time dependent changes in gene expression, each cell must be segmented and tracked by applying image analysis routines. Uncertainty in the measured intensity data can originate from a number of complex sources including the instrument hardware, the mis-segmentation cells and incorrectly tracking cells between frames of the time lapse image series. To estimate the uncertainty in these data we have examined the application of a mean squared displacement (MSD) analysis. The choice of this method was motivated by previous observations within the Cell Systems Science group at NIST suggesting that changes in the fluorescent protein expression follow a diffusive pattern. The diffusive pattern is similar to a particle's motion undergoing random diffusion in a medium. In particle tracking measurements, the uncertainty in the measurement of each particle's position can be computed by analyzing the MSD over a large number of particles. By analogy, we adopted this analysis procedure to estimate the uncertainty of our cellular fluorescence intensity measurements. We found that the computed uncertainty depended on slope of the MSD plot and was more accurate for smaller slopes. In other words, the rate of change of the biological process affects the accuracy of the uncertainty estimation. This relationship was confirmed by simulating time dependent data and systematically examining the relationship of the MSD slope and the measurement uncertainty. We also examined an automated approach for determining the parameters of the cell tracking algorithm based minimizing the uncertainty computed by the MSD analysis. This study represents the application of a MSD analysis computed over large sets of time series data to estimate the uncertainty in complex biological data.

Bridgewater College

Structural Studies of Important Industrial Gases Adsorbed in Zeolites
Matthew Cline

The control of greenhouse gases is one of the most critical issues for industry as emission regulations are tightened and concern about impact on the environment rises. The capture and sequestering of greenhouse gases is one of the many potential solutions that have been presented. In order to capture these gases a material is needed with high adsorption capacity and high selectivity for gases such as carbon dioxide and methane over other light gases. Additionally, the energy cost for both capture and subsequent removal of gases should be low; while pressure and temperature stability of the material are important considerations. A class of inorganic materials, known as zeolites, show promise for greenhouse gas capture due to their ability to physisorb carbon dioxide and their mechanical and thermal stability. In zeolites, pore window sizes, charge compensating ions and their positions, and overall structure affect the gas adsorption profile. Two zeolites of recent interest are cation-exchanged SSZ-13 and ZK-5, which have shown promising adsorption profiles in previous studies[1-2]. We have used synchrotron x-ray powder diffraction and neutron powder diffraction to determine the equilibrium adsorption positions of carbon dioxide and related gases in a series of SSZ-13 and ZK-5 zeolites. Understanding the relative influences of the framework, extra-framework charge compensating ions, and geometrical features of the framework will allow us to determine the most effective zeolite composition for this application.

[1] Hudson, M. R.; Queen, W. L.; Mason, J. A.; Fickel, D. W.; Lobo, R. F.; Brown, C. M. *J. Am. Chem. Soc.* **2012**, *134*, 1970-1973.
[2] Liu, Q.; Pam, T.; Porosoff, M. D.; Lobo, R. F. ChemSusChem (Accepted) **2012**.

Brigham Young University

Shape Evaluation of Nanoparticles Using the TSOM Method
Lisa Bendall

With the growth of nanotechnologies, methods of measuring and determining properties of nanoparticles are becoming increasingly important. Traditional methods, such as atomic force microscopy or scanning electron microscopy, are often time-consuming, expensive, and may require sample preparation which could damage the specimen. A new method called through-focus scanning optical microscopy (TSOM), which has been shown to be useful in measuring particle size, has also shown promise as a method for determining particle shape.

In this talk, I will discuss using differential TSOM images in order to determine the shape of nanoparticles. The TSOM method uses a traditional optical microscope with images taken at different focal positions along the vertical axis. These images are compiled to form a 3-D TSOM image. In order to evaluate the shape of an object, the symmetries of the TSOM image are examined. We use differential images of the target object and a basis for comparison and compare the slices at different angles about the vertical axis. We then plot the angle versus the correlation between the differential images and using the maxima and minima of the plot, we can deduce symmetries at certain angles to infer the overall shape.

The results of our simulations indicate that this method could be useful in identifying the shape of a particle or the configuration of multiple particles. We were able to identify significant changes in differential TSOM image patterns, which corresponded to the symmetries expected in our sample objects. This demonstrates the potential that this method has in evaluating the shape of an unknown target. Additional analyses of differential TSOM images could add to our understanding of the images and potentially make the TSOM method an option for characterizing nanostructures.

Multi-Split HVAC Unit Testing and Analysis

David Richardson

Multi-split Heat Pump units are tested according to a Department Of Energy test procedure which incorporates most of the elements of Air Conditioning Heating and Refrigeration Institute Standard 210/240-2008. Multi-split heat pumps are a new type of product that has not seen wide use in the United States until recently. As a result the operating characteristics of this equipment are not familiar to standards organizations and raters. As a result, system testing must be performed to determine operating characteristics and to determine the most appropriate way perform standard tests. Therefore, NIST was asked by the Department Of Energy to perform some system testing to determine the characteristics of a 3-ton nominal cooling capacity, multi-split heat pump. Air Conditioning Heating and Refrigeration Institute standard tests were performed along with tests according to a comparable standard, Air Conditioning Heating and Refrigeration Institute 1230-2009. The standard tests were performed along with more tests at different indoor and outdoor air conditions to determine operating characteristics. Manufacturer representatives aided NIST in setting up the multi-split system and ensured proper installation of their equipment in NIST's psychometric chambers. Other tests explored the possibility of accounting for the off mode power consumption when calculating a systems efficiency. A draft standard for rating systems for off-mode power was used to determine an off-mode power rating for the multi-split system. The off mode power consumption was measured by conducting various off mode tests at temperatures from 37.78°C to 0°C. These tests showed that even though the indoor units were off the outdoor unit would use up to 100 watts of power. This power was used to keep the compressor in the outdoor unit warm enough so the refrigerant would not condense inside of it. By taking the average power consumption at the different temperatures the off mode power rating was found to be 31 watts.

Brown University

A Discussion of the Efficacy of the Coulter Principle for Counting Micron-Scale Particles and Protein Aggregates in Comparison to Other Current Methods

Joshua Cohen

Many papers have recently been published about the possible immunogenic or other undesirable effects caused in vivo by aggregation of proteins. The concern that modern biopharmaceuticals may result in aggregation in vivo has led to a focus on characterizing these aggregates. Other labs have found that current market devices such as flow imaging devices, light obscuration devices and Electrical Sensing Zone devices provide different distributions and counts for aggregated proteins which led to a lack of a standard in measurement for these aggregates. To understand this problem, my lab began by producing an FEM multiphysics model for an ESZ device. Running many virtual particles showed ESZ measurement effects resulting from particle size to aperture size ratio, non-spherical geometry, orientation in the ESZ, porosity, and trajectory. Experimentally, the relative volume effect appears to be accounted for by the ESZ device we used (<5% error). Manufactured rods of known volume yielded error of about 38.1%. In the FEM fluid flow module, particles generally align their major axis with the flow field and approach the middle of the fluid field rendering trajectory and orientation effects less concerning. Furthermore, many modern devices disregard signals of recognizably non central trajectories, or hydro-dynamically focus particles to the center of the orifice. Rods, polystyrene beads, protein aggregates, and abraded particles meant to approximate the shapes of protein aggregates were compared in light obscuration, flow imaging and ESV devices. Our results agreed with other labs on the large discrepancies these measurements produce between machines. ESZ consistently counted more aggregates than Fluid flow in a small size range and less in a larger size range suggesting skew to the left of ESZ measurements of aggregates. A similar trend was noted for abraded particles suggesting that geometry rather than composition is causing this discrepancy. It is possible that fluid devices measure a bulk volume while ESZ measures a material volume, since these materials are porous. Future work for our lab includes testing a fabricated device equipped to both record an ESZ signal and a light microscopy photograph. Orthogonal testing may allow correction of differing measurements.

Modeling the Temperature of Panels Exposed to the Outdoors

Jonathan Schear

In the last decade, there has been a movement to invest in "cool roofs": roofing made out of materials that absorb less heat from the sun. Commercially available polymer roof coatings drive down energy costs from air conditioning in the summer, but can also raise heating costs in the winter. In order to determine the amount of energy savings a "cool roof" affords, it is useful to model the temperature of the roof under different weather conditions – a reflective, white roof might decrease energy use significantly in a high temperature climate but do the opposite in a cooler region.

Recent research at NIST produced an accurate method for modeling the temperature of polymer coated panels exposed to the outdoors given basic weather data and a few laboratory measurements of the panels. The model, which had been previously tested for black and white coated panels, was validated for blue, yellow, and red coated panels. Concurrently, a web application was developed in JavaFX to model the temperature of a panel exposed to the outdoors anywhere in the US. The application allows users to select the closest available weather station from a map, calculates average monthly outdoor conditions from the Department of Energy's EnergyPlus weather data, and finally calculates the temperature of the panel coating described by the user's input parameters.

Beyond roof coatings, polymer films are used throughout industry to improve the safety and functionality of numerous devices. They prevent the fracturing of glass in windows and windshields, strengthen building materials, and protect the paint on automobiles, among many other applications. Extreme temperature is one of the key environmental factors that contribute to the degradation and premature failure of polymer coatings. The severity of outdoor heat exposure is often characterized by the ambient air temperature, but the actual coating temperature is linked to other measurements intrinsic to the coating. Intuitively, a black coating will reach a much higher temperature than a white one – and this difference can lead to inaccurate service life predictions. The presented model and accompanying web tool will also be used to aid in the modeling of polymer degradation mechanisms and service life predictions.

<u>California State University Fresno</u>

Post-Column Counter-Gradients for Better LC/MS Analysis
Pahoua Xiong

Electrospray ionization (ESI) is a soft ionization technique used as an interface of liquid chromatography (LC) and mass spectrometry (MS) to analyze a variety of chemicals. ESI responses are frequently unstable in reverse-phase gradient separations when the amount of organic in the mobile phase is very low (or very high). Several experiments were performed to find the optimum percent of organic in the solvent mixture to get the best ESI signals. We proposed a new LC method that uses a post-column counter-gradient (PCCG) to keep the amount of organic solvent that reaches the spray needle near to its optimum value.

To test the efficiency of the ionization, while varying the amount of organic solvent in the liquid phase, we infused equimolar solutions (~ 1 andM) of the amino phenylalanine dissolved in acetonitrile/water in a Mass Spectrometer at a flow rate of 300 nL/min. Reverse-phase LC/MS separations of a mixture of the three amino acids were repeatedly performed to compare the PCCG method with the conventional separations without post-column addition.

The relative ESI-signal intensity dependence on the organic/water ratio for all three amino acids was a bell-shaped curve with a maximum between 40-50 % of acetonitrile. For the chromatographic separation we used a 60 min linear gradient (2 to 60% organic) and a 60 min linear counter-gradient (60 to 2% organic) to maintain an organic/water ratio of 50/50.

The PCCG method proposed in this work increases the sensitivity of the LC/MS analysis.

<u>Carnegie Mellon University</u>

Molecular Dynamics Simulations of Aluminum Nanoparticles
Madeline Cramer

Nanoparticles have attracted much interest in recent years due to their many potential applications in biomedical, optical and electronic fields, as well as in materials science. Aluminum nanoparticles, in particular, are being used in propellants, munitions, pyrotechnics, and powder metallurgy. These particles, between 1 and 100 nanometers, have been shown to display size-dependent properties that differ from the bulk. Due to the small size of the nanoparticles, it is often difficult or impossible to obtain reliable experimental data to characterize how properties vary. In part due to these limitations, molecular dynamics simulations are becoming increasingly popular as a way to visualize and examine the properties of materials.

In this work, multiple embedded-atom models are used to simulate the behavior of pure aluminum particles between 2 and 17 nanometers in diameter. Thermodynamic data, as well as the radial distribution function and centrosymmetry parameter, are recorded in order to characterize the spherical nanoparticles. The collected data is compared to the bulk FCC solid and liquid values of aluminum. The models are also compared against each other and experimental measurements in order to quantify their accuracy and how much the results depend on choice of model.

Hands Off!: Using Gesture Recognition to Manipulate 3D Visualizations
Divya Mouli

The RAVE, located right here on the NIST campus, is an interactive 3D Immersive Environment which can be used to view large scientific visualizations in a precise and intricate manner. Currently a wand is used to interact with the visualizations in the RAVE. However, in order to convey a wider variety of commands to increasingly complex visualizations, additional methods of interaction between the user and the RAVE are desirable. For this reason, a system of gesture recognition is being generated, in which gestures carried out by the user are recorded, recognized, and subsequently linked with certain customizable actions the user wishes to carry out.

In this talk, I will explain the steps that were necessary to adapt a previously existing gesture recognition software for a new system, generate a series of new recognizable gestures, and link certain gestures with desired user actions.

With this technology, users can manipulate programs and visualizations in a completely interactive manner, without ever having to step out of the RAVE.

Optimizing Photonic Crystals Using Computer Simulation
Tom Mullins

The fabrication of photonic structures, nano- to micro-size structures used to manipulate the propagation of light, is an expensive and time consuming process. In addition, the effect such structures have on the electromagnetic field is strongly dependent on the material and geometry. For example, increasing the radius of a gallium arsenide cylinder from 160 nm to 220 nm can increase the power through the cylinder by a factor of 5. Therefore, it is important to determine the exact shape, dimensions, and material of the photonic structure before fabrication. In this talk, I will discuss the use of computer simulation to optimize these structures. I will first present the different methods of simulation used and the verification of these simulations by comparison of simple geometries to analytical or known results. Then I will discuss two specific examples of interest, the enhancement of the number of photons emitted from the top of a cylinder and the maximization of the reflectivity of a thin membrane.

Fabrication of Nanopores in Anodized Aluminum Oxide
Graham Spicer

The study of protein structure remains one of the largest challenges in biology today. Many proteins cannot be crystallized, so the traditional method of x-ray diffraction to determine structure cannot be used. However, neutron diffraction can provide important structural information of proteins and other large molecules, provided they are constrained in an ordered lattice. We experimented with the fabrication of arrays of self-ordered nanopores in anodized aluminum oxide (AAO) films that can be tailored to constrain different molecules in an ordered lattice. These arrays form in specific regimes of the anodizing parameters used to grow the AAO film, and the varying of these parameters dictates the size, shape, and density of the nanopores. Nanopores having diameters of 10-70 nm were imaged in an environmental scanning electron microscope (ESEM) and results will be discussed.

College of William and Mary

It's a Secret to Nobody: Using a Public Source of Randomness For Cryptography and Zero-Knowledge Protocols

Matthew Blum

Random numbers have an impressive variety of applications in real world situations. From gambling to statistical sampling to encryption and more, random numbers have become an important resource in many different fields. Many simple random number generators have been created for people to use in settling bets or selecting data, but most of these random numbers are generated to be used as secret values. The NIST randomness beacon, on the other hand, is a public source of random numbers. Each number is generated and openly published and stored for the entire world to use. Although it is improper to use these random numbers for use as secret cryptographic keys, there are some unique and interesting applications for random numbers that anyone can access.

My project was based on discovering these applications for public random values and creating demonstrations showing how published random values can make many tasks significantly simpler. To make the demos as universal and easy to understand as possible, I programmed apps for iPad and iPhone devices. During this talk I will explain the specific advantages of publicly generated random numbers and discuss the challenges I faced in utilizing them. Finally, I will show the applications I have created to demonstrate these advantages.

Colorado School of Mines

*Electronic Transport Properties of the Metal Organic Framework $Cu_3(BTC_2)$*TCNQ*

Bryce Thurston

Metal organic frameworks (MOFs) represent a novel class of highly porous materials made up of a long range, crystalline network of organic ligands coordinated to metal ions, such as Zn^{2+}, Cu^{2+}, or In^{3+}. Also known as coordination polymers, MOFs have achieved record values of specific surface area, exceeding 5000 m^2/g. The high surface area has made MOFs primarily of interest for applications in gas storage and separation. The focus of my project has been the measurement of electronic transport in thin films of $Cu_3(BTC_2)$ treated with TCNQ (tetracyanoquinodimethane). The MOF $Cu_3(BTC)_2$, also known as HKUST-1 (this compound was discovered at the Hong Kong University of Science and Technology, *Science* 1999, 283, 1148), consists of Cu(II) ions linked by benzenetricarboxylate (BTC) ligands. $Cu_3(BTC_2)*(H_2O)_2$ films with a nominal thickness of 100 nm were grown on Si/SiO_2 substrates in a liquid cell reactor. Pt pads with dimensions of 800 μm by 400 μm and gaps of 100 μm, 150 μm, and 200 μm were prepatterned on the Si/SiO_2 wafer using electron beam evaporation and were used as electrical contacts. I-V curves were collected using a computer controlled high precision current-voltage source/measure unit and micromanipulator probes used to contact the Pt pads. After synthesis $Cu_3(BTC_2)*(H_2O)_2$ films were heated to 180 °C in vacuum for 30 minutes to remove the water molecules bonded to the Cu ions and transferred immediately into a solution of methanol saturated with TCNQ. As-synthesized $Cu_3(BTC_2)*(H_2O)_2$ film behaves as an insulator, measuring a current <5 pA at 5 V with non-linear I-V characteristics and a pronounced hysteresis. However, when treated with TCNQ, the I-V characteristic becomes Ohmic (linear), with a resistivity of $\approx 2\times10^5$ Ωcm, or approximately one order of magnitude lower compared to untreated films. Using temperature dependent measurements, we extracted an activation energy of 0.23 eV for electrical conduction. We believe that the increased electrical conductivity is due to the interaction between the Cu d-orbital and the pi* level of the TCNQ bridging ligands, which have displaced the water molecules. The electrical resistivity of $Cu_3(BTC_2)$*TCNQ film increased slowly over time when left in the laboratory ambient from $\approx 2\times10^5$ Ωcm to $\approx 6\times10^5$ Ωcm over a period of 26 days, probably due to water molecules displacing the TCNQ ligands.

Lunar Spectral Irradiance: Calibration of the Moon

Joseph Whalen

In space, Earth imaging satellites are exposed to a variety of harsh conditions that can degrade the sensitivity of the instruments they carry. We can understand how these instruments are degrading by using the moon as a calibration source and use these better calibrated instruments to gather more accurate data. Before our experiment, relative changes in brightness of the moon due to phase and libration angle were well understood using the model provided by the RObotic Lunar Observatory (ROLO), but only photometric measurements of lunar spectral irradiance been made. We present a spectroscopic method for calculating lunar spectral irradiance with precision of 1-2% and data that could provide a calibration of lunar spectral irradiance for use by satellites for wavelengths between 345 and 875 nm.

Raw lunar spectra were collected from the roof of NIST and processed by the USGS (US Geological Survey) with the ROLO model to adjust for changes in brightness through the night due to changes in phase and libration angle. As the moon moves through the sky the atmosphere absorbs different amounts of light based on the elevation of the moon. Using lunar position data from the US Naval Observatory (USNO) we performed Langley analysis at each wavelength in order to remove the effects of atmospheric absorption. Langley analysis applies the Beer-Lambert law and produces a linear relationship between relative airmass (the relative amount of atmosphere between the celestial object and the observer) and the log of the measured irradiance at each wavelength. This linear relationship allows for easy extrapolation to zero relative airmass to produce a true spectrum for the spectral irradiance of the moon.

Columbia University

Transfer Efficiency of Explosive and Narcotic Residue from Bytac®

Ashley Newton

Trace analysis of explosive and narcotic residues is of growing interest in national security and customs applications, especially considering the extensive and increasing deployment of trace particle screening devices designed for airport security applications. The Transportation Security Administration (TSA) maintains standards for both detection and calibration of trace screening devices, including Ion-Mobility Spectrometry (IMS) devices, using known standards provided by the National Institute of Standards and Technology (NIST). Of particular interest to this study is the ability of these devices to detect samples of explosive and narcotic compounds transferred from Bytac ®. Therefore, an extraction and quantification method was developed to determine the transfer efficiency of cyclotrimethylenetrinitramine (RDX), pentaerythritol tetranitrate (PETN), cocaine and methamphetamine from Bytac to various substrates (vinyl, cardboard and laminate).

A study was conducted to develop a method to extract nanogram levels of common explosive and narcotic compounds from the Bytac ® substrate in order to maximize extraction efficiency while maintaining detection efficiency. Analysis of the resulting extract solution was performed using high-performance liquid chromatography (HPLC) with UV-Vis detection. Data collected from the extraction study were subsequently quantified using calibration curves in which area versus concentration was determined to be linear over the region of interest using a least squares regression line. The extraction and quantification methodology derived from the preliminary extraction study was then utilized to determine the transfer efficiency of the explosive and narcotic standards provided by NIST. Samples of four explosive and narcotic compounds were printed onto Bytac ® strips in an approximation of NIST-provided standards before being transferred by a short swiping motion onto three different substrates, cardboard, laminate, and vinyl. In addition, three different force profiles, approximating a soft, medium, and hard swipe respectively, were utilized, thus creating a sample set of nine possible transfer methods. The methodology determined in the previous study was then used to extract and quantify any remaining narcotic or explosive residue on the Bytac ® strip in order to determine the transfer efficiency of NIST standards.

Techniques in Signal Processing for Chirped-Pulse Broadband Trace Gas Sensor

John Orthwein

In the wake of developments to a new broadband trace gas sensor that uses chirped-pulse spectroscopy in the terahertz frequency region, members of the project in PML, my advisor, and I have searched for improvements in both iterative-concurrent and post-procedural methods to process and refine the system's out-coming data. Current limits on receiving and sending ideal signals in the experiment lower the precision and sensitivity of the system's measurements as well as the amount of information that is able to be gathered from the gas sample. These limitations arise from errors inherent in any experimental set-up (these include errors associated with non-noiseless chambers, the discrete nature of data, and non-instantaneous data acquisition -- causing problems of convolution and phase shifts in the signal) as well as challenges that are unique to our own experiment (that is, problems associated with the broad, quadratic phase sweeps in our excitation chirped-pulse, and the large range of frequencies scanned by the sensor, which involves the analysis of many peaks in a spectrum at once).

In this talk I plan to outline some of the methods that we are currently implementing to tackle these problems in the refinement of the system's data signals, and, as well, to sketch the theory behind a few techniques that may be implemented in the future to further improve the system's sensitivity, precision, and functionality.

<u>DePauw University</u>

Calculating Graph Toughness
Catherine Baker

When evaluating networks, an important metric is its robustness. Less robust networks are more vulnerable to splintering when nodes are removed. Therefore it is important to be able to calculate how robust your network is. As part of my project, I wrote an algorithm that finds the toughness (robustness) of the network. In general, the calculation of toughness is considered a hard problem due to the lack of efficient algorithms for the worst case scenario, so we looked for cases where we could decrease the calculation time. In particular, we looked at a special class of networks to develop a closed form formula to calculate the toughness. From the study of this special class we were able to find a lower bound of the toughness for a more general version of that class.

Modeling the Spread of Infection
Zachary Keller

Computer viruses, influenza, and other diseases spread. Modeling the spread of infections and possible responses helps researchers understand both. In this work we represent the environment with nodes and edges (graphs) in three dimensions. In general, these graphs are not small. In order to look at and interact with large graphs, we use shaders, i.e. GPU programs, to visualize the nodes as well as to interact with the network. In this talk, we describe the different visualization and interaction tools that we have developed, as well as future possibilities for the visualization and interaction.

<u>George Washington University</u>

Monitoring the Power Grid
Shelly Bagchi

As part of the 'Smart Grid' effort, power plants are beginning to monitor the power they produce to detect and prevent large issues. Meters known as Phasor Measurement Units (PMUs) take data several times per second, and timestamp each data set according to a GPS reference. The high precision of the timestamps means that data can be collected from different areas and then matched up by time in order to provide a big picture of the current status of the power grid. PMUs also have the ability to transmit over a network, enabling real-time grid monitoring.

The standards for PMUs are still being established, especially with regard to network data transmission. My project involved configuring a special network analysis card to timestamp the data packets as they were received by the computer. I then wrote a LabVIEW program which decoded the packets to obtain the time when the individual data points were taken by the PMU. The program then calculated the latencies between the time when the data was recorded and the time when it was actually received. By creating histograms and other plots of these latencies, we can see if the PMU is transmitting data regularly or if there are any excessive delays in transmission. NIST can then provide this feedback to PMU manufacturers in order for them to improve their systems.

Calibrating Calibrators
Caroline Litchfield

In order to build products that rely on electricity it must be possible to make accurate and precise measurements of electricity. NIST holds the official standards of many physical quantities, and those standards need to be distributed throughout the rest of the world. The official Volt is held by the Josephson Junction, which comes in arrays with voltages up to 10 Volts. The challenge is calibrating machines on larger voltage ranges than the Josephson Junction can offer, as well as AC Voltages which depend on DC Voltage standards.

The tests necessary to perform the calibrations are repeated many times over a period of about a month to account for any environmental changes and to reveal any drifting of the instrument. For higher voltage ranges, resistance ratios were used to determine the error of the voltage supply. LabVIEW programs were written for long series of calibration tests that involved the interaction of several instruments. The specific meters and calibrators that were tested using these methods were found to have gains that were consistent to about 2 parts per million, with gains ranging up to 11 parts per million in some cases. After these procedures, the instruments are ready to be sent back to the clients along with reports of any gains, errors, or drifting patterns.

Georgetown University

Faithful to the Original? The Impact of Latent Fingerprint Enhancement
Julian Lee

With the increased use of digital image enhancement technology, fingerprint examiners can make forensic latent fingerprints look much clearer than before using enhancement software such as Adobe Photoshop, but even so, there have been a lot of caveats and controversy surrounding the methods that such software implements to preserve the fidelity of the evidence. This is especially true software packages introduce fancier operations to apply a certain transformation, such as color inversion, grayscale conversion and the like. With all of these issues in mind, it would be reasonable to believe that even though technology can make latent fingerprints look clearer, it can also corrupt such vital evidence subtly enough to the point where it may actually lead to the wrong person, resulting in a miscarriage of justice and possibly wrongful conviction. In light of this issue, one of the objectives of the project is to provide some specifications as unambiguous, reproducible, and universal referent for the forensic latent fingerprint image enhancement.

To deal with this issue, I initially scripted or automated common image transformation commands in a way that can effectively reproduce a sequence of image enhancement operations that each software package uses to complete the operation. Then, I examined how various close-and open-source software packages, such as Adobe Photoshop, ImagePro, IrfanView and ImageJ, consummate common image-enhancing commands. State-of-the-art and historical mathematical formulas were used to determine how those software packages implement those operations differently by determining to what extent the output images (which result from each software's application of a certain command) really differ. Much to my surprise, some software packages indeed use different implementations to complete a certain image enhancement procedure, such as converting images from RGB to grayscale, yet the resulting images are different in respect to pixel values/image histograms. However, the algorithms behind such operation remain highly similar and the results show that it is necessary for us to provide some specification on the algorithms to determine whether the actual fingerprints have been incorrectly manipulated or not. While our results are inconclusive in terms of the impact on the final verdict based on presenting the latent fingerprint in a court of law, we have been able to quantify the difference between original and enhanced latent fingerprint evidence.

Georgia Institute of Technology

Data Visualization for Analysis of the NCNR Cold Source Operation

Max Carlson

The cold neutron source at NCNR is a critical system as it provides neutrons for all the researchers in the guide hall (G-100). The operation of the cold source is tied to the operation of the NBSR - the reactor can run at full power only if the cold source is functional. To date the cold source has been highly reliable, but when unexpected events occur it is important to quickly diagnose the cause so that neutron beam experiments at NCNR can continue. If the cold source has to be shut down, the reactor has to be run at a low power, and if it is not restarted within a few minutes a longer outage will be necessary. For this reason, a tool is needed to provide quick access to information on the functioning of the cold source.

The cold source is electronically controlled using a Programmable Logic Controller (PLC) which is programmed using a computer and subsequently can run the refrigerator without user input. This PLC uses data from a multitude of sensors to control the system. For diagnostic purposes, this sensor data from the PLC is logged electronically as a "Dbase IV" format file and then accessed using a software tool that enables data analysis. This type of file cannot be easily interpreted with common software such as Excel.

The existing software used for analysis has a number of drawbacks, including only being accessible from a computer in the reactor room (C-100), a pre-set selection of data trends, and no ability to save or export data for future reference. The CSPlot software project intends to overcome these drawbacks and provide a fast and powerful analysis tool to the Cold Source Operation team to help the team troubleshoot any issues. The CSScreens software project is an additional component in improving the cold source data accessibility that allows reactor operators to obtain data on cold source operation without having to leave the control room to use the cold source dedicated computer.

Finally, to allow for early detection of malfunctions that could cause a shutdown, methods of including more of the existing Cold Source instrumentation under electronic PLC control are proposed.

Gonzaga University

An Investigation into the Enhancement of Vesicle-Based Glycan Arrays
Taylor Brown

The field of glycosciences is a developing discipline holding promising opportunity to elucidatecritical biological processes including intercellular signaling, molecular recognition, immune response, and pathological mechanisms. As such, a facile and robust analytical method to characterize the binding specificity of carbohydrate-binding proteins, or lectins, can facilitate research efforts across the field. Several array based systems have been developed to date, but many fall short in that they offer no method to accurately modulate the distribution of carbohydrate density, a necessary property to control as lectin binding depends not only on the type of glycan present, but also the physical spacing between glycans. To create an array system capable of modulated glycan density, surfactant vesicles have been functionalized with glycans and immobilized onto a nitrocellulose surface. However, previous data suggests that this technique gives rise to nonspecific binding of lectins. The goal of this study was to develop a method to reduce the non-specific binding in this vesicle-based array system.

Two interfaces inherit to the array system were considered as surfaces capable of nonspecific interactions; the vesicle interface and the nitrocellulose interface. Early data suggested that nonspecific binding at the nitrocellulose interface could be reduced with the use of either BSA or commercially available Carbo-Free Blocking Solution. Despite the use of Carbo-Free Blocking Solution on the full array, nonspecific binding was not decreased to the point at which specific binding was clear. Furthermore, the proportion of nonspecific binding ateach interface remained uncertain, thus the interface that contributed the most nonspecific binding was unknown.

In an attempt to localize the source of nonspecific binding, a simpler system, involving only the esicle interface, was pursued. Carbohydrate functionalized vesicles were incubated with biotinylated-lectin and fluorescently labeled NeutrAvidin. Size exclusion chromatography was utilized to separate vesicle-lectin conjugates from unbound lectin. BCA protein assay techniques as well as fluorescence measurements were tested to determine whether specific binding of lectin to carbohydrate vesicles could be localized at the vesicle interface. The results suggest that BCA protein assay techniques are impractical while fluorescent measurements hold more promise to characterized lectin interactions at the vesicle interface. Furthermore, fluorescently labeled NeutrAvidin appears to fluoresce more intensely upon intercalation to vesicles, which may give rise to enhanced signal quality in the context of a future, refined array system.

Rheological Properties of Sustainable Ternary Binders
Samantha Engel

As humans deplete natural and economic resources, sustainability is becoming a priority across the world. Specifically in construction, researchers are developing sustainable cement mixtures to be used in concrete. One possible sustainable solution involves fly ash-- a byproduct of coal production--as a mineral admixture to replace a fraction of the cement; however, additional materials are often necessary to achieve desired qualities similar to those of portland cement when using these more sustainable binders. The focus of this talk is on measurement of rheology, a characteristic that describes workability, of ternary, sustainable cement mixtures containing portland cement, fly ash, and a fine limestone powder.

This project is part of a large goal to optimize a ternary mixture of portland cement, fly ash, and limestone. Cement pastes according to a matrix of previously determined mixtures were prepared and tested for heat flow (calorimetry), bleeding percentages, and viscosity and yield stress (rheology). The calorimetry data was compared to previous measurements to assure comparability between materials and mixtures from past experiments. Due to its higher early age reactivity, viscosities and yield stresses of mixtures with Class C fly ash are higher than those of equivalent mixtures containing Class F fly ash mixtures. As limestone mean particle size decreases and the exposed surface area of limestone powder increases, higher viscosities and yield stresses are expected.

The results from this research will be used to form a methodology to choose the most appropriate mixture ratios for ideal rheology between the three aforementioned components. Conclusions from this research will supplement a broader project investigating several characteristics of the same matrix of cement mixtures.

Goucher University

Tunnel Junction Measurements of Spin Currents

Julian Irwin

Magneto-resistance first order reversal curve (MR-FORC) analysis, a technique used to characterize the magnetic properties of a material, is applied to magnetic tunnel junctions (MTJs) engineered for use as magnetic memory or sensors. MTJs are made of two layers of ferromagnetic material, one high and one low coercivity, separated by a thin tunnel barrier. MTJs have an electrical resistance which depends on an external magnetic field and which exhibits hysteresis, making FORC analysis an applicable tool for characterization of these devices. Experimental MR-FORC data is presented for MTJs of varying sizes and geometries in the 10 μm^2 range. A comparison between FORC data taken on an array of devices and MR-FORC data for a single device is also presented.

Gustavus Adolphus College

Shine on Me

Jenna Legatt

A variety of novel video imagers have recently been developed and employed for clinical applications such as image-guided intervention and optical biopsy, but the scenes appear quite challenging when they involve 3D surface topography. Most wide-field video imagers produce only 2D images containing glares, shadows, and spectral shift from backscattering. Thus, it is crucial to understand the surface topography of the sample in order to correctly reconstruct topographical information from the 2D projected scene.

This project focuses on developing an optical imaging technique to measure the topography of the sample using patterned light created by a spatial light modulator (SLM). The SLM is composed of a 2D array of pixels containing a few hundred million liquid crystal display. An electrical field is applied on a pixel-by-pixel basis to tilt the liquid crystal molecules; therefore, inducing phase shifts in the reflected light. This generates a pattern output which is illuminated onto a sample with a surface curvature. The distortion of the pattern can be analyzed to compute the topography of the sample.

In clinical applications, the 3D image will help surgeons locate anatomical features with higher precision without introducing more obstacles to the operating room. The SLM is a handy, flexible, and universal device with a broad potential impact in other optical technologies including optical tweezers, 3D profiling, light shaping, and beam steering. A potential application of the structured light illumination on the multi-trap optical tweezers application will also be discussed.

Hampton University

Diagraph Method in Detecting Rule Faults for Attribute Based Access Control Policies

Charles Scott

The Computer Security Division is developing and researching Diagraph methods for Access Control (AC) polices verification. The objective of this project is to detect and fix AC rule faults which include privilege assignments, leakage of privileges, as well as Conflict of Interest (COI). Access Control (AC) is used in many principals such as users and or processes that have access to various resources in a system. Operating systems and database management systems incorporate AC to control which user(s) can access which resource. These AC policies are composed by independent AC rules in propositions of privilege assignments described by attributes of subjects, actions, objects as well as environment variables of these protected systems. The AC polices are described as Attribute Based Access Control (ABAC) policies which consists of a set of rules that either contain a permission or denial action(s) on specific resources. The proposed research is capable of detecting these rule faults before an additional rule is added to the policy. This allows faults to be detected automatically when a specific AC rule is added to the policy other than generic computing principles, in which later computing results overwrite the previous one. One of my many tasks this summer was to develop algorithms and create diagraphs for any given ABAC policy(s) using subjects, actions, and resources. The research provides policy authors visible images for the structure of ABAC rules intuitively as well as interactively. The research has hopes on improving the composition of ABAC polices by using this Diagraphical approach.

Video Stream Face Detection

Courtney Smith

Video Stream Face Detection is vital in today’s society as far as safety and security in crowded areas such as airports, train stations, or shopping malls. Face detection and tracking technology in video streams can potentially help monitor such activities. These technologies have been around for quite some time and the big question now is how good they are? This project tries to answer this question by implementing an evaluation pipeline by selecting appropriate video streams, annotating the ground truth, and applying face and tracking systems/algorithms, results from the system can be compared with the ground truth and accessed via evaluation scoring software. In this presentation you will hear about how the scoring evaluation pipeline works by using various tools such as FFMPeg, FaceDetect software program developed based from the OpenCV library, ViperGT, and F4DE. FFMPeg provides video viewing and frames extraction. FaceDetect for image face detection. ViperGT provides actual face location annotation as the ground truth from the video clips. F4DE will compare the results from the FaceDetect against the ground truth to calculate the scoring evaluation and determine the performance of the face detector. If time allows and tools are available, I would also like to present the human tracking aspect of the project.

Hood College

Determining Important Control Parameters of a Genetic Algorithm

Andrea Haines

Genetic algorithms (GAs), a type of heuristic search, are useful for many computational problems that require finding a good solution among a large number of possible solutions. GAs represent possible solutions to a problem as individuals in a population and classic GAs represent the solutions' components as a collection of genes. GAs start with a randomly generated population of individuals and converge to a good solution, according to the "fitness" of the individuals and other evolution-mimicking factors within the algorithm. GAs mimic the success of natural evolution by allowing many different possibilities to be explored simultaneously, while driving the population towards solutions with high fitness.

Successful evolution toward highly fit solutions depends on control parameters that can be varied within a GA, but existing literature lacks a definitive study about the relative importance and best settings for these parameters. We conducted a robustness study and analysis of a GA's performance against 60 numerical optimization problems, examining seven control parameters under 1024 orthogonal fractional factorial combinations of settings. This study produced a relative ranking of the control parameters by their influence on the GA's performance and identified the parameter settings that yielded best performance.

The best parameter settings derived from the 60-problem study will be applied to control a GA steering a population of cloud-computing simulations (i.e., *Koala*) toward extreme outcomes. In particular, by steering *Koala* simulations, a GA will seek to identify behavioral directions and parameter combinations that could cause degraded operations and/or catastrophic failures in cloud computing systems.

Synthesis of Thiolated Tether Compound to Improve the Properties of tBLM Used in the Study of Integral Membrane Proteins

Rachel Meyer

Membranes are an essential structure in the functioning of cells. A complex mixture of lipids and proteins, membranes create a selectively permeable barrier between the cell and the environment, as well as compartmentalize areas in the cell for vital processes to take place (i.e., redox reactions, chemical gradients, etc). Membranes also regulate and facilitate the flow of substances into and out of the cell, generate chemical or electrical signals, participate in the transduction of these signals, and play a key role in the generation and utilization of chemical energy. Integral membrane proteins (IMPs), proteins that are imbedded in the membrane, play a major role in these activities. A protein's ability to function is closely related to its structure, and, in turn, the structure of the protein is dependent on the environment within which it resides. Therefore, IMPs become denatured outside of the membrane, and thus are exceedingly difficult to characterize using traditional methods. Tethered bilayer lipid membranes (tBLMs), synthetic membranes tethered to a surface, in our case gold, by thiolated tether compounds, are a tool that can be used in the study of IMPs. Possible applications for tBLMs include structure and function determination of IMPs that cannot be crystallized, studies with regards to the electrical properties of the tBLMs with different chemical compositions, and diagnosis of diseases that affect a cell's membrane. The goal of my project this summer is to engage in the synthesis of new tether compounds in an effort to improve tBLM fluidity, an important property of membranes, and stability.

Louisiana State University

Quantum Metrology with Nonclassical Light

Chase Brignac

Fabry-Perot interferometers have been used in metrology for almost one-hundred years. The interference pattern of coherent laser light passed through a Fabry-Perot cavity allows for very precise phase measurements. Phase measurements are useful for precise measurements of cavity length and light wavelength. The uncertainty of a phase measurement, also called the phase sensitivity, is classically limited by the random fluctuations in the number of photons that the photo detector receives. This is called the Shot Noise Limit of a Poisson process.

In the 1980's it was found that using nonclassical light allows for measurements that beat the Shot Noise Limit and in principle are bound by the Heisenberg Limit. Nonclassical light is light that cannot be described using classical electromagnetism. It is instead described by the quantized electromagnetic field of quantum mechanics. This study examined the use of nonclassical light in interferometry to advance the field of quantum metrology.

In this talk we introduce the basic principles of quantum metrology, particularly using photon number states in a Fabry-Perot interferometer. An overview of interferometry with coherent light as well as nonclassical light with number resolving measurements and average intensity measurements will be given.

Loyola University Maryland

Web Based Applications for Machine Tools
Andrew Gorbaty

Are you aware that the manufacturing industry spends millions of dollars a year building machines that are later scrapped? And are you aware of the workers and NIST scientists who have to do repetitive tests for certain machines just because there is no easier way to do this? What if there were some computer applications to rectify this? Listen to how Web Based Technologies can help industry, NIST workers, and NIST scientists to be more efficient in their work. The virtual machine tool designed this summer will be discussed at length, featuring a Computer-Aided Design simulator, graphical tools, XML parsers, and more. Future creation of freeware applications with programming languages such as JavaScript and WebGL for the manufacturing industry will also be discussed.

Calibrating Laser Range Scanners for Robot Safety
Allison Rose

The importance of robot safety has grown with the increased use of robots in manufacturing. Real-time sensors can improve human safety by detecting people's location on the shop floor and enabling robots to interact appropriately. Currently there is a lack of standards for calibration of these real-time sensors. The purpose of the project was to develop algorithms and procedures for easy and accurate calibration in relation to the environment and other sensors.

The project designed, implemented and tested programs for calibrating static sensors such as cameras and planar laser scanners using winged planar targets. The scanners read the time of flight of a laser beam to measure distances to objects and produce a one-dimensional array of distances in a plane. The winged targets were constructed of two white foam core boards forming a 90 degree angle. The objective was to use the targets to determine the geometric transformation between two laser scanners.

Experiments were conducted by collecting data from Hokuyo and SICK laser scanners, and analysis and algorithms were performed in MATLAB. The experiments were aimed at validating the developed methods.

Miami University of Ohio

Validation Measurements for Optical Remote Sensing of Greenhouse Gases
Alexis Denton

Emission quantification of greenhouse gases (GHG) from distributed sources poses a significant measurement challenge. Accurate measurements are critical for providing better models for global climate change, informing policy makers, and providing a solid footing for carbon economies. A distributed source is a poorly defined region of about 0.5–5 square kilometers, and examples are coalmines, landfills, large scale industrial sites, and carbon sequestration facilities. Problems include cost and availability of instruments, poorly defined measurement uncertainties, and deviation in measurements from models. We are pursuing the method of Differential Absorption Light Detection and Ranging (DIAL). DIAL measurements are made by sending out a pulse of light with a stabilized wavelength centered on an absorption peak corresponding to the species of interest (CO_2 CH_4). As the pulse of light travels through the atmosphere some photons are backscattered and collected using a telescope and imaged onto a sensitive detector. This step is repeated with the laser tuned off of the absorption peak, and from the ratio of these measurements the range resolved, species specific concentration can be determined. The concentration of CO_2 is calculated using Beer's Law and the absorption coefficients obtained from the HITRAN database. Two methods were developed for measuring the concentration of CO_2: a commercially available CO_2 gas analyzer and a home built absorption spectroscopy system. These different experimental approaches will provide multiple points of comparison and validation for the DIAL system.

Millersvillle University of Pennsylvania

A Cases Study for Sustainability Modeling and Optimization
Ryan Consylman

Sustainability has recently become an important issue due to the depletion of energy and natural resources. Manufacturers need to achieve sustainable manufacturing through optimizing energy and material usage at different operational levels. To avoid duplicated efforts, a systematic and reusable approach for sustainable process representation was proposed. The Sustainable Process Description Model (SPDM) was developed for efficient definition/storage/exchange of manufacturing process sustainability information, which provides basis for analysis of sustainability assessment using optimization and simulation. As one of the case studies to validate the methodology, this SURF project performs optimization based on an application scenario and manufacturing data (process, product, resources, and sustainability factor) represented using SPDM. The case study models a simplified representation of a patent binding line that produces phone books and it utilizes material (paper) as the sustainability factor and focuses on the optimization of material waste ratios and cost. IBM ILOG's CPLEX Optimization Studio was chosen as the optimization tool, in which Optimization Programming Language (OPL) is used. A partial SPDM instantiation has been developed for this case study. Java was used to develop the user interface and translate the SPDM to OPL recognizable format.

Crypto-Graphics: Visual Applications of the NIST Randomness Beacon
Edward Kimmel

Random Selection is a common solution used for many important or sensitive decisions. Finding a method of securely choosing the random numbers, however, is not. The NIST Randomness Beacon can solve this problem by producing secure public random numbers. These numbers cannot be predetermined and are made public to allow for verification of events that used them. Any scenario which relies on a secure random number not yet known can utilize the Beacon for Random Selection.

The concept of utilizing this Beacon for Random Selection is more understandable through examples. It was decided that iOS applications would be created as a means of visually presenting some applications of the Beacon. The focus of my project was to create these iOS applications. Through my project, I have created 4 applications showing usage of the Beacon for Random Selection through various graphical means as well as a graphical demonstration of the Birthday Paradox as a visualization of how common hash collisions are. I have also directly modified the Beacon to utilize 2 hardware cryptographic tokens in generating the random numbers.

The talk will explain a little bit about the Beacon and the technologies used within, but will mostly present the applications I have created and explain the communication protocol between the applications and the Beacon.

Implementing and Optimizing Calculations of In-Plane Scattering off of Thin Films
Wayne Treible

Off-Specular Reflectometry is an important probing technique for studying ordered and unordered thin materials because it provides unique in-plane contrast information that cannot be acquired through specular reflectometry or small angle neutron scattering (SANS). This allows for even more insight into thin films than the existing array of probing techniques provide.

The OSRefl codebase, previously developed at the NCNR for the analysis of the in-plane components of near-specular neutron scattering, was extended and modified to allow for the calculation of in-plane scattering for a collection of thin film test samples. Two approximations were used, the Born Approximation, which models plane waves interacting with the samples, and the Distorted Wave Born Approximation (DWBA), which models plane waves modified by the specular scattering off of the samples (math used from Kentzinger, *et al* in Physical Review B **77**).

Montgomery College

Enhancing the NIST Chemistry WebBook with Optimized 3D Structures – Part 2
Katie Hafner

This summer we have been working on the National Institute of Standards and Technologies online chemical database, the NIST Chemistry WebBook. The WebBook is one of NIST's most frequented and well-known databases. It includes over 200,000 structures and contains standard chemical information such as Chemical Abstract Services (CAS) number, molecular weight, chemical formula, 2d structure and International Chemical Identifier number, as well as experimental data. Our specific project has been to validate the WebBook's chemical information to make sure it is correct and to optimize 3d structures of its gas-phase molecules using quantum chemistry calculations: in doing this, we are ensuring that the WebBook continues to be a reliable, useful and sustainable database. The optimized structures are a useful addition to the WebBook because the output files contain information that can be extracted and used to derive chemical properties such as thermodynamics and vibrational frequencies. Our process has been to take 2d structures of molecules and run them through a series of semi-empirical methods and quantum calculations. We roughly optimize structures using PM6 (a semi-empirical method) and then more accurately optimize them using B3LYP/6-31G(d) (a quantum method). The structures are efficiently and quickly computed using PM6 methods, but go through the quantum calculations at a much slower rate. So far we have 30,000 and 5,000 structures that have completed PM6 and B3LYP calculations, respectively. The overall goal is for each compound in the WebBook to have a corresponding 3d optimized structure. Through our work this summer, we are making a considerable contribution to the number of optimized and validated structures present in the WebBook, thereby strengthening its reliability and sustainability as a NIST database.

Mount Saint Mary's University

Analysis of CO_2 Loss in Gas Cylinders and Changing Concentrations over Time in NIST Gas SRMs
Lance Dockery

The National Institute of Standard (NIST) gas metrology group is primarily responsible for the identification and measurement of gases and the development of gas standards which can be used by industry, other government agencies, and scientists for research. The National Oceanic and Atmospheric Administration (NOAA) prepares its own gas standards which have a bias of .2% or approximately 700 parts per billion when compared to standards developed by NIST. One aim of this study is to better understand CO_2 loss which may account for the bias between NIST and NOAA standards. Studying this bias involves using a mother/daughter study. Gas from one (mother) cylinder is transferred to another evacuated (daughter) cylinder. These cylinders were analyzed against each other using a cavity ring-down spectrometer. It was observed that there was always less CO2 in the daughter cylinder than the mother. It was expected that at high pressure more CO_2 would be lost into the walls than at lower pressures however the loss was found to be even across all pressures. This loss is more than the measurement uncertainty and it can account for some of the bias between NIST and NOAA however some of the still remains unaccounted for.

An additional aspect of the study will examine the change in the concentration of standard reference materials (SRMs) over time as the pressure in the cylinder decreases. This study is important to better understand the long-term stability of NIST standards as the pressure in the standard decreases from use. Cavity ring-down spectrometry, UV-Vis spectrometry and chemiluminescence were used to measure CO_2, CO, SO_2, NO, and H_2S species continuously as the cylinder pressure decreases. Knowledge of what happens to cylinders over time is important for the ability of NIST to certify old standards used by government agencies, industry and scientists where the concentrations may be outside of the initial standard concentration developed by NIST.

New College of Florida

Bench Scale Measurements of Toxic Effluents n Fire Smoke
Sophie Lang

Smoke inhalation is the leading cause of death from structural fires. By studying the toxic products evolved during combustion of common household items, the toxicity of the smoke can be evaluated. The concentrations of toxic products in smoke depend on a variety of factors, one of which is the yield of each product when a certain fuel is burned. Knowing the toxic product yield under specific fire conditions helps predict smoke toxicity in a large scale structure fire. Much of the data on toxic products has come from room scale and other large scale tests in the past, but these tests require a great deal of resources, so bench scale tests have been developed to collect similar data on a much more practical scale. This project is focused on vetting an experimental method to ensure that the data it yields is consistent with the data obtained by other labs using similar methods. This method uses a tube furnace to burn samples and FTIR spectroscopy to analyze the composition of the smoke. After calibrating the instrument and burning PMMA—chosen because it is a well-known material with a great deal of previous research done on it—a variety of polymers were burned and the data from those experiments analyzed.

North Georgia College & State University

Measurement of Material Thermal and Chemical Characteristics with the Laser-Driven Thermal Reactor

Matthew Jones

A state-of-the-art, rapid-heating technique, referred to as the Laser-Driven Thermal Reactor, is used to characterize multiphase, multicomponent materials of all types. For climate change applications, we are currently developing the technique to measure the absorption coefficient of filters coated with atmospheric aerosol particles [Presser, J. of Quant. Spect. & Rad. Trans, 2012]. For forensics applications, the technique is being used to develop a database of thermal and chemical signatures for energetic materials [Nazarian and Presser, Int'l J. Heat Mass Transfer, 51:1365, 2008]. The technique provides quantitative measurements of various relevant thermophysical and chemical properties, including sample heat release rate, chemical kinetics rates, total heat value, specific heat/energy release, and chemical reaction byproduct identification. As a 2012 SURF student, I assisted in the acquisition and analysis of data generated by the nigrosin-coated filter experiments, as well as helped in the preliminary work necessary for the future development of a homemade explosives database of thermophysical and chemical properties. Furthermore, my work included modeling the reactor, simulating the laser-heating process, and investigating potential modifications to the reactor design that would better our experiments.

Determination of Polymer/Fullerene Bilayer Miscibility

Deborah Leman

The fuel demands of the modern world have prompted the development of solar cell technologies that can be used on a large scale. Organic photovoltaics (OPV's) are compatible with inexpensive, low energy budget roll to roll manufacturing and can enable novel energy harvesting applications such as semi-transparent windows and self-powered indoor signage, though the current OPV device technologies lag behind their inorganic counterparts in efficiency. In order to increase performance of OPV's, the materials, morphologies, and properties of the active layer have been studied. The active layer in high performance OPV's is often a Bulk Heterojunction (BHJ) structure, in which a light absorbing/electron donating polymer and an electron accepting fullerene self-organize into a nanoscale network. The kinetics of the formation of the network and the thermal stability of this network are influenced by the molecular mixing (miscibility) of the two components, which can lead to alteration of device performance simply from temperature change. We are developing the protocols to measure donor/acceptor mixing by creating a bilayer of film and measuring the temperature dependence of thickness and composition using an automated spectroscopic ellipsometer with a heating element. We are making a comparison of materials that are widely used in OPV research, namely the donor polymers, P3HT and PCDTBT, and the acceptor fullerenes, PCBM-61, PCBM-71, bis-PCBM-61, and bis-indene-PCBM-61. The two polymers, P3HT and PCDTBT, have different glass transition temperatures (T_g) and crystallinities which affect the knitting process. Our results establish that the polymer T_g strongly influences the mixing and suggest that crystallinity may play a secondary role in determining the kinetics of mixing. In general, the larger fullerenes result in less mixing.

Oklahoma State University

Empirical Calibration Curves for Concrete
Danielle Artmayer

Potassium, chloride, and sulfur can accelerate the oxidation of steel reinforcement in concrete, thus weakening the structure and causing premature failure. Knowing the percentage of certain ions in concrete is useful for determining the likelihood for damage to the structure. While traditional, bulk XRF is commonly used to determine the relative abundances of these ions, µXRF was the analytical method chosen because µXRF can be extended to imaging applications. The ability to produce x-ray images from which quantitative elemental data can be derived is very useful for imaging ion ingress into distressed structures. To develop the calibration curves necessary to predict concentration from spectral response, samples were made with known concentrations of ions and analyzed with a µXRF. The samples contained well characterized cement (Lehigh Low Alkali Cement), water, and the analyte ion, and were mixed in a standardized process which is easily reproducible. After mixing, samples were placed into a mold to harden overnight. Data collected from these samples were processed using DTSA ll and then imported into R to produce a regression fit line. This talk will discuss the process of making and developing curves for empirical calibration curve development, and discuss ways of improving empirical calibration curve development.

Prairie View A&M University

Effect of Interlayer in Organic Tandem Solar Cell
Shahin Amini

Organic Photovoltaic Devices are a promising technology for converting sunlight into electricity by employing thin films of organic semiconductor. The goal is to reduce the cost of producing electricity by increasing overall efficiency close to 10-15%. The highest efficiencies of bulk-hetero junction solar cells from poly (3-hexylthiophene) (P3HT) and [Phenyl C-61-butyric acid methyl ester (PCBM) reported so far are close to 5%. Phenomena occurring during the photovoltaic process, such as the creation, diffusion and separation of exactions, as well as charge carrier transport, are governed by the active layer morphology. We want to create a tandem cell by stacking two layers of solar cells. Tandem solar cells provide an effective way to harvest a broader spectrum of solar radiation by combining two or more solar cells with different absorption bands.

We wanted to demonstrate an efficient tandem organic solar cell and we investigated the effect of the interlayer of efficiency of tandem cell. We fabricated several different interlayers to join the two cells to study the effect of device structure on efficiency. Materials are spin coated onto a glass substrate from solution. We fabricated polymer tandem PV cells using interlayers of the thin films of Aluminum/MoO_3, Aluminum/PEDOT: PSS, or TIO_x on the separate glass ITO substrate. The interlayer fabrication procedure was optimized and the efficiency was measured for the various device structures.

Novel Capillary Viscometry Protein Therapeutic Formulation
Anh-Tuan Le

Pharmaceutical companies are developing protein-based therapeutic treatments for a wide range of diseases. In many cases, these are in the form of viscous solutions that are injected into the body. It is critical that the viscous properties of the fluids, as well as their stability can be accurately tested. We developed two simple viscometer methods that utilize very small amounts of fluid and that can test the stability of the solution over a long period of time (months). We developed two methods: rising capillary viscometry and capillary plug viscometry. In both cases, we need to account for the complicating effects of the interface between air and solution. We studied these effects by varying the length of fluid in the capillary. We find that the capillary plug method is superior, because it is easier to account for these interfacial air/solution effects. We present results on the accuracy of these methods by measuring the viscosity of water as a function of capillary diameter, tube angle and fluid plug length. Preliminary results for protein solutions that show "shear thinning" will also be presented.

Purdue University

Assembly and Measurement of Quadruplex DNA Nanomaterials
Victoria Savikhin

Double-stranded DNA is a predictable, synthesizable, and self-assembling molecule, making it an ideal material for development of nanoscale devices for manufacturing and medicine. It is currently being used as a building block for increasingly complex nanoscale structures including logic gates, scaffolds, and 3-dimensional objects. Less work has focused on four-stranded guanine quadruplex DNA. This structural motif has the additional advantages of high thermal stability, resistance to enzymatic digestion, and increased structural rigidity. My project has focused on reproducibly creating quadruplex structures and controlling their assembly into larger structures.

Using gel electrophoresis, circular dichroism spectroscopy, atomic force microscopy, and fluorescence spectroscopy, I have shown that quadruplex self-assembly can be controlled reliably by changing cation identity; that single-stranded ends of quadruplexes bind to complementary DNA sequences; and that larger structures form from two quadruplex building blocks designed to interlock.

Reed College

Verification of Computational Fluid Dynamics Program for Fire Modeling
Max Gould

The effectiveness of the computational methods used to simulate complex fluid dynamics in the Fire Dynamic Simulator (FDS) is evaluated by means of two test cases. The first, a two dimensional vortex in a constant flow field, is a theoretically stable flow pattern. The computational methods are shown to be second-order accurate through analysis of the simulation's divergence from this theoretical vortex over time for a range of computational grid-resolutions.

The second case evaluates the accuracy of turbulence simulation in FDS. The case initializes two bands of opposing fluid flow that create a stratified mixing layer at their interface, generating turbulence along the layer. This case is particularly relevant to FDS with regards to the behavior and evolution of smoke layers. A comparison of the bulk Richardson numbers between FDS simulations, other CFD (computational fluid dynamics) simulations, and experimental results demonstrates the sophistication of FDS fluid modeling and provides further verification for the accuracy of its computational methods.

Rochester Institute of Technology

Finding Numerical Solutions of the Fourier Modal Method to Measure Two Dimensional Gratings
Jonathan Beaumariage

As modern electronics continue to shrink towards the nanoscale, the old methods of precision measurement are no longer sufficient. The semiconductor industry finds itself searching for a new method of extremely accurate measurement to ensure quality production. Here we present an improvement to one of these newer methods: spectroscopic ellipsometry. By measuring the change in polarization of light shone onto a silicon wafer, and then comparing that change to a computational model of said light, it is possible to precisely measure the nanostructure of the wafer. However, this method is typically held back by the computational complexity of the simulation. By exploiting symmetry in the silicon wafer pattern, it is possible to significantly decrease computational time. The method of doing so is presented, along with numerical examples highlighting the reduction of computational time. The method is also employed to measure some two dimensional crossed gratings.

Exploring Real-Time Web-Based 3D Mathematical Function Rendering and Manipulation
Brian Clanton

"The NIST Handbook of Mathematical Functions," together with its Web counterpart, the NIST Digital Library of Mathematical Functions (DLMF), is the culmination of a project that was conceived in 1996 at the National Institute of Standards and Technology (NIST)." The current online DLMF contains a collection of extensive visualizations of these mathematical functions.

This SURF project seeks to extend these visualizations to implement capabilities not yet available in the production version of the DLMF website.

The current digital versions of the functions are stored in files that can individually downloaded and viewed using computer software. While highly functional, we are looking to improve upon the existing capabilities and move towards more modern web architecture for 3D graphics.

In this presentation, we will discuss how we enhanced the display of three-dimensional functions using WebGL, a 3D graphics programming library that allows for GPU accelerated rendering in web browsers. In addition, we will cover functionality we created for this web application, including the unified environment for all of the models, the creation of shader programs for coloring and the implementation of an arbitrary clipping plane.

Tunability of Photon Entanglement
Dylan Heberle

Quantum entanglement has applications in fields such as quantum computing, quantum cryptography, and quantum teleportation. As such, it is a key application of nonlinear optics. In this study, we are interested in polarization entanglement, which can be achieved by sending laser light through a nonlinear optical crystal. Due to phase matching, entanglement is only efficient at a specific frequency of light for a given crystal. However, this frequency is a function of angle, which leads to a range of frequencies at which a particular crystal can produce entangled photons.

This study focuses on the production of Type-II entangled photon pairs in periodically poled rubidium-doped potassium titanyl phosphate (Rb:KTP) and titanium-indiffused lithium niobate (Ti:LN) waveguides. By fabricating waveguides at different angles relative to the crystal axes, a range of phase-matching frequencies is realized, allowing entanglement to be achieved throughout a range of operational frequencies. For the Rb:KTP waveguide, we found that the output wavelength can be tuned from 1122 nm to 1230 nm as the structure is rotated through 90°. Tunability of Ti:LN is comparable, but with an output closer to 2000 nm. This tunability shows promise for the generation of entangled-photon pairs by realizing frequencies that were previously unavailable.

Neutron Imaging of Chemical Phase Transitions in Alkaline Batteries
Joshua Kahn

Neutron Radiography provides a way to nondestructively study materials and devices in situ. This is a process similar to X-Ray imaging, but has advantages in certain situations. Neutrons pass through most metals quite easily and are sensitive to other materials, making them ideal for studying many materials that X-Rays cannot effectively be applied to. In this experiment, the phase changes of a standard AA alkaline battery are studied at various levels of discharge using neutrons.

Neutrons are scattered and absorbed by materials, and the transmitted intensity allows one to quantitatively measure the density of material that the beam passes thorough. However, the chemical composition may still be undetermined. If the material has a crystalline phase, then it may be possible to identify the composition using an energy selective neutron imaging method. Neutrons of a particular energy selected from a beam with a wide range of energies have a specific de Broglie wavelength. Neutron waves scatter from the planes of a crystal lattice in a phenomenon known as Bragg scattering, resulting in lower neutron transmission. As the wavelength increases, reflections become forbidden, leading to sharp drops in scattering known as Bragg edges. As the Bragg edges are based on the crystal structure of a material, neutron images taken at different wavelengths show contrast due to the different crystalline phases that are scattering neutrons.

Here we image the Zinc and Zinc Oxide in the anode of an alkaline battery. We will talk about modeling Bragg edges in the macroscopic cross section of the material, which takes into account all scattering and absorption of the neutrons by the material. Data for the transmission through both a homogeneous Zinc Oxide sample and a standard AA Battery will be presented for a range of wavelengths from 0.1 nm to 0.3 nm, in order to confirm the modeled scattering cross section. Data will also be presented for a three dimensional reconstruction of the battery using tomography, at different states of discharge. In addition, results will be presented for samples of a transparent ceramic, Spinel, which were analyzed during the course of the project.

<u>Saint Mary's College of Maryland</u>

Effects of Film Processing Parameters on Organic Photovoltaic Device Performance

Lucas Carneiro

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

During the summer we studied BHJs prepared by a film deposition technique called doctor-blading. Drawing on our project from last year, we were able to determine the optimal doctor blade speed, blade height, and solvent for film deposition. Keeping these parameters constant, we were able to independently change the solution concentration and the substrate temperature in order to determine their effects on film thickness, BHJ morphology, and, ultimately, device efficiency. Film thicknesses were measured via spectroscopic ellipsometry, and polymer order was characterized via UV-Vis spectroscopy and grazing-incidence x-ray diffraction. The impact of film processing on OPV device efficiency was determined by fabricating devices with constant thickness (≈ 120 nm). Variations in efficiency were related to morphological changes in the BHJ active layer.

Using Arbitrary Waveform Controlled Lasers and Cavity Ring-Down Spectroscopy to Determine Greenhouse Gas Concentrations
Pasquale Raico III

It is widely believed that increases in greenhouse gas concentrations in the Earth's atmosphere contribute heavily to Global Warming. Providing fast methods to monitor absolute concentrations of these gases without calibration gases gives us a means of tracking the Global Warming's "advancement". Dr. David Plusquellic has been developing a new fast scan technique using arbitrary waveform generators, electro-optic modulators and cavity ring-down techniques in the near-IR to probe the atmosphere in real time and determine absolute concentrations of carbon dioxide and methane. In this talk I will give a brief description of new technique and discuss the data analysis for retrieving absorption line shapes and concentrations.

Detecting Malware on Smart Phones
Alexander Roca

Smart phones are an integral part of daily life for many people. Thanks to the varied applications available for them, smart phones are useful tools that can be used for pretty much anything. Because of their ubiquity, however, smart phones are increasingly tempting targets for cybercriminals. One of the ways to attack a smart phone is to create a seemingly innocuous application with the intent of stealing data, disabling important functions, or fulfilling other malicious goals.

These applications are usually discovered, analyzed, and publicized in a process that takes roughly three to six months. However, during this time the application is free to cause havoc. Detecting malicious applications as soon as they appear is therefore an important goal. To facilitate this, we have developed programs that obtain and analyze free applications from the Windows Phone Marketplace. Once the applications are analyzed, the data is collected and stored centrally. By comparing this data with features of known malicious apps, we can hopefully identify new malware as soon as it is released to the Marketplace.

This talk will focus on the second half of our process: examining the applications once they have been obtained from the Windows Phone Marketplace.

Saint Olaf College

Testing Shapes and Sizes of the Diamagnetic Lateral Force Calibrator
Sarice Barkley

The atomic force microscope (AFM) is commonly used to perform nanoscale friction measurements, or friction force microscopy (FFM), but there are many different methods for calibrating these experiments. The diamagnetic lateral force calibrator (D-LFC) method, developed by Li et al., utilizes a precalibrated magnetic levitation spring system to directly convert the AFM friction signal in volts to force in Newtons, making it a robust and accessible method for lateral force calibration. Because of its novelty, however, there are many aspects that need to be optimized and limits to be tested, namely, which geometric dimensions are ideal for a variety of applications. In this study, various geometric combinations of the D-LFC are compared and tested against a theoretical model with the goal of improving FFM methodology. Experimental data are proving consistent with the theoretical model to within 5%.

Savannah State University

Catalyst Structure Investigated by In-Situ HRTEM Measurement During CNT Growth

Sterling Brooks

Carbon nanotube (CNT) growth has been studied extensively for the better part of the last 20 because of their outstanding electronic, mechanical and optical properties. However, no major industrial application has emerged as of yet due to a lack of control in the growth of these Nano-structures. The forecasted potential of this new form of carbon is the main reason behind the incessant need to elucidate its growth mechanisms. With the use of a carbonaceous gas, e.g. Acetylene, Methane or Ethanol and metallic nanoparticles of materials such as Cobalt, Iron or Nickel, growth of these nanotubes can be initiated. This synthesis method also known as CVD (Chemical Vapor Deposition) is performed at elevated temperatures (500 to 900 ºC). By using a High Resolution TEM (Transmission Electron Microscope) it is possible to record videos of the CNT's evolution from beginning to end. During my internship I have analyzed the structure of the active catalyst particles (size, morphology, chemical nature…) and measured the growth rates of the CNT's. I then tried to correlate these nanoparticle structural changes to their growth kinetics.

Southern University

Fabrication, Optimization, and Analysis of PLGA Nanoparticle for Potential Advancing in Stem Cell Therapy

John White

Nanotechnology has open up a world of studies that leads to a wide range of inventions. Through further development of nanotechnology, clinical medicine will advance to further dimensions past its current limitations. Therapeutic opportunities such as medical imaging, medical diagnosis, drug delivery, and cancer treatment can be improved. Stem cell research is becoming a popular discipline due to the development of biotechnology. Cell activity can be observed on a molecular level, which can lead to potentially enhancing the effects of diagnosing and treating diseases. Nanoparticles such as manganese, polystyrene, silica, titanium oxide, carbon, and quantum dots provided assistance in targeting and fixing stem cells to their desired site in addition to guiding stem cells to a specific direction. The properties of nanoparticles allow them to penetrate through the semi-permeable lipid bilayer. However, the limitations of nanoparticles relative to stem cells involve the toxicity, the targeting of unwanted cells, and the mechanisms of the various nanoparticles attached to stem cells. The goal is to discover new information and techniques necessary to alleviate the limitations of bionanotechnology. Nanoparticles will be created manipulating several parameters to determine optimal effects in terms of them differentiating them into osteogenic cells. The nanoparticles will be created by electrospinning, collected, and analyzed using confocal, SEM, and fluorescent microscopy. In electrospinning, particle concentration and flow rate are varying, but voltage and gradient will remain constant.

State University of New York at Albany

Space Charge Limited Current Spectroscopy in Organic Single Crystal Semiconductors

Michael Briggs

Organic electronics is a field of increasing popularity. Research is conducted on organic materials and their application in semiconductor devices because of their low cost and high mobility. Although single crystals are not a low cost production technique, they help understand the underlying physics, which is important to design and improve technologically relevant devices. A less understood aspect of single crystal organic materials is the charge transfer mechanism that gives rise to such high mobilities at room temperature.

For temperature dependent space charge limited current [TD-SCLC] spectroscopy the current/voltage characteristic is measured across the semiconducting crystal at various temperatures between room temperature and 77K. Space charge limited current [SCLC] occurs in the single crystals when a gate voltage is applied and charge carriers are formed. These carriers form a continuum of charge that is conductive through the crystal due to a potential difference across the source and drain. As the gate voltage increases, trap states caused by impurities and imperfections in the crystal are filled and changes in current density are observed as a result.

The growth of single crystal rubrene is commonly done by physical vapor transport. The weak attractive forces in the rubrene molecules cause it to sublime, travel down the growth tube in vapor phase, nucleate and grow into high-purity single crystals. These single crystals are then laminated onto prefabricated substrates with evaporated gold bottom contacts. The rubrene single crystals adhere to the gold contacts by electrostatic attraction. A gold top contact is the deposited and the field-effect transistor structure is completed. The I-V characteristics of the new devices are then measured at temperatures ranging from 100K to 300K using a cryogenics system. The mobility and density of states can be determined by analyzing the transistors' electronic properties.

My project first involved setting up a new crystal growth system and optimizing growth conditions to obtain usable crystals. Thermal evaporation was done to create the gold contacts needed to build the devices. Characterization of the cryostat was also needed in order to confidently measure the I-V characteristics of the devices at low temperature. Finally, analysis of the devices' characteristics was done to determine the mobility and density of states as a function of temperature.

Fluidity at Oil-Water Interfaces

Pascal Garczynski

Studying the Brownian motion of particles confined to fluid interfaces tells us about the properties of the interface. We employ particle tracking to study the microrheology of a layer of protein surfactant adsorbing at an oil-water interface. After the initial introduction of the protein surfactant, the oil-water interface undergoes a viscoelastic transition and the particles become trapped in a gel. We are especially working on developing a procedure and setup to accurately determine the diffusion coefficients as a function of age from the time the protein is introduced to the system. Among the many variables that affect the diffusion coefficient are the particle size and the solution characteristics (such as pH and protein concentration). An optical microscope and camera can capture a video of fluorescent polystyrene nanoparticles at the interface. We can then use Interactive Data Language (IDL) programming to analyze the data and track particles from the captured sequence of images. Following the calculation of the mean square displacements of the particles, the diffusion coefficient can be calculated.

Chemical Surface Patterning
Brian Janiszewski

Surface patterning is the process of creating geometric structures on surfaces by using lithography and etching technologies. Those physically patterned surface structures are used in making electronic/optical chips, magnetic media, MEMS and countless other micro/nano devices.

Surface chemical patterning is a relatively new research field. Instead of etching surfaces to create geometric contrast patterns, chemical patterning is used to selectively modify surfaces, forming chemical contrast areas on the substrate. This chemical contrast is useful in various applications. Examples include collecting moisture in air, defining water/liquid movement path on surfaces, assembling colloids or fluorescent dyes to activated areas, selectively immobilizing DNA fragments for biochip applications and developing new bottom-up nanofabrication processes.

For our research, hydrophilic “islands” were created on a hydrophobic surface using two different approaches, shadowmask lithography and nanoimprinting. The engineered islands varied in diameter and spacing, from the micro to the nano level. The islands were then used to grow zinc selenide crystals which were characterized according to their structure and properties, which differ, depending on the pattern used.

Characterization of SAMs on Cobalt and Gold
Leigh Kent Lydecker IV

The incorporation of organic molecules into electronics offers a wide range of functionality for use in devices. In order to discover the potential for use of various molecules, these molecules need to be able to be physically and electrically characterized.

Flip-Chip Lamination (FCL) is a multi-step process that produces test structures that allow us to investigate the electrical properties of molecular junctions. First, a metal is deposited onto a silicon substrate that contains a fluorinated release layer. Polyethylene terephthalate (PET) is laminated over the metal surface and the metal layer is “template stripped”, revealing the smooth underside of the deposited metal which is ideal for self-assembled monolayer (SAM) formation. Different molecular monolayers are then formed in solution onto the smooth metal surface and pressed to a wafer of hydrogen-terminated silicon to form a silicon-SAM-metal "sandwich" structure that allows for electrical measurement.

For my project, we utilized FCL to investigate well-known molecules on complex substrates, and complex molecules on commonly studied substrates. As a complex substrate, cobalt is a ferromagnetic metal and has potential use in spintronic devices, but its use as a substrate for SAMs is understudied. We successfully assembled octadecanethiol (ODT) and mercaptohexadecanoic acid (MHA) monolayers onto Co as shown by X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR). Co-SAM-Si junctions will be electrically characterized and compared to Au-SAM-Si junctions in order to understand the role of SAM/Co. For complex molecules on a commonly studied surface, we attempt to form molecular layers by click chemistry onto a gold substrate. Results from FTIR and XPS will be presented which show the successful incorporation of a molecular layer by click chemistry.

<u>State University of New York Binghamton</u>

Massively Parallel TDDB Test Systems
Lei Cao

Time-dependent dielectric breakdown, TDDB, is a failure mechanism in MOSFETs when the gate oxide breaks down due to long-time application of a low electric field. It is caused by formation of a conducting path through the gate oxide to the substrate due to a tunneling current when MOSFETs operate close to or beyond their maximum voltages. Building this system allows us to measure the TDDB of tens to hundreds of devices at the same time.

My task on this project started with designing the system and performing circuit simulations. After I finished selecting components (mainly op-amps), I simulated different situations that could happen during measurements. When one or more test devices breakdown, large amounts of current will be drawn from the op-amp providing the stress voltage, which will cause the stress voltage to drop. From the simulation, we want to see if the op-amps are capable of handling this drop. The result shows that the op-amps I selected are able to handle these situations so that system performance will not suffer much when they happen.

My next task was to design a temperature PID control circuit. I started by designing schematics and running simulations. After that, I drew the PCB layout and had it fabricated. I assembled the board and wrote the program for the PID controller. The purpose of making this board is to provide the high temperature needed for the stress test.

Now I am working on the code and testing the PID board.

Spin Current Polarization in Amorphous CoFeB Measured via the Spin-Wave Doppler-Effect
Jason Gus

The electron's spin is the root of magnetization in ferromagnets, and if we move the spins by flowing a current, we can actually move the magnetization. In our experiment, we measure the magnetization motion and use it to calculate the current polarization of the material. The current polarization is directly related to the difference between the currents carried by up-spin electrons and down-spin electrons and it tells us how easily we can move that magnetization. The current polarization is important for the performance of memory devices and the efficiency of field sensors. In our experiment, an antenna inductively launches electromagnetic waves and spin waves into a ferromagnetic wire with a current applied. A spin wave is a "wiggle" in the magnetization that propagates as a result of magnetic interactions. The speed of propagation is shifted by the current-driven drifty velocity of the magnetization, resulting in a Doppler shift of the spin wave's frequency of $\Delta f = v/\lambda$ where λ is the spin-wave wavelength and $v = J\mu_B P/(eM_s)$ is the spin drift velocity, which is a function of the current density J, the magnetization M_s, and the spin polarization of the current (P). We have optimized this process and have used this spin-wave Doppler technique to measure and compare the spin current polarization (P) of Co72Fe18B10 before and after thermal annealing.

Measurement Systems for Additive Manufacturing Processes
Keith Hebenstreit

Additive Manufacturing (AM) is defined as the process of joining materials from three-dimensional (3D) model data, usually layer upon layer, as opposed to subtractive manufacturing technologies [1]. The customized, complex, high value parts produced using AM are going to revolutionize the aerospace, medical, and dental industries as well as provide the United States the manufacturing presence it no longer has from producing commercial commodities. The impact of AM is predicted to be so great that people are calling it "The Next (Third) Industrial Revolution" [2].

The National Institute of Standards and Technology (NIST) has a Direct Metal Laser Sintering (DMLS) Machine that additively forms parts by melting and fusing individual layers of powdered metal. Being a revolutionary process in its early stages, DMLS has abundant room for improvement. Uncertainties with the process and the machine itself are hindering it from more wide-spread adoption in commercial use for improving parts that affect human lives, like those in an airplane or a medical implant. It is NIST's research goal to develop the measurement methods and resulting standards that will allow AM and DMLS to propel the United States into this manufacturing revolution.

The uncertainties mentioned above include laser beam path, dimensions of internal features, melt pool size and geometry, point temperature gradients, and porosity of fabricated parts. This talk will address the design and implementation of a high speed camera for Machine Vision (MV), an infrared imaging system for Thermal Imaging (TI), and an ultrasonic transducer for porosity measurements (UT) that will allow for *in-situ* data collection and machine calibration to further understand this process. The talk will also address measurements that were done on the DMLS machine as well as experiments conducted on a polymer based additive machine recently purchased by NIST called the MakerBot.

[1] ASTM, F2792-0e1: Standard Terminology for Additive Manufacturing Technologies. (2010).
[2] L. Rhoades, The Transformation of Manufacturing in the 21st Century, The Bridge. 35 (1), (2005).

A Low-Cost 3D Safety System for Robot Applications
Evan Kesten

The development and implementation of machine vision has become an important aspect of robotic safety systems. Current safety systems use line-scanners to view the ranges of objects in a single plane, but are not capable of capturing full 3D images. Until the development of the Kinect by PrimeSense, systems that could capture full 3D images were too expensive for use in safety applications. The low cost of this new sensor in addition to its broad functionality makes it a viable option for the replacement of line-scanners.

In this project, we developed methods for the use of the Kinect sensor as a low-cost, full 3D range-imager in robotic safety applications. We also created a simulated Kinect using the Unified System for Automation and Robot Simulation (USARSim) to examine the ability of the sensor to perform in various environments. The Robot Operating System (ROS) was used in conjunction with both the real and simulated sensor to handle, analyze, and process the incoming data.

Lastly, we performed performance evaluations by testing the sensor in both the real and virtual worlds to assess its limitations and establish the drawbacks of using this low-cost sensor over current, existing systems.

Charge-Based Capacitance Measurements and SCM on a Chip
Timothy Kohler

As semiconductor technology continues to shrink, measuring on-chip device capacitances have become increasingly difficult. Integrated circuits make use of transistors at the nano-scale with capacitances in the atto-farad range(10^{-18}). Accurately measuring these ultra-small capacitances is necessary to write model circuits in computer aided simulations. Computer models can be developed to simulate the behavior of nano-scale devices, for that we need measurement techniques to measure capacitances in the atto-farad range. Charged Based Capacitance Measurement (CBCM) is such a technique to achieve that goal.

CBCM is a differential technique to measure small capacitances. The rationale behind CBCM is to measures the average current necessary to fully charge (or discharge) the capacitance of interest at a fixed bias and at the fixed rate. To obtain the average current a differential measurement is taken between two identical branches in the circuit. The load branch contains a parasitic capacitance along with the load capacitance while the other branch acts as a reference, containing only the parasitic capacitance. By subtracting the reference branch current from the load branch current the load current is known, since the parasitic capacitance is common in each branch. The load capacitance can then be calculated since capacitance is equal to the average current divided by the voltage applied multiplied by the frequency. While the differential measurement is accurate, the method is limited by charge injection from the switching transistors and stray capacitances from the wires and bonding pads.

My project goal was to research CBCM, determine the equipment needed to make accurate measurements, write scripts to control the measurement and to test the CBCM circuit on a chip. Tests were done to see if present measuring instrument modules could measure low capacitances.

After failing to measure femto farads it was concluded that the present modules would not be sufficient. Scripts were then written to easily control the different measuring modules and input signals to the CBCM circuit. The chip is currently being probed and results are on the way.

Investigations of DNA Transport in Nanofluidic Slits
Ryan Lake

MEMS lab-on-a-chip technology for the preparation and characterization of biological samples is a high value growth area for the semiconductor industry, simultaneously addressing urgent national needs for advanced manufacturing and improved healthcare. Nanofluidic devices have enormous potential for integration into lab-on-a-chip systems to manipulate and measure biological molecules, such as DNA, at relevant nanoscale dimensions. However, the physical behavior of DNA molecules in nanofluidic confinement must be better understood in order to establish engineering design principles, which are necessary to implement such devices. In particular, the slitlike confinement of DNA is a topic of enduring interest in soft matter physics and current controversy in nanofluidics.

The specific purpose of this research activity is to study the physical behavior of individual DNA molecules in the Odijk regime of strong nanofluidic slitlike confinement as influenced by simultaneous hydrodynamic and electrokinetic transport. The effects of a Poiseuille flow on DNA conformation in strong slitlike confinement are not well understood. Any DNA deformation from equilibrium due to shear forces has not been characterized at slit depths $d<\approx 100$ nm. The relation between hydrodynamic and electrokinetic drive in this regime of nanofluidic slitlike confinement is also of interest. Multilayer nanofluidic devices with nominal slit depths of ≈50 nm, ≈100 nm, ≈250 nm, and ≈500 nm have been fabricated and characterized, and an experimental procedure and apparatus has been designed. This research activity will encompass more time and effort to complete and will be continued at Binghamton University by Mr. Ryan C. Lake under the supervision of Dr. Stephen L. Levy.

Through Silicon Via (TSV) Reliability Monitoring System
Adam Morgan

Our daily lives are now completely surrounded with electronics, from computers to smartphones. These devices are continuously getting smaller and faster as it seems that each month brings about something new, thanks to Moore's Law. Yet, Moore's Law seems to have reached its end. Circuits can only become nanometers in scale as you approach the atomic level. A new wave of System-on-Package (SOP) microchips has taken over to continue to allow these devices to become more sophisticated. The rise of the 3D microchip has begun.

SOP designs allow for increased functionality within a single package. No longer are multiple chips needed to achieve different operations. SOP enables all branches of circuit design to be layered one on top of the other, all within one stacked microchip. The main component of these circuits that makes SOP's possible is TSV. TSV's are what allow the electrons to flow back and forth between the multiple layers of a 3D circuit. Performance is faster and more efficient compared to chip-to-chip communication. However, if this new 3D circuit technology is to become popular, then designers and manufacturers need to know its capabilities, limits, and reliability in order for a transition into the "More than Moore's Law" era to be complete. Our goal is to determine the reliability aspect of these new circuits, especially the TSV's, by measuring and analyzing their lifetime over periods of induced heat and current stress.

My project was to develop data collection environments using an automatic data acquisition tool with a graphical user interface that would allow researchers to configure experimental parameters, view the data in real-time on plotted graphs, and save the data in a clear format for later analysis. I also aided in the setup of our experiment that uses Kelvin four-terminal measurement techniques. Originally, we began testing only one device. Currently, we are on track to test 10 devices at once in order to speed up data collection. Overall, we want to extract Thermal Coefficient of Resistance (TCR) curves from each of these devices at different temperatures and currents. Reliability information on these TSV's can then be extracted using Black's Equation. This could give us insight into the likely occurring electromigration caused by thermal and current stress. Initial data collection proved promising as we captured exponentially increasing resistances. However, in order to come to a valid conclusion about how reliable these TSV's are, more device-testing under a multiplexing scheme is required. Hopefully, similar informative results will occur that will allow researchers to grasp the true reliability aspect of this TSV technology and its effects on future 3D microchip design.

Benefits and Costs of Energy Efficiency in New Buildings
Brian Presser

In the modern world, few commodities are more important than energy. With fuel prices on the rise and the threat of global warming ever-present, the push for buildings to become more energy efficient has grown stronger than ever before. The energy efficiency of a building is a product of numerous interacting factors, including its construction materials and equipment. In addition, the location of the structure and the prevailing building codes play a major role. The goal of my project is to create a database of energy consumption, life-cycle cost, and environmental impacts for new buildings with varying levels of energy efficiency. Known as Building Industry Reporting and Design for Sustainability (BIRDS), this resource will contain information for both new construction and operation of buildings.

Creation of the BIRDS database required an effective way to create and execute large quantities of whole building energy simulations. As a result, a large part of my work at NIST has been to write code to produce and expand building simulation files for numerous designs. This summer, I expanded 30 generic residential prototype files to account for differing state building energy requirements and climate zones. After simulating each of the resulting 6900 files, I estimated the construction costs for each building design.

Expanding on work from last summer, I wrote code to estimate the environmental impacts for each of the prototype commercial buildings in the BIRDS database. All of these estimates were made using a cradle-to-grave approach. This means that the impacts of a particular building were considered through all stages of life, starting with raw material acquisition and ending with disposal.

My talk will discuss the approaches employed to incorporate simulation results, construction cost data sources, and environmental data sources into the BIRDS database. I will also discuss the impact that my contributions to the BIRDS database may have on national building practices.

Sustainability Analysis of a Die Casting Process
Megan Watkins

Manufacturing plays a major role, accounting for approximately one-third of the total energy consumption in the United States. Sustainable manufacturing has therefore become an area of increasing interest, as companies look to reduce their manufacturing footprint and become more environmentally friendly. A science-based methodology, known as sustainability characterization, is a new idea that will give companies a way to "measure" the sustainability of their manufacturing processes. This methodology was used as a baseline for this project to evaluate the sustainability of die casting unit manufacturing processes. More specifically, sustainable performance indicators were determined and a way to theoretically model sustainability, based on energy use, was investigated. Using the fundamentals of die casting processes, corresponding input-outputs were mapped in terms of sustainability and equations to theoretically calculate the energy used in a die casting machine were identified/formulated. The theoretical energy equations provide a baseline for creating an information model that will eventually lead to creating a science-based methodology standard for sustainable characterization of unit manufacturing processes.

State University of New York Buffalo

Characterizing the Structural and Rheological Properties of Triblock Coplymer Solutions
Michelle Reele

The understanding of the structural and dynamical properties of triblock copolymer solution are the key for many applications, such as shampoos, drug delivery, fuel cell membrane, surface modifications. Pluronic L64, $(\text{polyethylene oxide})_{13}$ $(\text{polypropylene oxide})_{30}$ $(\text{polyethylene oxide})_{13,}$ is a commercial block copolymer. The overall goal of our project is to investigate the bulk and surface properties of this tri-block copolymer solution by using dynamic light scattering (DLS), small angle neutron scattering (SANS), rheometry, and reflectometry. There has been a debate regarding the mechanism of the observed viscosity change in Pluronic L64 aqueous solutions near cloudy point conditions. Here, we use both DLS and SANS to measure the collective motions of micelles in bulk solution and investigate the phase transition close to its cloudy points. Our SANS results indicate that L64 maintains a spherical micelle structure. This refutes the argument that L64 forms worm-like micelles near the cloudy point and suggests that the observed viscosity increase is due to intermicellar interactions. SANS and DLS results will be used in combination with ongoing investigations to establish a link between micellar structure and physical mechanisms for this rheological behavior.

State University of New York Stony Brook

Fate of Carbon Nanotubes in Polymer Nanocomposites Exposed to UV Radiation

James Ging

Because of their novel properties nanomaterials are increasingly incorporated in polymer matrices for a variety of industrial applications. Although a substantial work has been put into the development and study of how nanomaterials can improve existing products, shockingly little has been done to examine how they are affected by environmental conditions such as exposure to ultraviolet light. The current industrial view is if there is a nanomaterial within a matrix, it is safe and would stay there indefinitely. This study seeks to identify if there is a potential for nanofiller release after the containing matrix degrades due to UV exposure.

Epoxies are used industrially in composites, coatings, and adhesives. Recent research showed that these materials gain new properties such as increased strength and resistance to ultraviolet radiation when carbon nanotubes (CNTs) are introduced into them. We are studying what happens to these nanocarbon fillers while the epoxy matrix breaks down and how it affects properties of the nanocomposites. To do this, we made samples of unfilled epoxy, nanocomposites of epoxy and unmodified multi-walled CNTs (MWCNTs), and nanocomposites of epoxy and amine-functionalized MWCNTs, then exposed them to long-term high intensity UV radiation using the NIST SPHERE environmental chamber. We then examined their mass loss, surface chemical properties, and surface morphology of the nanocomposites over time using a variety of analytical techniques, including FTIR spectroscopy, confocal microscopy, AFM, SEM, dynamic mechanical analysis (DMA), and XPS.

Nanoscale Imaging Using Spectral Domain Optical Coherence Tomography

Julian Hassinger

A central goal of nano-biophotonics is to provide quantitative imaging capabilities of biological specimens on a molecular scale. In recent decades, many optical measurement techniques have been developed to investigate molecular interactions and processes in single cells. For instance, a variety of dynamic fluorescence imaging techniques have been used to measure the effect of malarial infection on the small-scale vibrations of red blood cell membranes. However, fluorescence labeling often causes undesirable perturbation to the biological process of the infection. In this talk, progress toward the construction of a label-free spectral domain optical coherence tomography imaging system capable of studying the infection mechanism at a single cell resolution without perturbation of the sample will be presented. In the system, a specimen is illuminated by a broadband source, and the interference pattern generated by combining the reflection from the sample with that of a reference arm allows for the determination of the position of a reflector within the sample (e.g. cell membranes). Additionally, the phase information contained within the interference pattern can be used to track nanometer scale fluctuations in reflector position. The progress toward single cell imaging capability of this system will be presented via preliminary studies of well-characterized samples. Potential applications of this system in conjunction with an optical trapping system will also be discussed.

Stevenson University

A Vision of the Future
Kristin Giauque

Having a secure cyberspace is critical for today's society. Most of our everyday transactions and processes are in some way involving the Internet. Yet, with the Internet comes threats that aim to steal and possess our secure and confidential information. NSTIC, which stands for the National Strategy for Trusted Identities in Cyberspace, is a program proposed by the Obama administration that will help with enhancing the security and privacy of our information. The main concept of NSTIC is an "Identity Ecosystem." This is an online environment where identities of individuals and organizations are secured and certified because they agreed to standards to obtain and authorize their digital identities. The Identity Ecosystem not only benefits organizations, but individuals as well. This summer, we reviewed proposals from several organizations that projected new solutions and frameworks that would adhere to NSTIC guidelines. We also researched different agencies and groups that would raise public awareness of NSTIC. In this talk, NSTIC and the Identity Ecosystem will be discussed.

Texas A & M University

Controlled Production of Highly Charged Ions in Rydberg States
Maxwell Zhou

Highly charged ions have many interesting applications. Our solar corona has been shown to consist of many highly charged ions and scientists have begun producing these ions in a controlled environment to study and understand them. In this project, we are working to produce one-electron ions in high angular momentum states, called Rydberg states, which can be used to measure the Rydberg constant.

In order to produce Rydberg states of these ions we must first extract fully stripped ions (bare nuclei) produced inside an electron beam ion trap, then transport them a beam-line to an experimental apparatus wherein they can be isolated, manipulated, and observed in a Penning trap. Ions emerging from the EBIT are slowed electrostatically while entering the Penning trap, then captured by pulsing closed the Penning trap upon arrival.

Recently, a compact Penning trap using two NdFeB magnets at room-temperature was used to capture and confine highly charged ions, opening new possibilities for manipulation and spectroscopy of highly charged ions in a controlled environment. We are now developing a rubidium oven that can be attached to the side of the Penning trap. A beam of rubidium atoms excited by lasers will propagate to the Penning trap and charge exchange with the stored ions. The rubidium atoms are sent into the Penning trap in controlled bursts using a shutter, and then are excited by three lasers at different wavelengths to put the valence electron in a very high energy level so that the stored ion can easily capture the loosely bound electron. This system is almost complete and experiments are about to begin.

Texas Southern University

Fire Proof Foams
Ray Mbonu

Fire is the cause behind several million dollars in damage, approximately 40,000 deaths worldwide and $12.5 billion in property loss, when not properly controlled. Polyurethane foams are used in the cushioning of many consumer and commercial products, it is also one of the many ways fire is helped spread.

To control this we used the Layer-by-layer assembly process to create 1nm thick fire retardant clay coatings. My mixture consisted of a trilayer which is 2 polymers; Polyacrylic Acid (PAA) and Polyethylenimine (PEI), and 1 clay; Layered Double Hydroxide (LDH), in different concentrations, ratios, and trilayer numbers. After coating, the foams were flame tested using a cone calorimeter, where they were set on fire under a controlled machine that measured different properties, such as the heat release rates. The results were compared to that of polyurethane foam without a coating, which was used as the control in the experiment.

After the test was completed we observed that LDH burned well in comparison to the control. The several coated foams showed lowered heat release rates during burning. Also the coated foams still "existed" after testing as to the controls that burned completely away, which is what we are trying to avoid from happening. The best coating ratio was low polymer to high clay.

In this talk we will discuss fire damage and retardants, the layer-by-layer process, the polymers and clay used, coating concentrations, the cone calorimeter test and the properties it measured, and compare results in detail.

Characterizing the Safety and Efficacy of Fluoride Dental Varnish with Applications for Standards Development and Clinical Relevance
Richard North III

Fluoride dental varnishes were analyzed to validate a standard method for measuring the total fluoride content of fluoride-releasing varnishes. The purpose of the varnish is to stop cavities from continual growth or to completely reverse formation. There are wide varieties of fluoride-releasing compounds in a dental varnish, they may contain sodium fluoride (NaF), sodium monofluorophosphate (MPF), amine fluoride (NH_3-F), stannous fluoride (SnF_2), or any combinations of these fluoride compounds; the evaluation method must be capable of analyzing any fluoride present. This validation method is part of a multi-lab International Standards Organization (ISO) standard drafting process. The ISO method needs to accurately determine the quantity of total fluoride in any fluoride varnish as dispensed from the commercial container in an accurate and preferably simple manner. Fluoride measurements were performed by ion selective electrode (ISE) properly diluted within total ionic strength adjustment buffer II (TISAB II). Fluoride ISEs are constructed from single-crystal sections of rare earth fluorides and respond to fluoride ion activity over five orders of magnitude while showing a high selectivity for fluoride over other common anions. Results from the study show that the digestion and measurement techniques proposed are repeatable and suitable for ISO method adoption. The methods were also adapted for the measurement of fluoride varnish release and fluoride uptake into a hydroxyapatite disk (the mineral form of dental enamel).

Towson University

Windows Phone Malware Detection
Michael Smith

As smartphones continue to become more incorporated in our daily activities, the amount of sensitive data that these phones access increases. At the same time, criminals are constantly attempting to exploit smartphone applications to access this data and create a profit for themselves. This malware, malicious software, is becoming harder to detect and continues to populate smartphone application stores. Unknowingly to the user, seemingly harmless applications could be accessing sensitive information or performing unwanted actions on the phone. Typically, an initial evaluation is performed to determine if an application may be malicious before entering an application store. However, malware continues to become more sophisticated and harder to detect. If malware can elude this initial evaluation, detecting and removing it is often a slow process that could take several months. Meanwhile, the malware is free to continue its malicious activity on unknowing users smartphones.

To assist in preventing and detecting malicious applications specifically on Windows Phone, we have developed a process that extracts and analyzes free applications from the Windows Phone Marketplace. The process involves automatic retrieval of applications from the marketplace and an analysis that determines whether an application is more likely to be malware by comparing its activity to known harmless and malicious activity. One key element of the process involves extracting domains that the application interacts with and evaluating how suspicious those domains are based on its known characteristics. Ultimately, each application will be given a rating on how likely it is to be malicious and will be stored in a database to aid those interested in mobile security and the detection of smartphone malware.

Tulane University

Frequency Stabilization of a Continuous Wave Dye Laser for Use as a Quantum Memory
John Ortmann, Jr.

A common challenge faced by those using lasers for high-precision measurements and experiments is the challenge of laser frequency stabilization. An ideal laser emits light at exactly one frequency. Of course, this is never true in practice, and a realistic laser instead emits light in a relatively narrow range of frequencies which tends to wander to some degree over time. In this work, we attempt to stabilize the frequency of a 606nm continuous wave (cw) dye laser through the fabrication of a piezoelectric-actuated mirror system consisting of a mirror attached to a piezoelectric transducer (PZT), which is in turn attached to a massive copper and lead mounting structure (much like the work presented in [1]). This PZT actuator is then used in conjunction with a Pound-Drever-Hall (PDH) scheme [2] to monitor the laser's frequency output and continuously adjust the length of a cavity within the laser accordingly, so as to minimize the change in laser frequency over time. The ultimate goal of this research is to make progress toward the realization of a solid state quantum memory.

In this talk, I will discuss the design of our PZT actuator as well as some preliminary results obtained after its installation in the laser. Also, I will present some basic results obtained from performing finite element analysis (FEA) on a model of the actuator. For background, I will present a theoretical description of a simplified scheme for a solid state quantum memory as well as an explanation of the PDH scheme.

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[2] R.W.P. Drever *et al*., "Laser phase and frequency stabilization using an optical resonator," Appl. Phys. B: Photophys. Laser Chem. **31**, 97-105 (1983).

Modeling Helium 3 Scintillation with MCNPX

Elizabeth Scott

Accurate neutron fluence measurements are critical for beam-based neutron lifetime experiments and the calibration of the emission rate of NBS-1, the NIST-maintained standard Ra-Be photoneutron source. To address these issues we are building a Helium 3 counter that will completely absorb a cold neutron beam and permit the counting of the resulting scintillation events in He3 with near 100% efficiency in order to measure the neutron fluence with 0.1% accuracy. In order to model the neutron capture in He3 and the scintillation we are using a program called Monte Carlo N-Particle eXtended (MCNPX). This model will help determine possible systematic effects with the geometry of the experiment and sources of uncertainty. In this talk I will discuss the physics and set up of the experiment, how to properly model it in MCNPX, and the results found from this modeling.

University of California Berkeley

Optimal Broadcast and Spread of Information In a Network with Limited Resources

Jason Wu

Efficiency is an issue to be considered when studying networks. One way to look at efficiency is how fast information spreads across a network. Specifically, a network can be represented with an undirected graph using nodes and edges, which the information must spread along. Ideally, one can simply give information directly to every node, but assuming a resource constraint where only K nodes can be informed, the rest of the nodes must undergo a random walk process to "reach" the information in those K nodes. In such a case, it is preferable to choose the K nodes such that the expected time by the rest of the nodes to obtain information from those K nodes (the mean first passage time) is minimized. While it is straightforward to calculate this mean first passage time for a given subset of nodes, there is no systematic way to find the best subset of size K without doing the calculation for all possible subsets. The investigation of this problem looked at various ways to make finding optimal sets easier by attempting to characterize the optimal set and by attempting to make smaller the number of subsets to be considered.

University of California San Diego

Structural Studies of Multiferroic Thin Films
Lisa Krayer

Magnetoelectric materials have interactions between magnetic and electric degrees of freedom, and these materials have prompted vigorous study due to their rich physics and potential for device applications. The ability to change the direction of the magnetic moment in a material by applying an electric field at room-temperature is one example of a multiferroic magnetoelectric that could revolutionize data storage devices. We present structural studies of magnetoelectric films with a perovskite structure in order to elucidate the correlation between their structure and ferroic orders towards optimizing the magnetoelectric effect. Specifically, $BiMnO_3$ synthesized in bulk has been observed to have both ferroelectric and ferromagnetic orders simultaneously, while thin film $BiMnO_3$ on $SrTiO_3$ has a reduced magnetic moment that lessens the ferromagnetism in the crystal, which may be due to stress induced on the film by the substrate. A combination of diffraction and reflectometry, from neutron and x-ray sources, is used to investigate the thin film structure of $BiMnO_3$ on a $SrTiO_3$ substrate, which we correlate to microscopy, magnetization, and polarization measurements.

University of Colorado at Boulder

Exploration of Big Data Technologies to Scale Up Cancer Prognosis System
Stetson Zirkelbach

Big Data is becoming an increasingly important topic in academia and the sciences. In many fields the data sets are growing so large that analysis can no longer be done easily on a single machine. This severely impacts the information that can be gathered from the data.

This project was focused on determining the best approach for extending a cancer classification technique to handle large cancer patient data. The investigation focused on two open-source Big Data platforms, Hadoop and HPCC, and addressed software engineering issues that scientific users are likely to encounter. While neither platform is a perfect solution, Hadoop offers some advantages to scientific Big Data researchers and is ultimately the recommended platform for further development of the cancer prognosis system.

University of Delaware

Are You Being Greenwashed
Anna D'Alessio

Sustainability has become a growing issue especially in the manufacturing industry. Sustainability indicators measure the impact of manufacturing processes and products. There is a variety of indicators but no one authoritative set, therefore we use coarse grain indicators. Along with the indicators, manufacturing information models need to be defined in order to develop a methodology which can identify relationships between sustainability indicators and manufacturing information. A product category rule (PCR) is an example of the methodology specifically designed for the carbon footprint indicator. However, other sustainability indicators do not have such a methodology due to the lack of understanding of relationships between sustainability indicators and manufacturing information.

This study developed a set of manufacturing information requirements for sustainability indicators. The focus was on sustainability indicators related to energy and materials. To measure each indicator, we had to know, within the manufacturing process, where it was to be measured. A material flow analysis was used to determine the flow of materials and where the indicators belonged. A PCR for transport equipment was used to determine the information necessary to calculate the indicators. Information requirements defined in this study can be used to develop manufacturing information models which can track sustainability impacts throughout the manufacturing process.

The Effect of Ambient Conditions on Solution-Cast Organic Photovoltaics
Jacqueline Johnson

Solar energy is becoming an increasingly popular energy choice because solar photovoltaics (solar cells) can harness the nearly-infinite power of the sun without releasing pollutant emissions. Organic photovoltaics (OPV) technology is an emerging alternative to traditional solar cells. OPV uses polymers as semiconductors, which permits fabrication by solution coating methods that are less expensive than traditional inorganic semiconductor processing. Polymer-fullerene solutions are cast onto flexible conducting substrates to create the bulk heterojunction (BHJ) light-harvesting layer of the OPV. The coating process determines the structural and electrical properties of the BHJ film, but processing-performance guidelines have been difficult to develop because the results are sensitive to a large variety of processing variables which must be controlled. In this work, we automated several aspects of the coating process and studied how the BHJ films form under various controlled ambient conditions, such as substrate and solution temperature, convection, and solvent partial pressure. The resulting morphology and crystallinity of the films were studied using spectroscopy and microscopy. Several variables exhibit clear impacts on BHJ film structure that can be used to construct processing-performance guidelines for this promising new solar power technology.

University of Maryland Baltimore County

Construction and Testing of the Next Generation Ozone Standard Reference Photometer
Peter Luu

Ozone is a powerful oxidizing agent that damages many materials, respiratory systems, and plant tissue. As a pollutant at ground level, ozone levels are monitored at air monitoring stations worldwide by commercial instruments. A worldwide network of NIST SRPs (Standard Reference Photometers) acting as primary ozone standards is used to calibrate these commercial instruments. Ultimately, theses ozone calibrations are traceable to NIST nationally and the BIPM (Bureau International des Poids et Mesures) internationally.

Each SRP contains a pneumatics module, an optical bench, and an electronics module. The pneumatics module generates ozone at varying levels and sends this gas sample to guest instruments being calibrated and the SRP's optical bench. In the optical bench, UV (ultraviolet) light from a mercury lamp is collimated into beams and passed through glass cells containing gas samples to photo-detectors on the other side which measure absorption. The electronic module controls the instrument and interfaces with a computer. Applying Beer-Lambert's Law, the ozone concentration of the sample is determined and compared to guest instrument readings.

The current project involves constructing and testing a prototype of the next generation SRP. This prototype has been constructed to replicate an existing generation SRP with the exception of being built on an optical table. This arrangement allows components to be easily replaced for research purposes. A new electronics module is being constructed to replace the current generation electronics module. The current generation electronics module use a chip that is no longer manufactured prompting an upgrade. In addition, this next generation electronics module can carry out calibrations without being connected to a desktop computer. This electronics module will be tested to observe its effect on ozone measurements. The optical bench is also being experimented on. The collimated UV beam is known to diverge beyond the outer diameter of the glass cells and be carried by total internal reflection to the detector. Various optical configurations using a different aperture sizes, collimating lenses and condenser lenses will be used to reduce the divergence of the collimated beam. The effect, if any, of reduced divergence on ozone measurements will be observed.

Performance Assessments of Tactical Handheld Android Applications for Warfighters
Matthew Newcomer

The Defense Advanced Research Projects Agency (DARPA) has been working for several years to develop and field tactical handheld applications running on Android-powered devices to the US military. These devices have been used in Afghanistan by US Soldiers for over a year now and are regularly met with a positive response. Some Soldiers have explicitly stated that the devices have saved their lives during combat situations.

The NIST evaluation team has a core expertise in evaluating advanced technology where some members have extensive experience in assessing user-interface. NIST's role in this effort is to lead the evaluation of these tactical applications. This includes identifying errors and faults in addition to offering suggested improvements. Extensive testing is done on the devices where the data is provided to the DARPA sponsor for review. This information aids DARPA in making informed decisions as to whether or not an application is ready to be field.

I have had two tasks this summer. The first is creating test plans that exercise nearly every feature of the handhelds under more operational scenarios (as compared to testing in an office). Extensive data sets will be gathered once these test plans are exercised. This data will provide the developers with richer information better enabling them to make improvements in the applications. This task required me to do some research on test methodologies, including those targeting handheld devices. My second task is simply testing the handheld, including regression testing. Regression testing is where you test an unchanged function or feature in a new application version to determine if unrelated changes have had negative consequences.

Measuring Electrochemically-Induced Oxidative Damage in DNA
Mofiyinfoluwa Obadina

Exposing mammalian cells to oxidative stress can result in structural changes to DNA, including strand breaks. The ability to measure such damage can provide information about the threshold for DNA damage as well as the susceptibility of certain DNA sequences in the presence of oxidation. An effective method of measuring this process is capillary electrophoresis (CE) where the DNA is driven, with high voltage, through a polymer gel solution in a capillary tube. As this occurs, the fragments are separated based on size such that smaller fragments run through the gel quicker; this results in an electropherogram where the CE peaks indicate fragments of increasing sizes. My project involves conducting DNA electrolysis under potentiostatic conditions. Bulk DNA electrolysis was performed using high surface area reticulated vitreous carbon electrodes. Calf thymus DNA and oligonucleotide standards were oxidized in the electrochemical cell and their damage assessed using CE. The DNA treatment was performed at a fixed potential ranging from 1-3V vs AgCl reference electrode for 1-2 hours. The CE measurements were performed using a Beckman P/ACE 5510 and an ABI PRISM 310. So far, the results have been consistent with our hypothesis that an increase in oxidation potential and time increases the amount of fragmentation. The next step will involve using sequence standards to determine which regions of DNA are more prone to oxidation.

Simple Analysis of Biometric Matchers
Lael Rayfield

What are biometric matchers? In Forensic Science, biometrics refers to technologies that measure and analyze human body characteristics, such as DNA, fingerprints, eye retinas and irises, voice patterns, and facial patterns, for authentication purposes. Biometric matchers compare a person's features against stored biometric features in a database to see if the computer can find a match and identify the subject. Modeling the performance of the automated matchers is important for recognizing abnormal behavior in test results, and predicting performance of matchers when the size of the database is greatly increased. In this talk I will present the results of comparing two different functions that model the performance of biometric matchers: 1) experimentally measured Cumulative Match Characteristic (CMC) curves; 2) and best-fit curves produced by the Power-law Distribution.

Assignment of Wyckoff Positions for Entries in the NIST Metals Database
Donald Richardson

The NIST Crystallographic Databases (NIST Crystal Data, NIST Metals Structural Database, and FIZ-NIST Inorganic Crystal Structure Database) provide researchers, diffraction instrument vendors, and materials developers with an invaluable tool for materials design and phase identification. One example is to use them for the creation of "Crystal Phase Identifiers" for uniquely identifying crystalline materials. However, some entries in the current Metals Database would be more useful if we could supply the missing information on Wyckoff positions. These positions tell us which sub-group of symmetry operation matrices is needed to generate a set of "equivalent" atoms in a crystal structure.

In this project, our goal was to generate the missing "Wyckoff position information". To accomplish this objective, we cross checked the atomic coordinates of each structure with the *International Tables for Crystallography*. This cross check allowed us to assign the appropriate Wyckoff letter, multiplicity, and site symmetry for each structure. The assignment of the appropriate "Wyckoff position information" generally involves generating a set of symmetrically equivalent positions after determining the correct space group setting, and matching with the Wyckoff position listed in the *International Tables for Crystallography*. However, in certain cases, difficulties were encountered due to the evolution of certain standards and conventions over the past decades. For these difficult cases, our work consisted of the determination of the appropriate conventional space group and unit cell setting by analyzing the original data and published editorial remarks.

Optimization and Modeling of Metal-Oxide-Semiconductor (MOS) Photoelectrochemical Cells

Nathan Smith

Solar energy represents one of the most promising and potentially useful fields in terms of renewable energy and thus the importance of developing and improving solar cell designs and technologies is extremely high. Photoelectrochemical cells are one of many innovations on the concept, and often utilize the classical method of gathering electricity from light via the photoelectric effect and then using that electricity to dissociate water to form hydrogen for subsequent electricity generation by fuel cells. This research focuses on the use of metal-oxide-semiconductors (MOS) with metallic Pt collectors on an oxide-covered p-type Si bulk. In order to maximize the energy harvested from the sun many aspects of semiconductor physics must be analyzed and optimized in these solar cells. Various design considerations such as direction of illumination, the geometry of catalytic collectors, the nature of the tunneling oxide layer, and the incorporation of a multiple junction (tandem) structure. Using MATLAB and the Python-based FiPy engine, the influence of changing these various cell design parameters can be analyzed and then tested on solar cells created in the laboratory. The trends determined will hopefully allow the development of more advanced and efficient PV and PEC cells. Silicon is the primary element being evaluated in the work due to its low cost, large elemental abundance, and ability to efficiently harvest solar energy. A thin SiO_2 layer serves as the tunneling oxide and the collectors are made by depositing platinum on the surface via electrodeposition (for smaller sizes) or a shadow mask technique (for larger sizes). The sun delivers a huge amount of energy to the Earth's surface every day (180 W/m^2), most of which is absorbed and dissipated instead of being put to proper use; improving PV and PEC technologies can change this.

Video Interpolation with FFMPEG VidAT Tool

Jeffrey Turner

The VidAT tool was developed in conjunction with the ClearDTScorer to place bounding boxes around objects of interest. The ClearDTScorer identifies coordinates and dimensions of the boxes; as well as color coding them depending on how the system identifies them. This is a somewhat time-expensive procedure and cannot realistically be done to every frame of a video. The VidAT tool can draw bounding boxes onto the video wherever identified by the tracking log provided by the ClearDTScorer, and when one in every fifteen frames is evaluated there was a significant improvement in processing time of the video. The tradeoff of this sparse frame evaluation was poor video quality in the transitions of the bounding boxes, which appeared to "jump" every half-second. The enhancement to the VidAT tool interpolates the data in between video frames, and produces a modified tracking log that can be drawn by the filter without the costly process of evaluating every individual frame of the video. VidAT is being developed as a video filter for the open source FFMPEG project, and is being designed to conform to the specifications so that it can be used in conjunction with other video filters.

University of Maryland College Park

Characterization of the Dose-Rate Effect for Alanine Ionizing-Radiation Dosimetry
Yasamin Abbaszadeh

The NIST-developed alanine dosimetry system is firmly established as a transfer service for high-dose ionizing-radiation dosimetry and is an integral part of the internal calibration scheme supporting services for healthcare and consumer materials manufacturing. Recently, a previously unknown absorbed-dose-dependent, dose-rate effect was discovered for the alanine system. Though the potential impact of this effect is anticipated to be minimal for NIST's customer-based transfer dosimetry service, much great implications may be realized for international measurement comparisons between National Measurement Institutes.

Currently the data describing this effect is very limited because NIST gamma-ray sources are fixed rate. The University of Maryland College Park Gamma Cell is designed in a manner that allows a broad range of rates to be tested. An optical bench was used to create an array of irradiation geometries with dose rates that varied with distance. Alanine dosimeters were measured at these calibrated irradiation geometries. The goal was to fully define the dose-rate effect for a complete range of rates. Knowledge of the dose-rate effect will improve the quality of international comparisons with national labs from other countries and will enable NIST to predict at what date their calibrated gamma sources will need to be replaced.

DNA Self-Assembly on 1-D and 2-D Carbon Lattices
Nicholas Arnold-Medabalimi

A key problem in the processing and purification of single walled carbon nanotubes (SWCNTs) is their hydrophobic nature. By wrapping SWCNTs with DNA we disperse SWCNTs in water making them easier to process. The exact nature of the binding of DNA to SWCNTs is unknown due to the one dimensional nature of nanotubes which hinders analysis. Recently it has been reported that under certain conditions DNA forms ordered structures with trigonal symmetry (120° angles) on graphite. Because of the similarity between the carbon lattice of graphite and SWCNTs, we can investigate the properties of DNA on graphite to learn about its structure on SWCNTs.

From testing the reported conditions we discovered that the creation of DNA structures on the surface of graphite may have been induced not by the warmth of the system as claimed but rather by the electrostatic forces that are created as DNA binds not only to the primary surface but also the back side of the substrate. Nevertheless, we have confirmed that DNA has a preferred trigonal symmetry on graphite which is likely to be true on SWCNTs as well. Having determined the appropriate conditions for DNA assembly, we investigated the possibility that SWCNTs would exhibit similar behavior. Under similar conditions SWCNTs form ordered domains with trigonal symmetry. In addition observations have shown a phenomenon where DNA bound to the SWCNTs would strip off and bind the graphite, sometimes creating ordered structures. This implies that DNA has a higher intrinsic affinity for graphite than for SWCNTs.

Dimensional Characterization of Si Nanogratings Formed by PS/PMMA Directed Self-Assembly

Elizabeth Ashley

Block copolymers (BCP) are known to phase separate into distinct morphologies including spheres, cylinders and lamella as a function of composition. If a lamella forming BCP is deposited on top of a patterned substrate consisting of lines of alternating chemical composition the BCP will align with and amplify the underlying pattern. This is referred to as directed self-assembly (DSA). Block copolymer DSA is of particular interest to the microprocessing industry because of its potential for forming patterned nanofeatures below the current resolution limits. Successful DSA techniques will enable a decrease in the feature size of semiconductor devices, allowing for greater memory and functionality in electronic devices. In this study, the accuracy of the PS/PMMA alignment as the pitch of the pattern deviates from the natural pitch of the polymers is explored.

PMMA was removed, and PS was used as a mask for etching the Si wafer. The structure of the nanogratings formed were characterized using small-angle x-ray scattering (SAXS). Using a stacked trapezoidal model to simulate the dimensions of the grating, a MATLAB algorithm was written to model the scattered intensity in the Qx and Qz directions for each sample. By fitting the SAXS data to the simulation in MATLAB, our group was able to determine the dimensions of the Si nanogratings. AFM and SEM measurements were made on samples at varying stages of development to confirm the accuracy of the pitch values obtained by SAXS.

Correcting Substrate Warp for X-Ray Reflectometry

Pavan Bhargava

Reflectometry is a technique used mainly to determine the depth profile of thin-films. The measurements are made assuming that the sample is totally flat and that all reflection is specular. However, the thin wafers used as substrates are often warped and act as curved mirrors that distort the reflected beam and alter the reflected intensity. This effect varies over the entire range of measurement angles, and must be accounted for to ensure accurate data fitting.

Two approaches to correct for this were taken: creating a sample holder that pulls the wafer down against a flat surface, and developing a measurement procedure and mathematical model to correct for the effects of warp in software. The vacuum system includes a very flat quartz block on which the wafers sit. The block was drilled with several holes to transmit pressure from the vacuum pump to the bottom of the sample and pull it flat against the quartz. The success of this device was evaluated using x-ray reflectivity measurements of the warp before and after application of the vacuum.

In order to develop a mathematical model to correct for the warp, the x-ray beam was first well characterized. The effect of sample warp is approximated as a convolution of the beam with a Gaussian shaped warp distribution. By measuring the spread of the beam with and without the sample, the Gaussian warp distribution was isolated and used to calculate the correction factor as detailed here.

Neutron Diffraction Studies of Reduced Perovskite Iron Oxides

Vikas Bhatia

Metal oxides offer a wide variety of scientific and technological applications and are often studied for their magnetic and electrical properties such as superconductivity and multiferroicity. Explored for their applications in sensors and data storage, multiferroics such as the perovskite $BiFeO_3$ couple ferromagnetism with ferroelectricity.

In this study, the iron oxides $AFeO_3$ (A = Ca, Sr, Bi) were synthesized by solid state reaction. They were then reduced topotactically with calcium hydride to achieve a square-planar or brownmillerite structures. $SrFeO_2$ was then reacted with a variety of ligands to intercalate between the iron oxide layers. The chemical compositions and structures of the iron oxides were characterized with neutron diffraction, a technique that is sensitive to oxygen stoichiometry, crystal structure, and magnetic ordering. The reduction of perovskite transition metal oxides via soft chemical, or *chimie douce*, methods allows one to control bonding and prepare metastable phases. We present results from these reactions and diffraction studies of these metastable iron oxides.

Building Consistent Nanomaterial Ontologies in a Federated Environment

Shir Boger

The current challenge to interoperable data is the development of terms that can be generated in a federated environment and that can be exchanged and understood globally to find related data. Development of such terminology need be web friendly and need be suitable for automated and manual intersection among terms. We propose a rule-based approach to build a vocabulary and ontology to overcome this challenge. A previously developed method called Chem-BLAST (http://xpdb.nist.gov/chemblast/pdb.pl) uses this approach to organize chemical structures into an ontological tree and uses the tree to classify, query, and compare chemical structures. Our proposed study aims to extend this method to text based nanotechnology and cell imaging data. Our approach is to select highly reusable words as roots, which are defined based on popularly used common words, to build ontology. These roots are conjugated to form terms to denote specific entities and these terms are conjugated to form blocks, which are used to define use cases. Rules are based on language development techniques (Latin, Sanskrit) in which a commonly used limited number of roots form a framework to make words on demand. The standardization of the terms used in building the blocks is the framework for building ontologies which can be used to superimpose related data.

Durability of Backsheet Polymers Used in Photovoltaic Applications
Kathryn Connolly

The paucity of standards for quantitatively characterizing the performance and predicting the service life of polymeric materials and components used in photovoltaic (PV) systems hinders the innovation, development, and application of PV technologies. The success of PV technologies will ultimately depend on a clear demonstration of their long-term reliability. Currently the scientific basis to assure the PV products meet the 25-30 years of life-time warranty is scarce. In addition, current standardized test methods used for quantifying long-term reliability of PV polymers do not apply the relevant environmental stressors simultaneously. Therefore, there is little knowledge of the synergistic/antagonistic relationships between the environmental factors. Polymer materials are widely used as the backsheet of PV modules, which provides mechanical support for the module and protection from environmental conditions, such as UV irradiation, temperature, and humidity. The backsheet is a multilayer polymer, which traditionally consists of layers of fluoropolymer, an adhesive known as ethyl vinyl acetate (EVA), and polyethylene terephthalate (PET). The degradation of these polymeric materials in the backsheet will eventually lead to the failure of the PV module. In this study, the durability of PV backsheet polymers is investigated under exposure in dry thermal chambers, wet thermal chambers, and the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) at different temperatures and relative humidities. The exposure methods are designed to be representative of accelerated weather conditions. The chemical, physical, and mechanical degradation of the backsheet polymer over periodic exposure times is analyzed through the use of Fourier Transform Infrared Spectroscopy (FTIR), Atomic Force Microscopy (AFM), Confocal Microscopy, Dynamic Mechanical Thermal Analysis (DMTA), and tensile strength instrumentation. The data collected from the tests will be correlated to the exposure conditions for the samples in order to provide a better understanding of the durability and life-time of PV backsheet polymers which can then be applied to PV product development.

High Resolution Displacement Metrology for Nanomechanical Properties
Luis Correa

Much work has been done in the research and development of nanomaterials in the last few decades, and there is now an increasing demand for methods of determining mechanical properties of micrometer-scale and even nanometer-scale specimens. Meeting this demand requires precise and reliable indentation measurements at very low forces and depths. Most commercial nanoindenters suffer with frame compliance and thermal drift, which compromise our ability to test time-dependent properties of materials and make repeatability a challenge. Frame compliance is the deformation of the indenter's frame in response to indentation force, while thermal drift refers to relative motion of the indenter tip and specimen resulting from thermal expansion and contraction that is unknown and uncharacterized. Both effects can introduce error into the force and displacement data that are used to determine the mechanical properties of the specimen. An effective method for eliminating these undesirable signals is indentation by surface tracking, where the indentation depth is calculated using the specimen's surface as reference.

This summer I worked on the first and second generations of the Precision Nanoindentation Platform (PNP), which aim to build metrological standards for nanomechanics. The first-generation PNP uses tuning forks to track the specimen's surface during indentation. It works very well, as it can produce high resolution and repeatable indentation curves, but it also can be cumbersome, as tuning forks may change their resonant frequency with time or environmental conditions. To eliminate this problem, the second generation PNP will use laser interferometry to track the surface, essentially eliminating environmental difficulties and reducing measurement uncertainty. I will discuss both generations of the PNP, my summer work and why this work matters.

Reasoning with PrIKL

Ryan Dorson

Automated theorem proving enables computers to reason using logical systems. Many existing reasoning systems are limited in power or use shortcuts that are superficial. PrIKL is a new approach to theorem proving that is based on human reasoning combined with the power of machine computation.

The goal of PrIKL is to allow developers to reason with ontologies. These ontologies are sets of concepts within a given domain which the reasoner uses to make logical conclusions. The proofs of these conclusions are used to help developers further understand and develop their ontologies.

I helped to develop a graphical user interface (GUI) as a means of providing a wide range of users with easy access to PrIKL. Though users can interact with PrIKL programatically, the GUI allows for easy experimentation with ontologies. The GUI also assists in onotology generation and validates that ontologies are written correctly.

We built the PrIKL GUI using the NetBeans platform, a rich and overly-complicated tool for developing applications. Despite frequent complications, we were able to build a self-contained application for easy distribution of PrIKL to developers.

Characterizing the Impact of a Single Interface Layer Defect in CMOS Devices

Serghei Drozdov

As MOSFETs (Metal-Oxide-Semiconductor Field-Effect Transistor) continue to rapidly scale in size, a single captured charge at the interface level is becoming an important issue. Previously, with larger devices, a single defect could not cause a drastic change in performance but with smaller devices if the defect is generated at a 'critical point' the MOSFET's performance could degrade significantly.

The defects can be created under regular operating conditions but we accelerate this process under accumulation stress. There is a small chance of generating a defect in a critical spot and the time to generate one defect can take very long. Moreover, some of the defects are not created in the interface layer and the device has a chance to recover from those if given enough time. A smart testing set-up had to be designed to stress the devices and track the changes of their parameters automatically. This testing is meant to run on hundreds of MOSFET devices to collect enough significant data.

In our testing design, during the stress phase, we make short stops to track device's parameters that should change if a defect is generated. We use charge pumping to track the number of defects in a device. Other parameters are extracted by analyzing I-V curves (measuring the current while sweeping the voltage) in between stresses.

The automatic testing program generates large amounts of raw data and not all of it is useful to us. A software tool was developed to collect all of the raw data from a particular run, parse it, and then display it in a practical manner.

We expect to come across some defects that change the ION (ON current) of a device as much as 100%. A defect like that in just one of the devices could compromise the functionality of an entire circuit.

Reduced Flammability of Polyurethane Foam Using a Layer-by-Layer Assembly with Natural Materials

Nicholas Faenza

Fires are the cause of many injuries, deaths, and massive amounts of property damage each year. In 2010, over 1.3 million fires were reported in the United States. These fires caused 3,120 deaths, over 17,700 injuries, and almost $12 billion in property damage. Polyurethane foam is a major factor in the potency of many fires because of its common use in consumer products and it's highly flammable nature. Polyurethane foam used in mattresses alone is the cause for thousands of fires and hundreds of deaths each year. To reduce the number and extent of these fires the flammability of polyurethane foam needs to be reduced. In addition, there has been a recent demand for sustainable products that are not harmful to the environment.

A layer-by-layer assembly method is used to provide a nanometer thick coating on the foam to reduce its flammability. All of the coatings used consisted of all natural materials like; Chitosan, Sodium Alginate, and Montmorillonite, which make the coating sustainable and environmentally friendly. A cone calorimeter was used to test the samples, and measure key characteristics like peak heat release rate (PHRR). When burned, the coating forms a protective char around the foam, which helps lower the PHRR. The cone calorimeter tests showed significantly improved flammability characteristics when compared to the control foam.

The presentation will cover the extent of polyurethane foam related fire damage, the layer-by-layer assembly process, and the coatings used to reduce the flammability of the foam. The testing method and results will also be discussed.

Effects of Key Environmental Factors on Degradation of Polymeric Films Used in Protective Glazing Systems

Patrick Gaume

Polymeric films (known as safety films) are widely used to reinforce glass to counter many threats to buildings and occupants, including natural disasters (e.g., hurricanes, tornadoes, severe wind storms, seismic activities), and manmade destruction (e.g., burglary, vandalism, terrorist bombings, industrial explosions). These films are designed to keep broken glass intact within the framing system by absorbing some or all of the energy that causes the glass to break. Thus, they have the ability to prevent shards of glass from becoming lethal projectiles, and reduce injuries as well as property damage. Variety of test methods and specifications are currently used to evaluate and validate the initial performance of safety films and glazing systems. However, surprisingly very little attention is placed on their long term durability performance. It is recognized that these safety films, as with all other polymers, may degrade upon prolonged exposure to ultraviolet radiation, moisture, or extreme temperature. Such undesirable weathering impacts the physical, chemical and mechanical properties of the materials, shortening their useful life spans. In this talk I will explain the various environmental factors that degrade safety films, and clarify the relative importance of each environmental factor contributing to the mechanisms of degradation. Changes in mechanical and chemical properties as a function of temperature and moisture during accelerated aging in an integrating sphere-based weathering chamber (Simulated Photodegradation via High Energy Radiant Exposure) were measured using Fourier transform infrared spectroscopy, ultraviolet-visible spectroscopy and quasi-static tensile tests. In addition, a linkage between accelerated tests and outdoor exposure tests were established because such a linkage is required for the accelerated test methodology to be meaningful.

Cloning, Expression, and Purification of TRPML-1
Addison Goodley

The Transient Receptor Potential (TRP) family of proteins is a group of ion channels regulating intracellular trafficking as well as mechano-, chemo-, thermo-, and photoreceptor activity within the body's sensory nervous system. TRP mucolipin (TRPML), one of the seven sub-families of the TRP transmembrane proteins, is associated with the neurodegenerative disease type IV Mucolipidosis resulting from mutated, non-functional protein channels. However, little is known about the structure or function of the TRPML-1 protein, and no structures have been solved for the TRP family. The goal of this specific project was to clone, express, and purify TRPML-1 within yeast cells. By transforming the yeast with a plasmid containing the TRPML-1 coding gene, the target protein was grown within the yeast's cellular membranes. This protein could be isolated and purified to produce amounts of TRPML-1 suitable for analysis. If successful, the structure and function of the TRPML-1 protein as an ion channel within the natural membrane environment can be investigated by neutron scattering techniques.

Measuring Inadequate Interoperability in the Manufacturing Industry
Adrian Hamins-Puertolas

Inadequate interoperability, the failure of software systems to seamlessly communicate, causes an economic loss of billions of dollars each year for manufacturers and consumers worldwide. The societal impacts are twofold, leading to an increased cost of design and production and a delayed release of products. Most manufactures are unaware of the high cost of inadequate interoperability and, as a result, are harmed by a lack of seamless information exchange in the design and fabrication stages of production. This study will identify ways to measure inefficiency caused by interoperability problems, and will result in the creation of a tool which allows organizational units to estimate the impact of interoperability failure. The goal is to increase manufacturer awareness of inadequate interoperability's economic cost, which could lead to support for standardization across product and manufacturing design software.

Computational Fluid Dynamics Simulations for Building Aerodynamics
Scott Hemley

This presentation will discuss results pertaining to NIST's continued research efforts in Structural Safety under Extreme Windstorms. Specifically, the presentation will highlight results obtained using NIST's CFD (Computational Fluid Dynamics) software, FDS, for modeling wind flow around buildings. CFD is a powerful tool for wind engineering applications. The use of CFD software for wind engineering applications could help engineers to design buildings that can better withstand extreme wind events. In this research, CFD calculations were performed using FDS (Fire Dynamics Simulator) and compared to available experimental data in order to evaluate FDS's capabilities for wind engineering problems. This talk will discuss numerical results obtained with FDS as well as steps taken to improve the computational accuracy and speed of FDS calculations.

Parallel LDPC Error Correction for Quantum Key Distribution on a GPU
Jeffrey Jacobs

Since the advent of the quantum computing paradigm in the 1980's, several protocols for secure communication either partially or entirely over quantum channels have been developed. The most notable of these is the BB84 protocol, which utilizes both a quantum and classical channel to establish a secret key which can then be used for secure classical communication between two parties. However, the quantum channel in this protocol is subject to high error rates and thus an error correction algorithm which does not reveal the secret keys is required for a quantum key distribution implementation.

To this end, Low-Density Parity Check (LDPC) codes are used. Introduced by Robert Gallagher in the 1960's, they have become extremely popular over the past decade and used in many recently developed networking protocols such as the 802.11n Wi-Fi and 10GBASE-T Ethernet standards. In the context of quantum key distribution, however, the LDPC algorithm requires several modifications.

Mink and Nakassis outline and compare the performance of their modified QKD error correction algorithm on canonical LDPC matrices given by IEEE and ETSI standards in their 2012 paper "LDPC for QKD Reconciliation". I will discuss my work on parallelizing Mink and Nakassis' algorithm using Nvidia's Compute Unified Device Architecture (CUDA) engine on a Graphical Processing Unit (GPU) and the performance achieved by this implementation, as well as future extensions to the algorithm which could allow for even greater efficiency.

Effects of Interfacial Roughness in Small Angle Neutron Scattering from Multiphase Polymers

Benjamin Jones

Polymer structure at the micro- and nanoscopic scales greatly affects the polymer's macroscopic bulk mechanical properties. However, this structure can be difficult to characterize due to the electrical properties of organic materials as well as the scales at which the structure occurs. Neutron scattering can provide good contrast in organic materials and the wavelengths of neutrons are appropriate for the micrometer scale of polymer structure. However, to extract critical information about the material, experimental neutron scattering data must be compared to rigorous models. While very simple models can be derived analytically, a higher level of information required for modern problems makes mathematical models intractable.

Existing code of scattering models, developed in Python, was used as a test bed for adding higher levels of complexity critical to polymer science projects here at NIST. As an example, analytical models often assume that fillers in composite materials have perfectly smooth surfaces. However, in reality, the fillers are often natural products such as clay particles that not only possess significant roughness, but the roughness is thought to be a key component in the composite mechanical properties.

The existing code was converted and streamlined from existing reflectivity code to use less computer memory and user time. A larger simulation provides a more accurate model, but requires much more time to provide data to analyze and these parameters were optimized. This converted simulation code was calibrated with polymer architectures whose scattering could be analytically calculated in order to prove the program's accuracy before adding complexity.

By using a generalized simulation model this program will provide insights into the scattering expected from roughened interface between semi-crystalline and amorphous regimes in polyolefins.

Phase Transition Measurement of Lipids by Nanocalorimetry

Il Kyoon Kim

Nanocalorimeter is a thermodynamic measurement technique using silicon micromachined sensors that measure the temperature, heating rate and heating capacity; nanocalorimetery has been utilized to analyze the thermodynamic properties such as the melting point and enthalpies of phase transitions. In this project, nanocalorimetry is used to quantify the phase transition temperatures of lipids from gel to liquid state. Lipids carry a highly hydrophilic head; this allows the investigation of the effect of moisture surrounding the lipids on the transition temperature. It has been hypothesized that the increase in observed transition temperature of lipids in the air is due to the moisture absorbed from the atmosphere. In order to verify the hypothesis, the phase transition of a lipid, 1,2-dihexadecanoyl-sn-glycero-3-phosphocholine (DPPC), was measured in air, dry nitrogen gas, and subsequently, in gases with different levels of humidity. Humidity was controlled by saturated solutions of LiCl, KSO_4, and NaCl. The correlation between moisture and phase transition of lipids found through the results can improve further understanding of cell morphology and interaction through cell walls, and biopharmaceutical applications.

Comparison of FDS Predictions with Gas Velocity Measurements in the Exhaust Duct of a Stationary Source

Kevin Li

Carbon dioxide released as a result of the burning of fossil fuels remains a major source of greenhouse gases that are responsible for the greenhouse effect and climate change. The mitigation of these emissions is dependent on proper measurement of the flow at or near the source, but these measurements can often be uncertain. The NIST Large Fire Laboratory runs such test through an exhaust duct, and these experiments can be simulated using computational fluid dynamics programs. NIST has developed a CFD software called Fire Dynamics Simulator (FDS). By validating the use of FDS as a measuring tool, NIST can not only verify its experimental results with CFD predictions, but also make recommendations about future experiments. The experiments run at the NIST lab were simulated within FDS and the results were qualitatively compared. The experimental results examined the velocities at two chords on a plane perpendicular to the flow, near the outlet of the duct; once the key components in the experimental duct were simulated in FDS, a similar measurement plane was used with the same two chords to evaluate velocity. This talk will elaborate on how the simulated results compare with the results of the previous experiment and make recommendations on future measurements. Conclusions will be made about the potential use of FDS as guidance for these measurements.

Dynamic Update of MySQL Database in Kitting

Lipeng Liang

Kitting is the process in which several related items are placed into a container as a unit. Kitting has not yet been automated in many industries where automation may be feasible and desirable. Industrial robots are introduced into the kitting process to enhance automation. The kitting problem is addressed by building models of the knowledge that would be required to operate an automated kitting workstation. An ontology represents knowledge as a set of concepts within a domain, and the relationships among those concepts. Ontology changes dynamically. When to update ontology and the mechanism to trigger ontology update are essential to the kitting process.

The MySQL database is used to process the Kitting objects and relationships among the objects. MySQL database is in a dynamic environment and it represents ontology. The operations and actions of kitting robots need to meet certain criteria. Every specific robot action requires valid preconditions and leads to specific effects. All the preconditions need to be verified before a robot action is implemented. One of the summer tasks is to create mapping of preconditions onto MySQL database and verify validity of preconditions in MySQL. MySQL database is in a dynamic environment. When changes in MySQL meet certain conditions, they should trigger ontology update.

Quantification of Human Bone Marrow Stromal Cell Shape Dynamics in Collagen Three-Dimensional Scaffolds

Karthikeya Menta

Human bone marrow stromal cells (hBMSCs) are sensitive to specific scaffold architectures. The scaffolds can vary in both chemistry and structure. Scaffold architecture affects cell shape, and as such cell shape needs to be quantified in order to better understand cell behavior response to scaffold architecture. In this study the dynamic change in cell shape from initial seeding into collagen scaffolds to 24 h was studied. At each time point (0, 0.5, 2, 5.5, 12, and 24 h) cells were fixed and stained for nucleus and actin cytoskeleton structure with 4',6-diamidino -2-phenylindole (DAPI) and AlexaFluor 546 Phalloidin stain, respectively. Using confocal microscopy, cells were identified and imaged. Using ImageJ software, cell shapes were quantified by measuring cell spread area, cell breadth, area distribution curves, and the principal moments of the gyration tensor. Initial results indicate hBMSCs do develop into highly branched and elongated structures by 24 h. Also, around time point 5.5 h, hBMSCs transform from spherical into mostly star shaped like structures. However, during this time point there is much more variety in cell shape than during any other time point. This study has been able to provide insight into the transformation of hBMSCs in a collagen scaffold which most closely resembles *in vivo* like conditions. The goal of this study is to develop a standard set of measurements for shape quantification of hBMSCs. By assessing cell shape, this approach will help tissue engineers determine the time scale in which cells adopt a 3D morphology (i.e. more relevant *in vivo* behavior) and in turn, design scaffolds that enhance 3D morphology, cell function, and tissue regeneration.

Expression, Crystallization, and Holographic Analysis of the Protein Rubredoxin

Stephanie Miller

X-ray fluorescence holography (XFH) differs from traditional crystallography in that it permits structural analysis of both crystalline and non-crystalline samples with orientational order. Preliminary analysis on a well-studied biomolecular crystal structure will demonstrate proof-of-principle for this proposed technique. Rubredoxin has been selected as a model protein because it is small (~5 kDa), it crystallizes with minimal symmetry, and it contains a single fluorescent iron atom.

A key portion of this project consisted of producing sufficient rubredoxin to accommodate the iterative optimization of protein crystallization. The Histidine-tagged gene of interest was expressed via T7 promoter in BL21 (DE3) E. coli expression cells. Protein purification was achieved on an immobilized metal ion affinity chromatography (IMAC) Ni column and the His-tag was cleaved with TEV protease. Crystal screening was conducted on purified protein to generate crystals of sufficient quality for the holography measurements. Rubredoxin crystals were then exposed to 0.17nm x-rays for measurement of complete holographic datasets. The resulting data were transformed to produce holographic images.

An Analytical Finite Element Model of Micro- and Nanoscale Electrostatic Beam Resonators

Erica Sanker

Micro- and nanoelectromechanical resonators are currently used as radio frequency (RF) oscillators and filters for applications including timing and synchronization of electronics, RF communications, and biochemical sensing. The electrostatic beam resonator is one class of mechanisms that has been widely studied for these applications due to its ease of fabrication and simplicity in actuating with electrostatic forces. As a result, nanoscale electrostatic beam resonators are under development as part of the NEMS Measurement Science project at NIST, which is examining the measurement and manufacturing challenges for the next generation of nanoelectromechanical systems (NEMS). In support of this work, an analytical finite element model of the dynamics of an electrostatically actuated doubly clamped beam has been developed. This model has been compared to numerical results from ANSYS and has been shown to be in good agreement. The analytical model is non-dimensional, providing the opportunity to study the dynamic behavior of the resonator without the need for defining the geometric parameters of the mechanism *a priori*. This model has been used to analyze three particular characteristics of the resonator. The first is the detuning of the resonant frequencies due to a static electrostatic force generated by a bias voltage to the actuator. The electrostatic force is nonlinear due to its dependence on the applied voltage and gap size between the beam and electrode, resulting in a negative stiffness effect. The second characteristic is the distorting of the vibration mode shapes caused by electrostatic actuation compared to the beam's free response. Finally, the model has been used to analyze the ability of the electrostatic actuator to excite the beam's vibration modes for a given electrode geometry. This analysis can be used to determine whether higher modes can be reached by appropriate design of the electrode. Higher modes provide a higher frequency, which allows for ultra-sensitive mass sensing and better overall sensitivity. Results from our analysis on all three of these characteristics will be presented with respect to mechanism parameters including bias voltage, and width and location of the actuation electrode. These results will aid the design of future MEMS/NEMS resonators by providing a systematic analysis of how to select design parameters to achieve a desired frequency, motion amplitude, and mode shape.

The Kinect: A Cheap and Accurate Depth Measurement Tool

Jacob Siegel

The most infamous XBOX 360 accessory is the Kinect Sensor, which provides a touch free gaming interface. Just as a regular digital camera returns a color image, the Kinect returns a color image and a depth map. The depth map is an image in which each pixel contains the information about scene depth. While Kinect is not as accurate as other laser based depth cameras, it has several distinct advantages: price (~$150), acquisition speed (~25 frames per second) and ease of use. In this project, I have explored the use of Kinect for scientific dynamic depth measurements, and specifically geodesic distance and area measurements.

The project has focused on developing software that would assist in measuring geodesic distance and area of human body parts. The work with Kinect cameras has leveraged drivers for Windows, Mac, and Linux, as well as the OpenNI library with functions for receiving color and depth video stream and tracking a human in the camera field of view. I have written code to calibrate depth measurement and designed a calibration object for this purpose with two parallel planes. I have also written to code to support user-driven selections of distance and area that are registered with the detected human ‘skeleton’ and tracked over time to report the geodesic measurements. I will talk about the geodesic measurement calculations derived from depth maps, technical challenges of working with Kinect cameras, and potential applications and implications of this new cheap depth camera.

Biomedical Image Analysis
Marissa Sileo

Over the last few decades, image analysis has been used to extract significant information from images and provide output in the form of another image or in the form of properties of the original image. Biomedical imaging and cell microscopy are just two example areas in which automated image analysis can be applied to improve the systems. One of the most important tasks the automated analysis systems can perform on the biomedical images is image segmentation. Segmentation is the process of separating objects, or regions of interest, in the image from the background. Currently, there are many known approaches to this process, with the most popular being region-based, edge-based, thresholding, cluster-based and model-based techniques. Scientists around the world are unrelenting when it comes to developing new methods and evaluating them based on their accuracy, reliability, repeatability, robustness and dependency on the operator. One way to evaluate these techniques is by comparing them to a “ground truth” image as a gold standard, which has been segmented manually. We conducted an experiment using five microscopy images of nuclei in aortas of rabbits from different age groups, with corresponding “ground truth” images, to evaluate these techniques. Approximately 150,000 objects, some containing multiple nuclei, were segmented using seven different techniques. Filters and other morphological operations were also applied to some of the images to improve the segmentation performance. After segmenting the images, we employed several different shape features, such as eccentricity, solidity, and convexity, to classify the nuclei. Finally, we use this information to separate the nuclei into their respective classes in an effort to prove that the shapes of the nuclei vary in different regions of the aorta, as they can be viewed as flow sensors, and also with respect to ages in the rabbits.

Phase Equilibria in Co-Al-W Ternary System
Jake Steiner

The recent discovery of a cuboidal γ/γ’ microstructure in Co-Al-W ternary alloys similar to that found in commercial Ni-based superalloys used in high-temperature applications has spurred significant research efforts into the development of Co-based superalloys. These materials have the potential to replace Ni-based superalloys currently used as turbine blade materials in aircraft engines and energy production. They can operate at higher temperatures, improving efficiency and ultimately production and operation costs. However, more information is required to accurately assess the thermodynamics of the base Co-Al-W system, including whether or not γ’ is a stable, equilibrium phase. We studied two different alloys, Co-11W-10Al and Co-10.8W-9.5Al, subject to various thermo-mechanical processing treatments to do so. X-ray diffraction, scanning electron microscopy and energy-dispersive X-ray spectroscopy were used characterize the phases present, their composition and their relative abundance. We found that the microstructure of each alloy greatly depends on its processing treatment. Preliminary results show the formation of regions of pure γ' along grain boundaries in some samples, suggesting that pure γ' may be a stable equilibrium phase in the ternary Co-Al-W system.

Estimation of the Uncertainty in Orientation Distribution Function Using Monte Carlo Technique

Komal Syed

Most materials found in nature are polycrystalline, and the crystallographic texture is defined as the preferred crystallographic orientation of the grains in a polycrystal. Crystallographic texture provides essential information about the material performance which can be controlled by material processing. Measurement of the crystallographic orientations in a sample can be performed by various diffraction techniques. Due to the availability of the NIST Center for Neutron Research (NCNR), neutron diffraction is used in our study. Neutron diffraction provides many advantages over x-ray diffraction, such as being able to irradiate larger sample volumes as well as obtain complete pole figures. Orientation Distribution Functions (ODFs), calculated from the pole figures, provide complete information about the orientation of the grains.

There has not been much research done yet to *quantify* the uncertainty in these calculated ODFs. The statistical analysis of the ODF in this project is crucial to understand how accurate the crystallographic texture is known. Different factors can contribute towards the uncertainty in an ODF; such as the effect of the number of discrete orientations used for ODF estimation and the propagation of the uncertainty in the pole figure data to the uncertainty in the ODF. The latter factor is the essence of this project and is estimated using a Monte Carlo technique. The effect of perturbed pole figures is analyzed on the calculated perturbed ODFs. Using texture analysis software (Mtex) in Matlab, the mean and standard deviation of the perturbed ODFs are calculated. The results quantify the confidence interval on an estimated ODF and give a basis for further research to analyze other components of the uncertainty in ODF.

Manufacturing Specific Process Information Models for Sustainability

Lina Valivullah

Sustainable manufacturing systems use processes, methodologies, and technologies that are energy efficient and environmentally friendly. To create and maintain such systems, well-defined measurement methodologies and corresponding manufacturing information models play a crucial role to consistently compute and evaluate sustainability performance indicators of manufacturing processes that will result in reliable comparisons. However, when it comes to describing sustainability of product manufacturing, the presently available methods and tools do not account for manufacturing processes explicitly and hence result in inaccurate and ambiguous comparisons. Furthermore, there are no formal methods for acquiring and exchanging sustainability related information that help establish a consolidated sustainability information base for decision support. This research work involves a study on the scope of the currently available manufacturing information models to incorporate sustainability. Identifying the requirements for information models that cater to sustainable manufacturing was done utilizing an earlier developed Systems Integration for Manufacturing Applications (SIMA) reference architecture model and the injection molding unit manufacturing process as a case study.

Analyzing Microblog Search Through an Ablation Study of TF-IDF

Mark Villarrubia

Search over microblog databases such as Twitter faces two major obstacles; the size of the database, and the size of the tweet. The relatively small tweet size means that traditional indicators of document relevance are less clearly indicative. In 140 characters, for example, a high number of query terms may not indicate relevance so much as spam. Each repetition of a term subtracts from the space available to discuss that term, making it more difficult to judge relevance from measures such as term frequency. The large database size, on the other hand, means that a slight misreading of a query can cause a search to return hundreds of at best tangentially related documents. Further, this provides a direct challenge to evaluating a search's effectiveness; in a small database, a large percentage of documents can be evaluated relevant or irrelevant for a topic by human assessors, providing a rigorous evaluation of the search. In a larger database, however, these judgments become sparse to the point where the first page may contain no judged documents, relevant or otherwise.

This project searches for characteristics of a superior microblog search algorithm through ablation analysis of Lucene's TF-IDF, a top search algorithm for other field of search. It investigates different factors within the TF-IDF algorithm, determining which component provides the search with the largest precision gain. Each component is weighted in varying degrees and the weightings are compared against each other. Because standard metrics cannot adequately evaluate sparsely judged searches over large indices, the searches are measured with bpref and map', measures of relevance which perform well even on topics for which large amounts of judgments are not available. Separately testing the individual parts of TF-IDF reveals which parts remain accurate indicators of relevance, while the use of judgment-independent metrics partially sidesteps the issue of database size, providing an analysis of the components of an optimal microblog search.

3D Geometry Photovoltaic Devices

Matthew Widstrom

There has been an increasing academic focus on researching sources of renewable energy as nonrenewable sources increase in price and scarcity. Photovoltaic devices that harness the energy of the sun show great promise as dependable renewable energy sources that may one day replace help replace fossil fuels. Cadmium selenide (CdSe)/cadmium telluride (CdTe) thin film photovoltaic devices with a dual back contact geometry show great promise as potential renewable energy sources. Device fabrication involves CdSe electrodeposition on one of two interdigitated electrodes on a prepatterned substrate followed by CdTe electrodeposition over the entire structure so that both electrodes are behind the active portion of the device. In contrast to traditional planar devices, illumination is on the electrode-free CdTe surface rather than through a window layer. This geometry serves to decrease the number of photons blocked by the absence of a window layer or top electrode and decouples the length scale for absorption and recombination of charge carriers. These devices were characterized by taking current-voltage and external quantum efficiency (EQE) measurements, showing promise for our geometry.

Building Evacuation of People with Mobility Impairments
Emily Wiess

During an emergency evacuation in high-rise buildings, disabled and elderly occupants are typically instructed to wait in a refuge area until they are rescued by the local fire department. The 2001 World Trade Center attacks and subsequent collapse presented a scenario in which all occupants, regardless of ability, had to evacuate. This incident prompted the safety community to reconsider previous evacuation strategies for people with mobility impairments. However, a negligible amount of egress movement data, such as speeds and flows through doors, has been collected for disabled and elderly occupants. The Engineering Laboratory at the National Institute of Standards and Technology (NIST) has gathered stairwell movement data for disabled individuals during fire drills of high-rise buildings to better understand disabled evacuee movement and behavior throughout emergencies. Video recordings of evacuation drills in two assisted living facilities provide raw data for a descriptive analysis of an array of disabled and elderly evacuees. Occupants whose movements and behavior were analyzed included those who were visually identified as elderly as well as individuals needing assistance to evacuate from canes, walkers, stair decent devices, and other people. As expected, the egress speeds of disabled and elderly individuals appeared to be significantly slower than those of able-bodied occupants. Through similar data analyses of additional observed building evacuations, NIST will be able to provide the technical foundation for egress requirements in buildings for a variety of population types, including people with mobility impairments.

Developing Analytical Tools for the Characterization of Protein Biomarkers Using Antibodies and Superparamagnetic Substrates
Jiemin Wu

Research in bioanalytical technologies has been gaining prevalence due to high demand for more efficient methods in detection and analysis of specific disease biomarkers in biofluids. Antibodies in particular are a common, but highly effective biomolecule in the capture of proteins of interest for specific assays. In order to achieve optimal measurements and characterization, these analyses require a robust design in antibody-substrate immobilization and biorecognition. Major challenges associated with biomarker detection are the low abundance of target molecules in clinically relevant-sized samples, the complexity and large dynamic range of sample matrices, and the propensity for non-specific molecular interactions. Therefore, current research seeks to investigate the best platforms to use for reliable target protein capture and separation from complex matrix solutions.

The objective of the project focused on the study of various techniques for conjugating antibodies to commercial superparamagnetic bead substrates to determine an optimal assay method. Three prominent factors studied in this process include the conjugation reaction type, antibody loading capacity, and bead particle size. Experiments were conducted using two different conjugation-chemistry bead types, which were conjugated to antibodies targeting two different human serum proteins: cardiac troponin I (present in diseased state) and C-reactive protein (CRP). In addition, different diameter sizes were investigated along with the ligand-particle coupling technique (passive versus crosslinking conjugation reactions). Both troponin and CRP were immunoprecipitated using antibody-conjugated particles and subsequently digested into peptides. Liquid chromatography and triple-quadrupole mass spectrometry were utilized to analyze peptide fragmentation transitions and quantitatively compare the immunoprecipitation efficiencies of the different bead types. This assay will be extended to isolation of target proteins from complex solutions such as serum with a relatively high degree of efficacy.

Dataflow: Web-Based Data Reduction

Alex Yee

To facilitate reduction for neutron experiments at the NCNR and similar research laboratories, a web-based tool, Dataflow, was designed and conceived. Dataflow's GUI allows users to create data reduction pipelines that model the reduction steps that the data will undergo. These reduction steps are each performed by various modules that are uniquely provided for each type of instrument. Dataflow is designed so that creating and adding new modules or even incorporating new instruments is feasible.

The majority of reduction steps applicable to Triple-Axis Spectrometers have been encoded and incorporated into Dataflow. Filereaders were written to read different Triple-Axis file formats, including those from other research facilities including HFBR and Chalk River Laboratories. Furthermore, re-binning code was written and employed to regularly grid data for plotting through Dataflow. Both 2-D pseudocolor data plots and n-d plots with variable axes are available throughout the reduction chain in Dataflow, allowing a visual plot of data before and after any step in the reduction. Numerous other improvements were added to the triple-axis module and tested on actual data.

University of Michigan

Chemical Heterogeneity of Wildfire Aerosol Emissions: Implications for Climate Change

Sean Collins

The frequency and magnitude of wildfires are projected to increase with changes in global climate. At the same time, wildfires represent a significant factor in aerosol and greenhouse gas emissions that alter atmospheric chemistry and physics. Consequently, understanding wildfire emissions is a key analytical parameter for assessing this reciprocal relationship. However, descriptions of wildfire emissions remain fraught with high uncertainties due to the compositional heterogeneity of the emissions. Despite a common fuel source, wildfire biomass burning occurs across a range of temperatures and combustion rates, yielding chemically diverse and often mixed emissions. Here, we present detailed chemical and structural analyses of complex, internally mixed wildfire aerosols from experimental burns of Canadian boreal forest. Transmission electron microscopy and electron energy loss spectroscopy probe the nanoscale structural and chemical composition of wildfire aerosols to elucidate size, mixing state, bonding character, and other physical constants of this emissions source. The particular occurrence and optical effects of metal species in carbon-based soot from smoldering-phase fires will be presented. These data, in turn, inform computational modeling of the optical properties of these atmospheric aerosols and elaborate the impacts of wildfire emissions for global climate change.

University of Nebraska Lincoln

Domain Size Dependence of Successive Alternating Layers of Co and Pd

Anton Lintel

In this work, we use scanning electron microscopy with polarization analysis (SEMPA) to image the three-dimensional magnetic nanostructure of perpendicularly magnetized multilayer thin films with graded anisotropy. These films are the basis of proposed magnetic memories and sensors that rely upon repeatedly switching perpendicular magnetic nanoelements over large wafer areas[1]. An important starting point for such devices is therefore the production of thin films with tunable micromagnetic characteristics. Previous studies[2] have found such useful magnetic properties in samples of alternating sub-nanometer thick layers of cobalt and palladium. Furthermore, the magnetic anisotropy of these multilayer samples is found to depend on the relative thicknesses of the cobalt and palladium layers. We have measured samples comprised of 0.6nm palladium and 0.4nm cobalt layers repeated 15 times followed by 0.6nm palladium and 0.8nm cobalt layers, again repeated 15 times. We use in-situ low energy ion bombardment to depth profile the magnetic nanostructure through the boundary between the two thickness ratios, and present high resolution magnetic images of the domain structure as a function of depth.

1) Joe Davies, NVE Corporation, personal communication, January 26, 2012.
2) H.J.G. Draaisma, W.J.M. de Jonge, F.J.A. den Broeder, *Jour. Magn. Magn. Mater.* **66**, 3, 2 (1987).

University of New Hampshire

Designing and Constructing Steel Cruciform Specimens for a Biaxial Tensile Machine

Newell Moser

Sheet metal processes, such as bending and deep drawing, are widely used in automotive industries. It is a constant challenge to manufacture lightweight, structural car parts, but it is necessary since this will lead to more efficient vehicles. Companies spend millions of dollars on forming equipment before an acceptable design is found. A biaxial tensile machine is used to aid in quantifying material properties. These data can then be incorporated into the design process to help develop lighter vehicles while also saving money for the manufacturer. Previous biaxial studies did not analyze large-strain behaviors of sheet metal because nearly all cruciform specimens prematurely failed. However, since sheet metals are exposed to high strains during forming processes, additional research is needed to understand precisely how these materials behave during these strain paths. In order to accomplish this, it is essential that the cruciform specimen being tested yields and ultimately fails within the center, or area of interest.

A list of previously-used cruciform designs was compiled and analyzed. It was believed that during an experiment, triaxial stresses were developing near the corners which eventually led to failure. The geometry that best suppressed these stresses was then chosen as the basis for future experiments. Because the thickness was thought to be tightly linked to these stresses, this parameter was solely changed between the four specimens. A CNC plasma cutter was calibrated and then used to cut out the mild steel cruciform specimens. The specimens were welded on top each other using high strength acrylic glue so as to achieve the desired thicknesses. By applying various surface finishes and cutting techniques to similar samples, Marciniak cup tests could be performed in an effort to understand the importance of edge effects and premature yielding. The surface finish that most prolonged the onset of failure was applied to the cruciform specimens. The biaxial machine located at NIST is unique in that it uses X-ray diffraction (XRD) to measure the stresses experienced by the specimen. This method provides more accurate data than common procedures, which are reliant on estimated cross-sectional areas. A random speckle pattern was spray painted over the area of interest of each specimen so that digital image correlation (DIC) could be employed to measure full-field strains. Initial experiments incorporated equibiaxial loadings, but various strain paths will be tested.

University of New Haven

Aging Effects on the Enzymatic Activity of Functionalized Gold Nanoparticles

Danielle Gorka

Biofunctionalized gold nanoparticles (AuNPs) are being investigated as next-generation cancer drugs and cancer drug carries due to the unique properties of nanoparticles. Currently, regulatory agencies, *i.e.* the FDA, review nanomedicines on a case-by-case basis. As nanomedicines become more prevalent, standard methodologies need to be created to test the efficacy of these drugs. Many novel nanotherapeutics contain ligands attached to the surface of the nanoparticle that specifically target tumor cells. It is important that the number of these ligands can be quantitatively determined on a single nanoparticle basis thus the amount of attached ligands can be optimized.

A model system of horseradish peroxidase, a well-studied enzyme, attached to the surface of a gold nanoparticle was used to create a broadly applicable methodology that can be used by drug manufacturers and regulatory agencies to test novel nanotherapeutics in preclinical trials. Enzyme kinetic measurements were performed using Ultraviolet-Visible Spectroscopy (UV-Vis) to determine the activity of the attached enzyme. Atomic force microscopy (AFM) was used to determine the number of attached enzymes through the use of gold immunolabeling which is a similar method traditionally used with transmission electron microscopy (TEM) samples. This causes the formation of a raspberry like structure, which were imaged and counted using AFM.

Nanofiltration Membranes and Their Swelling Properties by Use of XR and QCM

Allison Young

Since the 1970's, polyamide membranes have been used for reverse osmosis and nanofiltration water purification technology, *i.e.* conversion of seawater and brackish water into fresh water. Although there has been a large amount of research done in the development of these materials, there is little knowledge about their structure-property relationships. In this research, we adapt X-ray reflectivity and Quartz crystal microbalance to investigate the swelling properties of polyamide nanofiltration membranes. With the aid of the classical Flory-Rehner theory traditionally used for the characterization of highly swollen polymer networks, we extract the physical properties of the nanofiltration polyamide network including the Flory interaction parameter and molecular mass between crosslinks swollen with water.

University of North Carolina Charlotte

Diamond Turning Machine Characterization
Luke Savage

The goal of this project is to employ precision machine design methods to facilitate the safe use and optimization of an existing diamond turning machine. Diamond turning refers to a process where a diamond is used to machine work pieces to extreme tolerances, e.g. 100 nm. An accurate and deterministic virtual model of the machine's performance allows simulation of work piece error to optimize tool paths. Generation of this type of model requires measurements with low uncertainties. Measurement uncertainty analyses and precision fixture design were performed to facilitate linear positioning measurements of the X- and Z-axes with displacement measuring interferometry and an expanded measurement uncertainty less than or equal to 50 nm.

Temperature control of both the diamond turning machine and the work piece are critical. Small fluctuations in temperature can cause errors due to thermal growth. For example, a 0.1^{o}C change in temperature can cause a 10 cm long aluminum work piece to grow approximately 220 nanometers. Therefore temperature control of the work piece requires precise control of the cutting fluid temperature. A new cutting fluid system was designed that has a large thermal capacitance to improve the control over the cutting fluid temperature. In addition the new cutting fluid system is designed to minimize leaks, which plagued the old system, and to improve the ease of replenishing the cutting fluid.

Before machining, the location of the single point diamond tool with respect to the work piece surface needs to be known with a tolerance of a few micrometers. The current method of locating the tool with respect to the work piece involves placing the operator close to the rotating spindle with a hand held magnifying glass and manually jogging the tool in 1 micrometer increments until the tool makes contact with the work piece. This presents a safety hazard and therefore a tool set station consisting of a microscope and video system was designed to accommodate remote tool placement to better than 1 micrometer within the machine work volume. In addition, the imaging system will double as a tool inspection station for monitoring. This presentation will discuss the results of this work.

University of Oklahoma

Solidification of Nanoparticles at High Rate
Maryam Sabeghi

In the Material Measurement Laboratory, thermal properties of nanoparticles are measured using nanocalorimetry. The large surface area of nanoparticles is known to alter their properties compared to bulk materials and expected to differ even from thin film. With a large surface area and ample nucleation sites, undercooling nanoparticles is difficult to achive experimentally and requires very high cooling rate. Detailed measurements on the solidification of nanoparticles will help on the understanding of other small scale and high rate transformations. In this study, I looked at the dynamics of solidification of Al nanoparticles (60 nm-80 nm) at high cooling rates and, demonstrated how the high rate can affect the measurements. Al nanoparticles were deposited on the nanocalorimeter chips using electrospray. Current pulses were applied to the nanocalorimeter chip, rapidly heating the sample above the melting point; the sample cooled at approximately 10^4 K/s. I also measured the enthalpy and, heat capacity. These kinds of studies can lead to advances in materials used for nanodevices that may soon have a huge impact on our daily life.

University of Pennsylvania

A Picturesque View of Sustainable Manufacturing Standards
Sean Reidy

Sustainable manufacturing is quickly becoming more critical and pervasive in the engineering world. Although there are standards to help companies improve their sustainability, they are overlapping, sparse, and not cohesive. Furthermore, this information is presented textually, which conflicts with the non-linear flow of information in these standards, as relevant information is not always grouped together. To address this problem, we are creating a single taxonomy that categorizes information from multiple standards in a way that makes understanding and searching quick and easy. By using a visualization tool to display a web of information that explicitly represents relationships between standard terms, sustainable manufacturing concepts, and other standards, the information retrieval process for engineers becomes less time-consuming and more comprehensive. In this talk, I will explain how presenting standards information in a visualized form using a Web Ontology eases the process of searching for data relevant to sustainable manufacturing standards. This will help to maximize efficiency for sustainable manufacturing and form a centralized, cohesive information repository for sustainable manufacturing standards, promoting their use, and furthering the goal of sustainable manufacturing.

University of Puerto Rico

Electrocatalytic Hydrogen Oxidation and Evolution at Pt Surfaces in Alkaline Solution
Desirée García Torres

Understanding electrocatalytic reduction and oxidation of hydrogen is crucial for a green energy economy in which polymer membrane fuel cells (PMFC) are envisioned to supply a significant portion of portable power demands. PMFC's are comprised of hydrogen oxidation reaction (HOR) at the anode and oxygen reduction reaction (ORR) at the cathode, suffering from the high cost of the platinum (Pt) electrocatalyst for both reactions, which can be exacerbated by low activities, poor durability, poisoning and Pt loss. Although the catalysts show higher stability in alkaline media than that in acid, the former exhibits orders of magnitude lower activity for HOR. The goal of this project was to develop novel HOR electrocatalysts for alkaline PMFC application. Additionally, the same catalysts were also tested for hydrogen evolution reaction (HER), the reaction involved in hydrogen fuel production.

More specifically, this work examined an electrochemical synthesis technique for Pt monolayer electrocatalysts supported by metal substrates. This approach was utilized to create Pt electrocatalysts with ultra-low Pt loadings, which can reduce the cost of fuel cells, and understand factors dictating their activity in alkaline media. In particular, nickel supported Pt coatings, which further reduce Pt content by introduction of a base metal, were examined for HOR and HER. The kinetics of HOR and HER on Pt and Pt alloy surfaces were analyzed by rotating disk electrochemical cyclic voltammetry in conjunction with the Koutecky-Levich and Butler-Volmer equations. Electrocatalyst activity was optimized by cation chemistry of the electrolyte and Pt loadings in terms of deposition time and number of monolayers. An electrochemical technique known as hydrogen underpotential deposition (UPD) was used to assess the Pt surface area, while complimentary tools such as scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectric spectroscopy (XPS), and ion scattering spectroscopy (ISS) were used to correlate structural information to activity measurements.

Durability Study of Polymer Nanocomposites
Jennifer Gil Acevedo

Nanoparticle filled polymeric composites are used in a variety of applications in the construction, building, automotive, and aerospace industries to increase the life cycle performance of products. Differences in the nanoparticle dispersion of these composites affect their durability when exposed to weathering conditions over time. To determine the correlation between degradation due to weathering and particle dispersion, nano-titanium oxide (TiO_2) filled acrylic urethane (AU) polymer films of different dispersions were exposed to simulated weathering conditions of high intensity ultraviolet (UV) radiation on the NIST SPHERE (Simulated Photodegradation Via High Energy Radiant Exposure) at 55 °C and 0 % relative humidity over a period of four weeks. Physical changes in surface morphology and mechanical property changes in degraded polymer samples were measured and analyzed using laser scanning confocal microscopy (LSCM) and tensile testing with dynamic mechanical analysis (DMA) instrument.

Generally, samples with poor particle dispersion exhibited the most severe degradation while samples with good particle dispersion showed least severe degradation. To understand how the UV radiation affected the whole samples or only on the surface of the samples, the mechanical properties measured by tensile testing were also compared to the surface mechanical properties measured by nanoindentation in the same exposure condition. The results of this experiment will be compared to previous studies in this nano-filled polymer system in different exposure conditions and provide the fundamental understanding for the improvement of nanoparticle filled polymeric composites.

Nano-Injector Based Direct Write Metal Deposition
Joseph Marcano Estévez

My project involves assembling and testing a nano-injector system for use as a direct write metal deposition system. The immediate purpose of this system is to deposit electrically conducting metal lines on existing advanced transistor test structures. This will facilitate transistor characterization not available to us due to the pre-existing design/layout of our test structures.

For example, the system can be used to deposit "ground-signal-ground" connections for RF based transistor measurements or connect many transistors to form different types of test circuits. Future uses of this system include direct write of nano-structures (pillars or fins) and direct write nano-lithography.

The system includes three different components; (1) A nano-pipette puller, which consists of a CO_2 laser heat source and mechanical "pullers". A glass pipette "blank" is pulled apart while being heated. This results in a reduction of the pipettes inner diameter (from 0.5mm to >50nm) depending on the desired use. (2) A digital injector which provides two independent control channels for providing positive or negative pressure to the nano-pipette. This can be used to draw liquid into and then inject liquid out of the nano-pipette. (3) A motorized 3-axis micromanipulator used to position the nano-pipette above a sample. The manipulator stepper motors can be software controlled to move in desired directions and speeds or can be operated manually.

In my presentation, I will first discuss in more detail the function and limitations of these three components. Next, I will discuss how they can be integrated into a direct write system capable of facilitating our transistor measurement needs. I will then discuss the progress made in assembling and testing the capabilities of this machine. Finally, I will briefly touch on the future use of this machine at NIST.

Wireless Sensor Networks for Machine Monitoring

Mairim Nieves-Nevárez

The Smart Manufacturing and Control Systems program provides measurement science and standards that enable plug-and-play sharing of real-time information between manufacturing equipment and the applications that monitor them, control them, and optimize their performance in the factory. MTConnect is an open protocol for data exchange between factory devices, such as machine tool and manufacturing equipment using Hyper Text Transfer Protocol (HTTP) as the underlying communication scheme. On the other hand, the Institute of Electrical and Electronics Engineers (IEEE) smart sensor and network standards define a set of metadata, data format and communication interfaces and protocols for wired and wireless sensor applications. They provide self-identification and self-description capabilities to sensors and actuators via electronic datasheets attached to the devices. Smart sensor networks can provide real-time information of the condition of the devices in a factory. However, due to a wide variety of sensors available in the market, sensor manufacturers are searching for open and standardized sensor and factory network protocols to enable plug-and-play capabilities and enhance interoperability of the devices. The ability of automated transfer of sensor metadata and characteristic data contained in the datasheets to a system for self-configuration reduces human errors by manual entering of data, thus help to increase the reliability of the system and ease the sensor installation and maintenance. This project focuses on the exploration of the MTConnect protocol and relevant IEEE 1451 smart sensor network protocols and the seamless, vertical integration of these standard protocols in a system, enabling the ease of real-time access of sensor information and validating the performance of the system.

Monitoring and Analyzing the Deployment of Resource Public Key Infrastructure (RPKI) Within the Internet

Luis Perez Cruz

The Border Gateway Protocol (BGP) is an Internet protocol that allows the exchange of routing information between different autonomous systems (AS). It keeps a logical table that states the path that a certain AS needs to follow in order to reach a specific IP address owned by another AS.

Over the past few years, misconfigurations and malicious attacks against BGP routers have resulted in sending routing information to the wrong direction. As a by-product, portions of the Internet have been knocked down, causing large losses to different Internet-based companies and placing sensitive information in danger. RPKI is an infrastructure designed to secure routing processes on the Internet. It contains Route Origination Authorization (ROA) objects that allow the router to verify whether a certain AS is authorized to announce a block of IP addresses.

This project aims to present an analysis of routing information downloaded from RouteViews on a daily basis and to determine its validity by comparing it against ROA objects downloaded on the same day. The objective is to build a web application that displays different graphs and statistics that will show how wide the RPKI is deployed, its characteristics and how much percentage of the routing information collected can be verified. The goal is to monitor RPKI deployment and provide statistics useful for the internet community that will help to foster the infrastructure development and deployment process.

The Advantage of Using TiO_2 in Improving the Performance of Dental Resins

Brismar Pinto-Pacheco

The durability of dental adhesives is one of the keys for success of the resin-composite restorations. Previously studies have showed the resin performance determined the durability of the adhesives. The purpose of this study is to improve the performance of dental resins currently used by adding a small amount of titanium dioxide nanoparticles (TiO_2 NPs), which have outstanding mechanical properties and unique photo activities. Not only is it inexpensive, with titanium being the fourth most abundant metal on earth (followed by aluminum, iron and magnesium), it is also non-toxic. In order to improve the mechanical properties of dental resins, unmodified TiO_2 NPs (P25 and P90) and acrylic acid modified TiO_2 NPs (AP25 and AP90) were prepared as organosols in ethanol and added to the two resins that were being studied in this project: Ethoxylated bis-phenol-A-dimethacrylate (EMDA) and a mixture of bis-phenol-A-dimethacrylate and hydroxy-ethyl-methacrylate (B+H) in a mass ratio of 1:1 (99.9% resin: 0.1% TiO_2 NPs). The mass fractions of TiO_2 NPs in organosols were determined using the Weight-Lost method, and the TiO_2 concentrations were also evaluated using the UV/Vis. The degree of vinyl conversion (DC) of resin bars made of the above resins were evaluated using FTIR before and 5 minutes, 1 hour, 24 hours and 1 week after being curing using blue light. The mechanical properties of the same resin bars were determined using the 3-point and dynamic mechanic analysis (DMA) to measure the elastic modulus and viscoelastic properties, respectively.

The FTIR confirmed the success of the acrylic acid functionalization. The DC of the AP25 increases about 2% versus the unmodified TiO_2 NP (P25). After curing, the DC remained the same at the four time points tested, proving that the reaction ends in a short period of time. The 3-point-bending and the DMA results confirmed the improvement of the modulus and the elasticity of the resins by adding TiO_2 NPs.

The results show that by adding a small amount of AP25 or AP90 to the resin, the DC and mechanical properties of the resins can be improved significantly, provoking a better performance when used as backbones for dental adhesives. In the future it should be determine if changing the concentration of modified and unmodified TiO_2 NPs has a positive effect on the durability and hardness of the resin.

Hydration Dynamics of Thin Nafion Films Studied with Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS)

Estefanía Quiñones Maléndez

Fuel cells, which consist of an anode, a cathode and an electrolyte, are electrochemical devices capable of converting chemical energy into electrical energy. They are usually distinguished by the type of electrolyte they use in charge transport. The one that inspired this project is well-known as the polymer electrolyte membrane (PEM) fuel cell since its electrolyte consists of a polymer membrane. These fuel cells, while facing cost and durability issues that inhibit their widespread commercial use, remain a promising technology for cleaner, renewable, and more efficient energy conversion. Understanding the hydration dynamics in thin films of Nafion, the most prevailing PEM material, is one of the key factors for addressing these issues and optimizing fuel cell performance. Hydration dynamics are important to understand because the solubility and mobility of water within the membrane material is intimately related to the fuel cell's conductivity and performance.

The focus of this talk is presenting the use of polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS) to investigate water diffusion and interfacial transport within Nafion thin films (5 -200 nm thick). Typically, the study of the kinetic processes of diffusion and interfacial transport are complicated by simultaneous polymer relaxation that occurs with water sorption in these materials. Due to the overlap of these three processes, it has been difficult to determine which one predominates and truly defines the kinetics of sorption in thin films. But by switching between H2O and D2O at constant relative humidity we manage to remove contributions from relaxation processes and thus provide a proof of concept in advancing the measurement science behind understanding the role of multiple processes involved in hydration kinetics of PEM materials.

Instrumentation of Geothermal Heat Pump Test System

Norman J. Rivera-Cotty

Geothermal HVAC systems use a heat pump coupled to the ground rather than the air to reduce energy consumption. The NIST Net-Zero Energy Research Test Facility (NZERTF) house uses a Geothermal HVAC system to reduce the electric load on the solar panels. Three different types of geothermal heat exchangers were instrumented to measure and compare their energy and economic performance.

Design of geothermal heat exchangers requires knowledge about the thermal conductivity and capacity of the soil they are installed in. These soil properties can be determined using a Thermal Response Test (TRT) which involves circulating hot water through the geothermal heat exchanger to simulate a heat pump load. The time evolution of the circulating water temperature can be used to infer the thermal properties of the soil, and to determine the effectiveness of the heat exchangers. A methodology was developed for determining the soil properties and comparative performance of the heat exchangers using a procedure established by the American Society of Heating, Refrigeration, and Air-conditioning Engineers (ASHRAE).

An experimental apparatus has been constructed to perform the TRT tests for the NIST Net-Zero Geothermal system. The test rig includes pressure, temperature, and flow sensors, as well as a variety of safety sensors to protect against over-pressure/temperature and leaks. The sensors were assembled and integrated with the TRT rig Control Cabinet and Data Acquisition System (DAS). Additional sensors were buried in the ground to monitor soil temperatures, these sensors were connected to the DAS. The data acquisition and recording is controlled using a program written using the LabVIEW software.

Testing and Traceability of Entropy Sources for Random Bit Generation

Angel J. Rosado Rosado

A random number or bit generator is a computational or physical device designed to generate a sequence of numbers or symbols that lack any pattern. Cryptography and security applications make extensive use of random numbers and random bits for generating keys and other critical security parameters. The most important requirement of a random bit generator is having a good, reliable source of entropy. However, the generation of random bits is problematic in many practical applications of cryptography. With this in mind a set of statistical tests has been created to measure the entropy in each output sample of an entropy source. NIST Special Publication 800-90B specifies the design and testing requirements for entropy sources that can be validated by NIST's CAVP and CMVP.

During my internship I have been working reviewing software that implements the statistical tests defined NIST Special Publication 800-90B for testing entropy sources used for Random Bit Generation. As part of my role in the summer, I went through the code, reviewing, commenting and verifying that it conforms to NIST SP 800-90B. I also created a UML diagram to visualize and document the structure of the application and started creating a Graphical User Interface (GUI) for running tests and creating reports.

In my presentation I will give a briefing about Random Bit Generators and how it is used in security and cryptography. Also a quick review of the different tests used to measure the entropy of an output sample of an entropy source. I will talk about the tools used in order to review the software and the tools used to create the UML Diagram and the GUI.

Test Lines Segmentation Performance Assessment Tool
Luis Rivera Santiago

Text line segmentation is considered to be an essential preprocessing step to decompose the document images to be used in other document analysis tasks such as text recognition. The Multimodal Information Group in the Information Access Division of ITL plans to conduct a benchmark test to survey the current state-of-the-art performance in document image text line segmentation. In this talk I will describe the software tool I developed to assess the system's ability to segment the text lines. I will explain the Munkres assignment algorithm and my implementation to find the optimal match between the line zones produced by the system and the ground truth. I will conclude with a demonstration of the tool features.

University of the Sciences

Characterization of Carbon Nanomaterials
Amanda Huon

Carbon nanomaterials such as nanotubes (CNTs) are electrically conductive nanomaterials with a diameter of several nanometers and lengths up to several hundred micrometers. Due to this highly anisotropic geometry, CNTs can conduct electricity along its long axis, while the small diameter makes them virtually transparent at optical wavelengths in the range of 400 nm to 800 nm. Networks of interconnected tubes maybe arranged into mechanically strong conducting films with high transparency whose performance may exceed existing transparent conductors, thin metal films or metal oxides. Understanding the fundamental relation that governs transparency and conductivity in such networks is of primary importance for both scientific and practical purposes. The transparency of these conductive films has been previously modeled based on their electromagnetic properties, and modified to describe CNT films [1]. In our earlier work, we had used these semi-empirical equations and found that the theoretical model did not agree with our experimental results for CNT density near the percolation transition, where the films are mechanically strong and highly conducting [2].

These results have motivated the present project, where the aim is to develop CNT growth conditions to control both length and density, and study the percolation threshold. The CNTs were grown by a catalyst Chemical Vapor Deposition process using alcohol as a carbon source. We found that utilizing cobalt as the catalyst and aluminum as the catalyst-support material enhanced the growth of the vertically aligned multi-walled carbon nanotubes network. In order to have reproducible growth of CNTs, control of the catalyst and catalyst support deposition conditions is critical and will be discussed. Further, the results of optical and SEM measurements done to characterize theses samples are presented.

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University of South Alabama

Enabling the Extraction of Publications Metadata
Adam Moore

The Computer Security Division of the ITL contains a large number of publications, including Internal Reports, Security Bulletins, and Special Publications. Currently, it is difficult to maintain an accurate representation of the information contained within these documents. Semantic technologies offer a method for organizing these documents. In particular, semantic technologies provide a method for encoding the relationships between documents in a machine-readable graph of information. This graph may be used to standardize terminology and easily visualize the relationships between documents. Additionally, the Resource Description Framework (RDF) specification provides a standard data format allowing the resulting data to be easily utilized by the Computer Security community.

I will present the prototype of a software system that utilizes semantic technology to extract metadata from CSD publications. I will present the architecture of the system, including third-party software applications that provide the metadata extraction and data-viewing capabilities. To conclude, I will discuss the challenges involved in the development of the system and strategies for utilizing the resulting semantic data.

University of South Carolina

Investigating ECM Biomolecule Interactions
Jillian Matson

The extracellular matrix (ECM) provides structural support and chemical cues to cells in order to maintain tissue function. The ECM is composed of three major classes of biomolecules: (1) structural proteins (2) specialized signaling proteins and (3) proteoglycans. Collagen is one of the major structural proteins in the ECM. Interactions between collagen and proteoglycans are important in tissue function but are not fully characterized. In this study we used a model ECM system composed of a collagen functionalized substrate and glycosaminoglycans (GAG), a major component of proteoglycans. To study the interactions between collagen and GAG, we used Quartz Crystal Microbalance with Dissipation monitoring (QCM-D) to study the effects of ionic strength and pH on collagen-GAG association. With QCM-D it is possible to qualitatively understand the strength and reversibility of the biomolecular interactions along with mechanical changes in the collagen substrate. Our results indicate that the association of GAG with collagen differs as a function of ionic strength. At physiological pH (7.4) and low ionic strength (0.1 M NaCl solution), interactions between collagen and GAG are strong and irreversible, however they are weaker and irreversible at higher ionic strength (1 M NaCl solution). Additionally, we found collagen fibrils were not stable at lower pH (5.5). These studies demonstrate the utility of QCM-D as a tool to observe the interactions of ECM biomolecules in varying conditions. By gaining a better understanding of ECM interactions in physiological and experimental conditions, new strategies in therapeutic and regenerative medicine, may emerge.

University of Texas Dallas

Quick Read Codes Made by Nanoindentation
Meagan Kelso

The Atomic Force Microscope, or AFM, has the capability of imaging the geographical characteristics of materials and manipulating their surfaces. With new technology and software today, it is possible to create small indentions of lines and shapes on a sample, but can the AFM pinpoint atoms on a surface to control them? The goal of my research is to create a micro-scale type of quick read code with the AFM by pushing dopants into a material in a random pattern. This will create a unique mark that is not easily replicable or noticeable by a third party, and can be printed on items sent to the military as a way to achieve a higher level of anticounterfeiting. By using an AFM to achieve this technique rather than other small-scale microscopes, the code could be cheaply and quickly printed onto items, and easily read by the desired recipient. In the process of becoming acquainted with how the AFM operates, I was also able to assist others in their research of analyzing Through-Silicon Vias, or TSVs. With the use of other, more common modes of the microscope, the height and potential of several TSVs were measured, which had been heated and cooled a different number of times. The collected data has helped in illustrating properties of SiO_2 that can be used to enhance future electronics.

Ghosts in the House
André R. Rosete

The Net Zero Residential Test Facility (NZERTF) is a residential home built on the NIST campus that enables the development and demonstration of measurement science needed to achieve net zero energy homes. NZERTF will be used to demonstrate that a residence typical of the size and aesthetic design of homes in the Washington, D.C. metropolitan area can produce as much energy as it consumes on an annual basis. Energy consumption inside the house must therefore be tested in a reliable and repeatable manner. For that purpose, the house occupants cannot be actual people; they must be simulated to ensure consistency. Appliances must also be simulated in order to represent the activities of the occupants, such as cooking, laundry, and domestic hot and cold water usage. In order to properly represent occupancy, both sensible and latent heat produced by the residence are also simulated. I have built and wired circuitry inside metal boxes with heat-generating resistors on top, which can be used to simulate electrical loads or people by adjusting the current using a dimmer on the side. I have also built similar metal boxes that have outlets, to which actual appliances can be connected so that they may be remotely turned on or off. The activities happening in the NZERTF are based on a pre-defined occupancy profile and hourly schedule, all remotely controlled by software and hardware. The control schedule is built around a narrative of the daily life of a family of four, including two adults and two children. I have programmed an interface that shows which appliances and lights are currently active, and also where the 'people' in the house are currently located, serving as a visual representation of the occupancy profile. The successful simulation of occupants is essential to ensuring the feasibility of building a net zero energy facility in the Washington, D.C. metropolitan area.

University of Virginia

Modeling Material Information Flow Through the Product Lifecycle
Arvind Harinder

The sustainability impact of a product is not determined at a single life cycle stage, but measured and aggregated across all stages of a product's life cycle. Material choice greatly affects sustainable impact of a product, and serves as a common thread between each stage of the life cycle. However, to leverage this common underpinning between life cycle stages, we first need to understand how material information flows through the life cycle. This project aims to understand this information flow by synthesizing commonly used information representations across different stages of the product life cycle. To accomplish this, the first step was to identify the stages of the product life cycle. Then, standards used in modeling product information were mapped to their respective stages on a life cycle chart. Finally, using three selected standards, I created an ontology to demonstrate the mapping of material information flow across the life cycle. This work contributes to the Generic Product Structure (GPS) under development in the Sustainability Metrics for Manufacturing (SMM) project under the Sustainable Manufacturing Program at NIST.

Virginia Polytechnic Institute and State University

Cavity Optomechanical Sensors for Atomic Force Microscopy
Stephen Epstein

Atomic force microscopy is a technique to image surface topology down the level of individual atoms and has been an essential tool for micro-/nanoscale studies in physics, chemistry and biology. Cavity optomechanical atomic force microscopy consists of an AFM probe in close proximity with a microfabricated optical cavity. The close proximity of the AFM probe and optical cavity creates an integrated interferometry optical readout. The integrated interferometry optical readout is possible because of the recent improvement in microfabrication techniques and optical readout schemes. Cavity optomechanical atomic force microscopy shows promise to extend the utility of conventional atomic force microscopy by being more sensitive and having a much faster acquisition speed than traditional atomic force microscopy.

The specific device approach being considered is a nanoscale elastic beam that wraps around an optical whispering gallery mode resonator. The geometric design of the nanoscale mechanical probe needs to be optimized while maintaining high optomechanical coupling for high sensitivity. The desired characteristics are a high resonant frequency for high acquisition speed, low probe stiffness for high sensitivity and high probe stability. One of the aims is a mechanical probe design that has a natural resonant frequency of 10 MHz. The probe design space is being studied by analytical and finite element modeling techniques. The geometric design space being considered is consistent with the limitations of current microfabrication techniques. Comparing the optical mechanical coupling of different probe geometries is achieved by numerically calculating the path integral of the normal distance between the optical whispering gallery mode resonator and the displaced mechanical probe.

How to Feed and Water Your Dishwasher
Kelly Webster

Residential appliances account for about 20% of the energy consumption in a household. When operated correctly, more energy efficient appliances not only reduce environmental impact, but can also decrease the homeowners' water and electricity expenses.

NIST supports the Department of Energy (DOE) in specifying the test procedure used to rate all machines sold in the United States. The Federal Trade Commission (FTC) specifies the Energy Guide label to post energy performance data on all new models. The Environmental Protection Agency (EPA) encourages reductions in the amount of energy and water used by home appliances through the Energy Star label, which identifies models that are 10% more efficient than standard dishwashers, according to the DOE test procedure. Manufacturers wishing to have an Energy Star label affixed on their product must meet specific requirements.

The focus of the dishwasher project is to investigate the quality of the test procedure: Is it representative of field use? Is it repeatable across labs? Are tests reproducible? Is there a way to minimize test burden? And although energy and water are conserved, does the dishwasher clean well?

With the Energy Guide and Energy Star distinction on manufacturers' products, consumers can make more educated purchases. Thus, this testing will have a direct and positive impact on the United States' energy consumption.

Virginia State University

Android Defense Science
Major McNair

TransApps is an ongoing research project by DARPA (Defense Advanced Research Projects Agency) to keep our soldiers safer in the field. Android based handheld devices are configured to use applications that would save much need time and effort on missions. TransApps provides the foundation for fast, high level communications. The system consists of android-based handheld devices, a tactical maps communication server, and an app-store. Currently over 1000 handheld units are being field tested with more expected to be deployed in the near future. NIST is tasked with regression testing the handheld devices, the web-based servers, and communication mechanism between these devices. Regression testing is a type of software testing that for bugs and glitches as well as testing whether previous bug fixes haven't made new bugs. The tactical maps communication server acts as a stationery or mobile headquarters. Independent test plans have been developed by NIST to test the capabilities of the system. In addition to the test plans, NIST testers provide feedback to the application developers on ease-of-use, and functionality. The Client (Server Operator) side of the project allows a user to gather information (e.g., exact location, general observations of their environment with and without geo-location) from many handheld users at the same time. I was tasked with testing the capability of Client-side of the system. For example, could a leader act quickly to change planned routes/destinations and provide up-to-date information gathered from different locations to squads that need it? Having access to instant information allows squads in hostile terrain to function more effectively by being able to make intelligent decisions quickly.

Virginia Wesleyan College

Investigation of Sample Matrix Effects Using Spinning Sampling Chamber Laser Ablation ICPMS
Matthew Boyce

Laser Ablation Inductively Coupled Plasma Mass Spectroscopy (LA-ICP-MS) is becoming an increasingly utilized tool in conducting direct elemental analysis of solid samples. While it is gaining popularity in geological, environmental, and forensic analysis, it is still limited in its analytical application. For current methods to produce quantitative results, they require reference materials that are matrix matched to the analyte, so the ablations can be considered comparable. This project seeks to overcome the need for matrix matched reference materials by utilizing a spinning sampling cell. By rotating the sample, multiple materials can be ablated at once, allowing for gas phase mixing followed by simultaneous ICP-MS analysis. Isotopically enriching one of the ablated materials allows for correction in the ablation differences between the materials' matrices. A rapid standard addition method can provide quantitative measurements of the elements present in a sample. This methodology can facilitate the analysis of many solid sample types that are typically difficult to analyze.

Developing a Library of Selenium Nanoparticles Based on Charge, Size and Stability
Darren Driscoll

Chemicals in their nanoparticle form have properties that are completely different from their bulk forms. Additionally, depending on size and charge, nanoparticles may exhibit different effects in biological or environmental systems. Also, stability plays an important role in the duration that these nanoparticles could affect a biological or environmental system. Little research has been done in accords to selenium nanoparticles and their possibilities within our environment. This classification is the first step into delving into the research of monodispersed selenium nanoparticles.

In order for necessary risk assessments and further hypothesis testing to occur for the differing sizes and charges, libraries of well-defined materials with systematic variations are required, for example various capping agents (with different surface charges) and various sizes. In this work, a single synthesis approach was used to create varying sizes of red selenium nanoparticles with different capping agents. Three different compounds, bovine serum albumin (BSA), cetyltrimethylammonium bromide (CTAB) and sodium dodecyl sulfate (SDS) were all used as capping agents in the selenium nanoparticles synthesis. With varying concentrations, each capping agent produced a range of monodispersed nanoparticles, each with varying stability. The nanoparticles were classified into three categories: small ≈ 30nm, medium ≈ 60nm and large ≈ 90nm. The focus of further experiments can be the hypothesis testing within each of the categories in order to test stability as well possible interactions within biological and environmental systems.

Wake Forest University

Exploring Organic Magnetoresistance in Spintronic Devices
Alyssa Brigeman

Organic spintronics is a promising field of research which combines desirable features of organic semiconductor devices such as low-cost, ease of fabrication and mechanical flexibility with the nonvolatility of spintronic devices. Recently, progress in the field led to the discovery of a new physical phenomenon unique to organic semiconductors, called organic magnetoresistance (OMAR). Magnetoresistance refers to a change in the electrical resistance of a material in response to an external magnetic field, and has been studied extensively in traditional electronics leading to the discoveries of giant (GMR) and tunnel (TMR) magnetoresistance—phenomena utilized in industries to increase storage density on hard disks by achieving high resolution read heads. Since OMAR provides great potential for applications in future organic spintronic technologies, it is important to understand OMAR and how we can control it.

Unlike other types of magnetoresistance, OMAR is observed in nonmagnetic organic devices, and therefore cannot be explained by the same mechanisms as GMR or TMR. OMAR research is thus directed towards determining a physical explanation for this unique and novel phenomenon. A few theories have been proposed, generally based on spin-mixing between singlet and triplet states due to hyperfine coupling and its dependence on an externally applied magnetic field. However, as the detailed and precise theory elucidating the physical mechanisms causing OMAR is still missing, the phenomenon remains an intriguing research topic.

In order to understand possible causes of OMAR, multiple devices with various structures were fabricated using a thermal deposition technique. The magnitude of OMAR (magnetic field dependence of electrical resistance) was measured against the thickness of the organic semiconducting layer in the device, the introduction of a self-assembled monolayer (SAM) between the anode and semiconductor to match the highest occupied molecular orbital (HOMO) level of the organic semiconductor with the Fermi level of the anode, and the insertion of hole-injection-assisting polymer layer between the anode and semiconductor. OMAR measurements were taken on a commercial probe station—a constant bias voltage was applied across the device, and an external magnetic field (up to 100mT in magnitude) was swept. We have observed significant OMAR in the fabricated devices, and have found that the strength of OMAR varies as the device structure or the applied voltage changes.

Weber State University

Glycoanalysis Using Universal Proteolysis and Mass Spectrometry: Showing Off the Sweet Side of Proteins
Nicholas Smith

Glycosylation is the post-translational modification of a protein that occurs when a carbohydrate chain, known as a glycan, is enzymatically added to the protein. The two most common types of glycosylation occur with N-linked and O-linked glycans that attach to asparagine and serine/threonine amino acids, respectively. Previous studies at NIST developed a proteolysis (protein digestion) workflow that identifies glycosylation sites, as well as chain sequence and branching information, of N-linked glycans. The first goal of this project was to assess the applicability of universal proteolysis (lysis of all peptide bonds) and mass spectrometry (MS) for relative quantification of N-linked glycans. LC-MS of a universal digest of RNase B yielded relative quantities of Man5 through Man9 glycans. These results were in good agreement with those obtained from the currently accepted technique of HPLC using fluorescently labeled glycans. Universal proteolysis and LC-MS minimize offline sample handling and reaction steps, thereby reducing user-dependent variability.

The second goal of the project was to expand universal proteolysis to O-linked glycoproteins. O-linked glycans have historically been more difficult to characterize due to unwanted side-reactions of commonly used glycan release methods. Universal proteolysis avoids these shortcomings by using much milder conditions and because the glycan reducing terminus remains protected by an amino acid after digestion. Universal proteolysis followed by permethylation was used to analyze the glycans of κ-casein. Two sialylated O-linked branching isomers were distinguished via MSn (multiple sequential stages of fragmentation) analysis. This demonstrates for the first time the potential of universal proteolysis for complete characterization of O-linked glycans. These efforts represent critical additions to the glycoanalytical toolbox and will be invaluable in the detailed characterization of future glycoslyated protein standard reference materials.

Westminster College

Simplifications and Generalizations of Generating Functions for Classical Orthogonal Polynomials with Definite Integrals

Connor MacKenzie

In this talk we dive into the world of classical orthogonal polynomials. We will cover simplifications and generalizations we derived this summer of important expansions, called generating functions, which are associated with these polynomials. We then use these expansions to derive definite integrals related to the generating functions and their generalizations. The classical orthogonal polynomials are used in fields like mathematical physics, approximation theory, and numerical analysis. Finding these simplifications and generalizations often gives us insight into the properties and interrelations for the classical orthogonal polynomials. The definite integrals can show up anywhere in applied mathematics, so finding them will provide a great resource to others. My research so far has found many interesting simplifications such as reducing some of the fundamental generating functions for orthogonal polynomials into elementary functions. I have also found interesting properties related to the even- and odd-ness of the degree of the polynomials.

Whitman College

The Effects of Helium Upscattering and Neutron Absorption on the Neutron Lifetime

Nathan Abrams

A free neutron is known to decay into a proton, electron, and an electron antineutrino. The current accepted lifetime for the unstable neutron is 881.5 ± 1.5 seconds. However, recent ultracold neutron bottle experiments have produced statistically different neutron lifetimes, indicating unknown systematics with measurements. Accurately knowing the neutron lifetime affects both the Standard Model of particle physics and our understanding of the Big Bang. The experiment I will discuss has a general procedure of creating ultracold neutrons, trapping the ultracold neutrons, and observing the ultracold neutrons decay. One of the experiment's systematic effects is helium upscattering. Another of the experiment's systematic effects is neutron absorption by helium-3. Both systematic effects cause a loss of neutrons in the trap. The specific goal of my project is to determine the systematic effects of the helium upscattering and neutron absorption. The presentation will explain why the neutron lifetime matters, outline how the experiment works, address helium upscattering and neutron absorption, and describe the process of determining the values of the systematic effects.

Whitworth University

Testing the Performance of 6LoWPAN-Based Wireless Sensor Network

Minh Trang Nguyen

Nowadays, the innovation of technology has made many progresses. Wireless sensor network technology is considered as one of the key technologies that will revolutionize the way we live in the 21st century. It is possible due to the recent advances in wireless communication, networking, micro-electronics, and low-cost and low-power microprocessors. Understanding the connectivity and communications between sensors and a network will improve the effective management of network strategies, especially for wireless networks. In order to do that, the performance of networks needs to be investigated and tested using a Factory Equipment Network Testing (FENT) Framework. One specific wireless sensor network called IPV6 over Low power Wireless Personal Area Network (6LoWPAN), is an upcoming protocol which will enable the deployment of wireless networks using the Internet Protocol Version 6 (IPv6) on the smallest devices.

This project focuses on exploring the characteristics of an IEEE 1451.5 - 6LoWPAN-based sensor network and developing a software solution to integrate this sensor network into the FENT testbed. Then the performance of the 6LoWPAN network could be assessed using Wireshark, a software package that is used for software and communication protocol development, network troubleshoot, and analysis. We are also active in developing the experimental FENT framework to further investigate the connectivity and performance of different types of factory equipment networks that would be used by many users and industry.

Worcester Polytechnic Institute

Studying Phase Transformations in Al/Ni Reactive Multilayers Using Nanocalorimetry
Bernadette Cannon

Many metal combinations exhibit exothermic mixing reactions. These reactions have applications as local heat sources, including joining and munitions. In this work, we study reactions in the Al/Ni system using a nanocalorimeter. The nanocalorimeter is a MEMS device that collects thermodynamic data from small samples with mass ranges of tens to hundreds of nanograms. It consists of a platinum heater/sensor across which a current is applied and voltage is measured using a four-point probe configuration; the temperature coefficient of resistance for each chip is calibrated optically using a pyrometer. The nanocalorimeter allows us to heat Al/Ni samples in a rapid but controlled manner and to monitor the energy released during the subsequent reactions. In these experiments, we have observed changes in the number of exothermic peaks as a function of heating rate, pointing to possible suppression of intermediate phases as the heating rate is increased. We hypothesize that this phase suppression may be due to large concentration gradients which develop at higher heating rates. In order to confirm or strengthen this hypothesis, the next step is to identify the phases which are forming at each exothermic peak. Plans are under way to conduct *in situ* nanocalorimetry experiments in a dynamic transmission electron microscope in order to simultaneously capture thermodynamic data and image and identify the phases as they form at various high heating rates.

Thin Film Deposition of Quantum Dots (Nanoscale Characterization of Photovoltaic Devices)
Anthony Gianfrancesco

Properties of thin-film semiconductor photovoltaic (PV) devices such as CdTe or CIGS are critically dependent on nanoscale structure and morphology. To improve the quality of such materials, characterization techniques are needed that probe the devices at the level of a single grain or grain boundary. Previous attempts at such a characterization have been the use of laser beam induced current (LBIC) images which have obtained as high as ~1 micrometer. In this work we use thin film quantum dots (616 nm) as a near-field optical source into a PV material. We first characterize the conditions necessary for creating a uniform thin film of quantum dots (QD) on CdTe and polycrystalline Si. We then use AFM to image the morphology of the surface, as well as an SEM to quantify the thickness of the thin films. Once a desirable, reproducible thin film has been created, we can then look forward to the nanoscale characterization of the PV materials. We do this by injecting an electron beam into the QD layer generates photons; these generate photo-carriers in the solar cell. The generated photo-carries are collected by the top and bottom contact on p-type and n-type semiconductors, respectively. Such sets of current images allow us to evaluate the impact of charge transport and recombination at the grain boundaries on device performance.

CFAST and the Incorporation of Uncertainty
Barbara Hall

Fire modeling is an efficient way to simulate fire situations for analysis. There are many reasons that modeling may be carried out, spanning from reconstruction of a fire scene for a criminal investigation to testing of a fire suppression system array during the design process of a building initially or while undergoing renovation, all correlating to the fact that it is too costly to physically build and destruct structures for every scenario. The Consolidated Model of Fire and Smoke Transport, commonly known as CFAST, was created at the National Institute of Standards and Technology. The creation of CFAST began in 1988 with the precursor program FAST. Improvements consisting of revisions and the addition of new components have occurred throughout the years since, resulting in new versions. Version 6.2, the most recent edition available to the public, was released in November of 2011. CFAST uses operator specified input parameters, such as building materials and the environment in which the situation occurs, to solve commonly used fire protection engineering equations. Calculations carried out during the simulation provide an insight to the buildup and spread of fire, heat, and gases throughout the compartments, the activation time of detectors, and the available time for an occupant to exit the structure or area. As with any other experiment there are always uncertainties that cause a variation in results produced. Currently, when using CFAST, there is no way to include the factor of uncertainty in a fire simulation. Uncertainty in this case may relate to the input parameters or to the equations used to calculate the output values resulting from the simulation. One way to combat doubt in produced results is to carry out multiple simulations. Up to this point a user must set up each simulation in CFAST, manually start it, then repeat the process for each simulation they carry out. Work was carried out at the National Institute of Standards and Technology and also at Worcester Polytechnic Institute that led to the development of a tool to aid in the automated initiation of numerous simulations, incorporating uncertainty, to produce results in a timely manner. The work carried out at NIST, based on knowledge of CFAST, involved the creation of an input file template, compatible with the most recent version of CFAST, and assessment of the functioning tool. The work carried out at WPI, based on knowledge of the FORTRAN programming language used to code the CFAST program, pertained to the coding of the tool.

Modeling Upholstered Furniture in Fire Environments with CFAST

Andrew Nelson

Statistically, upholstered furniture has been shown to play a major role in fire-related deaths. The NIST-developed fire modeling program CFAST (Consolidated Model of Fire and Smoke Transport) was used with the ignition literature to characterize the contribution of upholstered furniture to fire spread and growth in residences. A particular focus was the potential development of untenable conditions and flashover. The project involved comparing fire growth scenarios on upholstered furniture and other types of materials typically found in residences, as well as secondary ignition of nearby items. Parameters varied included fire size and growth rates, floor area and room volume, ventilation parameters, and ignition behavior. Realistic ranges of these parameters were chosen to represent a broad range of fires that may occur in residences.

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2012

SURF STUDENTS BY

ORGANIZATIONAL UNIT

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UNIVERSITY	STUDENT	TITLE OF TALK	OU
St. Olaf College	Barkley, Sarice	Testing Shapes and Sizes of the Diamagnetic Lateral Force Calibrator	CNST
Savannah State University	Brooks, Sterling	Catalyst Structure Investigated by In-Situ HRTEM Measurement During CNT Growth	CNST
University of Michigan	Collins, Sean	Chemical Heterogeneity of Wildfire Aerosol Emissions: Implications for Climate Change	CNST
Virginia Polytechnic Institute and state University	Epstein, Stephen	Cavity Optomechanical Sensors for Atomic Force Microscopy	CNST
Worcester Polytechnic Institute	Gianfrancesco, Anthony	Thin Film Deposition of Quatum Dots (Nanoscale Characterization of Photovoltaic Devices)	CNST
State University of New York Binghamton	Guss, Jason	Spin Current Polarization in Amorphous CoFeB Measured via the Spin-Wave Doppler-Effect	CNST
State University of New York Albany	Janiszewski, Brian	Chemical Surface Patterning	CNST
University of Nebraska Lincoln	Lintel, Anton	Domain Size Dependence of Sucessive Alternating Layers of Co and Pd	CNST
Purdue University	Savikhin, Victoria	Assembly and Measurement of Quadruplex DNA Nanomaterials	CNST
Colorado School of Mines	Thurston, Bryce	Electronic Transport Properties of the etal Organic Framework $Cu_3(BTC_2)$*TCNQ	CNST
University of Delaware	D'Alessio, Anna	Are You Being Greenwashed	EL
University of Maryland College Park	Connolly, Kathryn	Durability of Backsheet Polymers Used in Photovoltaic Applications	EL
Millersville University of Pennsylvania	Consylman, Ryan	A Case Study for Sustainability Modeling and Optimization	EL
University of Maryland College Park	Dorson, Ryan	Reasoning with PrIKL	EL
Gonzaga University Washington State	Engel, Samantha	Rheological Properties of Sustainable Ternary Binders	EL
University of Maryland College Park	Faenza,Nicholas	Reduced Flammability of Polyurethane Foam Using a Layer-by-Layer Assembly with Natural Materials	EL
University of Maryland College Park	Gaume, Patrick	Effects of Key Environmental Factors on Degradation of Polymeric Films Used in Protective Glazing Systems	EL
University of Puerto Rico	Gil Acevedo, Jennifer	Durability Study of Polymer Nanocomposites	EL
State University of New York Stony Brook	Ging, James	Fate of Carbon Nanotubes in Polymer Nanocomposites Exposed to UV Radiation	EL
Loyola University Maryland	Gorbaty, Andrew	Web Based Applications for Machine Tools	EL
Reed College	Gould, Max	Verification of Computational Fluid Dynamics Program for Fire Modeling	EL
Worcester Polytechnic Institute	Barbara Hall	CFAST and the Incorporation of Uncertainty	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Hamins-Puertolas, Adrian	Measuring Inadequate Interoperability in the Manufacturing Industry	EL
University of Virginia	Harinder, Arvind	Modeling Material Information Flow Through the Product Lifecycle	EL
State University of New York Binghamton	Hebenstreit, Keith	Measurement Systems for Additive Manufacturing Processes	EL
University of Maryland College Park	Hemley, Scott	Computational Fluid Dynamics Simulations for Building Aerodynamics	EL
Alabama A&M University	Hines, Shannon	Fire Resistant Foam	EL
Arizona State University	Jaber, Abbas	Parsing COLLADA: A Robust Method for Inputting Geometry Into FDS	EL
Arizona State University	Keberle, Katelyn	Environmentally-Friendly Flame Retardant Coating for Polyurethane Foam	EL
State University of New York Binghamton	Kesten, Evan	A Low-Cost 3D Safety System for Robot Applications	EL
New College of Florida	Lang, Sophie	Bench Scale Measurements of Toxic Effluents in Fire Smoke	EL
University of Maryland College Park	Li, Kevin	Comparison of FDS Predictions with Gas Velocity Measurement sin the Exhaust Duct of a Stationary Source	EL
University of Maryland College Park	Liang, Lipeng	Dynamic Update of MySQL Database in Kitting	EL
Texas Southern University	Mbonu, Ray	Fire Proof Foams	EL
Virginia State University	McNair, Major	Android Defense Science	EL
Worcester Polytechnic Institute	Nelson, Andrew	Modeling Upholstered Furniture in Fire Environments with CFAST	EL
University of Maryland Baltimore County	Newcomer, Matthew	Performance Assessments of Tactical Handheld Android Applications for Warfighters	EL
Whitworth University	Nguyen, Minh Trang	Testing the Performance of 6LoWPAN-Bassed Wireless Sensor Network	EL
University of Puerto Rico	Nieves-Nevárez, Mairim	Wireless Sensor Networks for Machine Monitoring	EL
State University of New York Binghamton	Presser, Brian	Benefits and Costs of Energy Efficiency in New Buildings	EL
University of Pennsylvania	Reidy, Sean	A Picturesque View of Sustainable Manufacturing Standards	EL
Brigham Young University	Richardson, David	Multi-Split HVAC Unit Testing and Analysis	EL
University of Puerto Rico	Rivera-Cotty, Norman	Instrumentation of Geothermal Heat Pump Test System	EL
Loyola University Maryland	Rose, Allison	Calibrating Laser Range Scanners for Robot Safety	EL
University of Texas Dallas	Rosete, André	Ghosts in the House	EL
University of Maryland College Park	Sanker, Erica	An Analytical Finite element Model of Micro- and Nanoscale Electrostatic Beam Resonators	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Brown University	Schear, Jonathan	Modeling the Temperature of Panels Exposed to the Outdoors	EL
University of North Carolina Charlotte	Savage, Luke	Diamond Turning Machine Characterization	EL
Arizona State University	Stehlik, Daniel	Beginning Standardization of Condition Monitoring Tests for Cables in Nuclear Power Plants	EL
University of Maryland College Park	Valivullah, Lina	Manufacturing Specific Process Information Models for Sustainability	EL
State University of New York Binghamton	Watkins, Megan	Sustainability Analysis of a Die Casting Process	EL
Virginia Polytechnic Institute and State University	Webster, Kelly	How to Feed and Water your Dishwasher	EL
University of Maryland College Park	Wiess, Emily	Building Evacuation of People with Mobility Impairments	EL
DePauw University	Baker, Catherine	Calculating Graph Toughness	ITL
College of William and Mary	Blum, Matthew	It's a Secret to Nobody: Using a Public Source of Randomness for Cryptography and Zero-Knowledge Protocols	ITL
Rochester Institute of Technology	Clanton, Brian	Exploring Real-Time Web-Based 3D Mathematical function Rendering and Manipulation	ITL
Stevenson University	Giauque, Kristin	A Vision of the Future	ITL
Hood College	Haines, Andrea	Determining Important Control Parameters of a Genetic Algorithm	ITL
University of Maryland College Park	Jacobs, Jeffrey	Parallel LDPC Error Correction for Quantum Key Distribution on a GPU	ITL
DePauw University	Keller, Zachary	Modeling the Spread of Infection	ITL
Millersville University of Pennsylvania	Kimmel, Edward	Crypto-Graphics: Visual Applications of the NIST Randomness Beacon	ITL
Georgetown University	Lee, Julian	Faithful to the Original? The Impact of Latent Fingerprint Enhancement	ITL
Westminster College	MacKenzie, Connor	Simplifications and Generalizations of Generating Functions for Classical Orthogonal Polynomials with Definite Integrals	ITL
University of South Alabama	Moore, Adam	Enabling the Extraction of Publications Metadata	ITL
Carnegie Mellon University	Mouli, Divya	Hands Off!: Using Gesture Recognition to Manipulate 3D Visualizations	ITL
Columbia University	Orthwein, John	Techniques in Signal Processing for Chirped-Pulse Broadband Trace Gas Sensor	ITL
University of Puerto Rico	Perez Cruz, Luuis	Monitoring and Analyzing the Deployment of Resource public Key Infrastructure (RPKI) Within the Internet	ITL
University of Maryland Baltimore County	Rayfield, Lael	Simple Analysis of Biometric Matchers	ITL
University of Puerto Rico	Rivera Santiago, Luis	Text Lines Segmentation Performance Assessment Tool	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
St. Mary's College of Maryland	Roca, Alexander	Detecting Malware on Smart Phones	ITL
University of Puerto Rico	Rosado Rosado, Angel	Testing and Traceability of Entropy Sources for Random Bit Generation	ITL
Hampton University	Scott, Charles	Diagraph Method in Detecting Rule Faults for Attribute Based Access Control Policies	ITL
University of Maryland College Park	Siegel, Jacob	The Kinect: A Cheap and Accurate Depth Measurement Tool	ITL
University of Maryland College Park	Sileo, Marissa	Biomedical Image Analysis	ITL
Hampton University	Smith, Courtney	Video Stream Face Detection	ITL
Towson University	Smith, Michael	Windows Phone Malware Detection	ITL
University of Maryland Baltimore County	Turner, Jeffrey	Video Interpolation with the FFMPEG VidAT Tool	ITL
University of Maryland College Park	Villarrubia, Mark	Analyzing Microblog Search Through an Ablation Study of TF-IDF	ITL
University of California Berkeley	Wu, Jason	Optimal Broadcast and Spread of Information in a Network with Limited Resources	ITL
University of Colorado Boulder	Zirkelbach, Stetson	Exploration of Big Data Technologies to Scale Up Cancer Prognosis System	ITL
Oklahoma State University	Artmayer, Danielle	Empirical Calibration Curves for Concrete	MML/NCNR ChemBio
University of Maryland College Park	Boger, Shir	Building Consistent Nanomaterial Ontologies in a Federated Environment	MML/NCNR ChemBio
Virginia Wesleyan College	Boyce, Matthew	Investigation of Sample Matrix Effects Using Spinning Sampling Chamber Laser Ablation ICPMS	MML/NCNR ChemBio
Gonzaga University Washington State	Brown, Taylor	An Investigation into the Enhancement of Vesicle-Based Glycan Arrays	MML/NCNR ChemBio
Brown University	Cohen, Joshua	A Discussion of the Efficacy of the Coulter Principle for Counting Micron-Scale Particles and Protein Aggregates in Comparison to Other Currents	MML/NCNR ChemBio
University of Michigan	Collins, Sean	Chemical Heterogeneity of Wildfire Aerosol Emissions: Implications for Climate Change	MML/NCNR ChemBio
Mount Saint Mary's University	Dockery, Lance	Analysis of CO_2 Loss in Gas Cylinders and changing Concentrations Over Time in NIST Gas SRMs	MML/NCNR ChemBio
Montgomery College	Hafner, Katie	Enhancing the NIST Chemistry Web Book with Optimized 3D Structures – Part 2	MML/NCNR ChemBio
North Georgia College and State University	Jones, Matthew	Measurement of Material Thermal and Chemical Characteristics with the Laser-Driven Thermal Reactor	MML/NCNR ChemBio
North Georgia College and State University	Leman, Deborah	Determination of Polymer/Fullerene Bilayer Miscibility	MML/NCNR ChemBio
University of Maryland Baltimore County	Luu, Peter	Construction and Testing of the Next Generation Ozone Sandard reference Photometer	MML/NCNR ChemBio

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Augsburg College	Ly, Nathaniel	Uncertainty in Live Cell Fluorescence Intensity Measurements Estimated With a Mean Squared Displacement Analysis	MML/NCNR ChemBio
Hood College	Meyer, Rachel	Synthesis of Thiolated Tether Compound to Improve the Properties of tBLM Usd in the Study of Integral Membrane Proteins	MML/NCNR ChemBio
University of Maryland College Park	Miller, Stephanie	Expression, Crystallization, and Holographic Analysis of the Protein Rubredoxin	MML/NCNR ChemBio
University of Maryland Baltimore County	Obadina, Mofiyinfoluwa	Measuring Electrochemically-Induced Oxidative Damage in DNA	MML/NCNR ChemBio
Arizona State University	Ness, Stuart	Enhancing the NIST Chemistry Web Book with Optimized 3D Structures – Part 1	MML/NCNR ChemBio
Columbia University	Newton, Ashley	Transfer Efficiency of Explosive and Narcotic Residue from Bytac®	MML/NCNR ChemBio
Alabama A & M University	Ragland, Tamika	Measurements of Vitamin A in Northern Fur Seals	MML/NCNR ChemBio
Weber State University	Smith, Nicholas	Glycoanalysis Using Universal Proteolysis and Mass spectrometry: Showing Off the Sweet Side of Proteins	MML/NCNR ChemBio
Carnegie Mellon University	Spicer, Graham	Fabrication of Nanopores in Anodized Aluminum Oxide	MML/NCNR ChemBio
University of Maryland College Park	Wu, Jiemin	Developing Analytical Tools for the Characterization of Protein Biomarkers Using Antibodies and Superparamagnetic Substrates	MML/NCNR ChemBio
California State University Fresno	Xiong, Pahoua	Post-Column Counter-Gradients for Better LC/MS Analysis	MML/NCNR ChemBio
University of Maryland College Park	Arnold-Medabalimi, Nicholas	DNA Self-Assembly on 1-D and 2-D Carbon Lattices	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Ashley, Elizabeth	Dimensional Characterization of Si Nanogratings Formed by PS/PMMA Directed Self Assembly	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Bhargava, Pavan	Correcting Substrate Warp for X-Ray Reflectometry	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Bhati, Vikas	Neutron Diffraction Studies of Reduced Perovskite Iron Oxides	MML/NCNR MML/NCNR MatSci
Worcester Polytechnic Institute	Cannon, Bernadette	Studying Phase Transformations in Al/Ni Reactive Multilayers Using Nanocalorimetry	MML/NCNR MML/NCNR MatSci
Georgia Institute of Technology	Carlson, Max	Data Visualization for Analysis of the NCNR Cold Source Operation	MML/NCNR MML/NCNR MatSci
Bridgewater College	Cline, Matthew	Structural Studies of Important Industrial Gases Adsorbed in Zeolites	MML/NCNR MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
St. Mary's College of Maryland	Carneiro, Lucas	Effects of Film Processing Parameters on Organic Photovoltaic Device Performance	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Correa, Luis	High Resolution Displacement Metrology for Nanomechanical Properties	MML/NCNR MML/NCNR MatSci
Carnegie Mellon University	Cramer, Madeline	Molecular Dynamics Simulations of Aluminum Nanoparticles	MML/NCNR MML/NCNR MatSci
Virginia Wesleyan College	Driscoll, Darren	Developing a Library of Selenium Nanoparticles Based on Charge, Size and Stability	MML/NCNR MML/NCNR MatSci
University of Puerto Rico	Garcia Torres, Desirée	Electrocatalytic Hydrogen Oxidation and Evolution at Pt Surfaces in Alkaline Solution	MML/NCNR MML/NCNR MatSci
State University of New York Albany	Garczynski, Pascal	Fluidity at Oil-Water Interfaces	MML/NCNR MML/NCNR MatSci
American University	Ghias, Elizabeth	Synthesis of PEG Compounds for CB2 Structure Characterization with Neutron Scattering and Reflectivity Techniques	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Goodley, Addison	Cloning, Expression, and Purification of TRPML-1	MML/NCNR MML/NCNR MatSci
University of New Haven	Gorka, Danielle	Aging Effects on the Enzymatic Activity of functionalized Gold Nanoparticles	MML/NCNR MML/NCNR MatSci
University of the Sciences Philadelphia	Huon, Amanda	Characterizationof Carbon Nanomaterials	MML/NCNR MML/NCNR MatSci
University of Delaware	Johnson, Jacqueline	The Effect of Ambient Conditions on Solution-Cast Organic Photovoltaics	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Jones, Benjamin	Effects of Interfacial Roughness in Small Angle Neutron Scattering from Multiphase Polymers	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Kim, Il Kyoon	Phase Transition Measurement of Lipids by Nanocalorimetry	MML/NCNR MML/NCNR MatSci
University of California San Diego	Krayer, Lisa	Structural Studies of Multiferroic Thin Films	MML/NCNR MML/NCNR MatSci
Prairie View A & M University	Le, Anh-Tuan	Novel Capillary Viscometry Protein Therapeutic Formulation	MML/NCNR MML/NCNR MatSci
Alabama A & M University	Lewis, Justin	Molecular Modeling Tools for Advanced Materials	MML/NCNR MML/NCNR MatSci
University of South Carolina	Matson, Jillian	Investigating ECM Biomolecule Interactions	MML/NCNR MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Menta, Karthikeya	Quantification of Human Bone Marrow Stromal Cell Shape Dynamics in Collagen Three-Dimensional Scaffolds	MML/NCNR MML/NCNR MatSci
University of New Hampshire	Moser, Newell	Designing and Constructing Steel Cruciform Specimens for a Biaxial Tensile Machine	MML/NCNR MML/NCNR MatSci
Texas Southern University	North III, Richard	Characterizing the Safety and Efficacy of Fluoride Dental Varnish with Applications for Standards Development and Clinical Relevance	MML/NCNR MML/NCNR MatSci
University of Puerto Rico	Pinto-Pacheco, Brismar	The Advantage of Using TiO_2 in Improving the Performance of Dental Resins	MML/NCNR MML/NCNR MatSci
University of Puerto Rico	Quiñones Meléndez, Estefania	Hydration Dynamics of Thin Nafion Films Studied with Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS)	MML/NCNR MML/NCNR MatSci
State University of New York Buffalo	Reele, Michelle	Characterizing the Structural and Rheological Properties of Triblock Copolymer Solutions	MML/NCNR MML/NCNR MatSci
University of Maryland Baltimore County	Richardson, Donald	Assignment of Wyckoff Positions for Entries in the NIST Metals Database	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Steiner, Jake	Phase Equilibria in Co-Al-W Ternary System	MML/NCNR MML/NCNR MatSci
University of Oklahoma	Sabeghi, Maryam	Solidification of Nanoparticles at High Rate	MML/NCNR MML/NCNR MatSci
University of Maryland Baltimore County	Smith, Nathan	Optimization and Modeling of Metal-Oxide-Semiconductor (MOS) Photoelectrochemical Cells	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Syed, Komal	Estimation of the Uncertainty in Orientation Distribution Function Using Monte Carlo Technique	MML/NCNR MML/NCNR MatSci
Millersville University of Pennsylvania	Treible, Wayne	Implementing and Optimizing Calculations of In-Plane Scattering Off of Thin Films	MML/NCNR MML/NCNR MatSci
Southern University	White, John	Fabrication, Optimization, and Analysis of PLGA Nanoparticle for Potential Advancing in Stem Cell Therapy	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Widstrom, Matthew	3D Geometry Photovoltaic Devices	MML/NCNR MML/NCNR MatSci
University of Maryland College Park	Yee, Alex	Dataflow: Web-Based Data Reduction	MML/NCNR MML/NCNR MatSci
University of New Haven	Young, Allision	Nanofiltration Membranes and Their Swelling Properties by Use of XR and QCM	MML/NCNR MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Abbaszadeh, Yasamin	Characterization of the Dose-Rate Effect for Alanine Ionizing-Radiation Dosimetry	PML
Whitman College	Abrams, Nathan	The Effects of Helium Upscattering and Neutron Absorption of the Neutron Lifetime	PML
Prairie View A & M University	Amini, Shahin	Effect of Interlayer in Organic Tandem Solar Cell	PML
George Washington University	Bagchi, Shelly	Monitoring the Power Grid	PML
Rochester Institute of Technology	Beaumariage, Jonathan	Finding Numerical solutions of the Fourier Modal Method to Measure two Dimensional Gratings	PML
Brigham Young University	Bendall, Lisa	Shape Evaluation of Nanoparticles Using the TSOM Method	PML
Wake Forest University	Brigeman, Alyssa	Exploring Organic Magnetoresistance in Spintronic Devices	PML
State University of New York Albany	Briggs, Michael	Space Charge Limited Current Spectroscopy in Organic Single Crystal Semiconductors	PML
Louisiana State University	Brignac, Chase	Quantum Metrology with Nonclassical Light	PML
State University of New York Binghamton	Cao, Lei	Massively Parallel TDDB Test System	PML
Miami University of Ohio	Denton, Alexis	Validation Measurements for Optical Remote Sensing of Greenhouse Gases	PML
University of Maryland College Park	Drozdov, Serghei	Characterizing the Impact of a Single Interface Layer Defect in CMOS Devices	PML
State University of New York Stony Brook	Hassinger, Julian	Nanoscale Imaging Using Spectral Domain Optical Coherence Tomograpy	PML
Rochester Institute of Technology	Heberle, Dylan	Tunability of Photon Entanglement	PML
Goucher College	Irwin, Julian	Tunnel Junction Measurements of Spin Currents	PML
Rochester Institute of Technology	Kahn, Joshua	Neutron Imaging of Chemical Phase Transitions in Alkaline Batteries	PML
University of Texas Dallas	Kelso, Meagan	Quick Read Codes Made by Nanoindentation	PML
State University of New York Binghamton	Kohler, Timothy	Charge-Based Capacitance Measurements and SCM on a Chip	PML
Arizona State University	Lajevardi-Kosh, Arad	Characterization and Preparation of Actin Surfaces and Tethered Bilayer Membranes	PML
State University of New York Binghamton	Lake,Ryan	Investigation of DNA Transport in Nanofluidic Slits	PML
Gustavus Adolphus College	Legatt,Jenna	Shine On Me	PML
George Washington University	Litchfield, Caroline	Calibrating Calibrators	PML
State University of New York Albany	Lydecker IV, Leigh	Characterization of SAMs on Cobalt and Gold	PML

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Puerto Rico	Marcano Estévez, Joseph	Nano-Injector Based Direct Writ Metal Deposition	PML
State University of New York Binghamton	Morgan, Adam	Through silicon Via (TSV) Reliability Monitoring System	PML
Carnegie Mellon University	Mullins, Tom	Optimizing Photonic Crystals Using Computer Simulation	PML
Tulane University	Ortmann Jr., John	Frequency Stabilization of a Continuous wave Dye Laser for Use as a Quantum Memory	PML
Appalachian State University	Pruett, Zachary	The Brightness of the Moon: Lunar Spectral Irradiance	PML
St. Mary's College of Maryland	Raico III, Pasquale	Using Arbitrary Waveform Controlled Lasers and Cavity ring-Down spectroscopy to Determine Greenhouse Gas Concentrations	PML
Tulane University	Scott, Elizabeth	Modeling Helium 3 Scintillation with MCNPX	PML
American University	Tweardy, Matthew	Creating Thermometers of the Future: Imaging Temperature Gradients Using Ultrasonic Transducers	PML
Appalachian State University	Villanova, John	Analysis of Toolmark Topographies from Ten Consecutively Manufactured Chisels	PML
American University	Weinstein, Brian	Temperature Monitoring and Control in Laser Cooling Laboratories	PML
Colorado School of Mines	Whalen, Joseph	Lunar Spectral Irradiance: Calibration of the Moon	PML
Texas A & M University	Zhou, Maxwell	Controlled Production of Highly Charged Ions in Rydberg States	PML
Andrews University	Zirkle, Thomas	Magnetic Field and Position Probe	PML