ABSTRACTS

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Alabama State University

Development of a Standard Toxicity Assay for Nanomaterials Using Caenorhabditis Elegans

Shayla Duncan

Engineered nanomaterials (ENMs) are being incorporated into consumer products as well as in different areas of industry due to their unique properties. Even though ENMs have been used in products such as sunscreen, paints and coatings, research is still being conducted on the possible toxicity of these materials and their effects on the environment. Our research focuses on evaluating the effects of ENMs on the growth and reproduction of *Caenorhabditis elegans* by using the international standard protocol 10872. *C. elegans* are easy to culture, reproduce rapidly and have a short life cycle making them ideal model organisms for toxicity assessment. Additionally, a standard toxicity assay protocol already exists for *C. elegans* (ISO 10872), however it does not include information on testing ENMs, which require special consideration. Our goal is to adapt this standard protocol for use with ENMs. We assessed different media types, feeding methods, and changes to the positive control benzylcetyldimethyl ammonium chloride (BAC-16). These modifications will aid in reducing variability in the toxicity assay and provide a standard platform for evaluating the potential toxicity of ENMs.

Assessing Antibacterial Properties of Novel Dental Resins Containing Titanium Nanoparticles

Shakeria Stewart

Dental caries (i.e., tooth decay and cavities) is one of the main causes of tooth loss and oral pain. There are methods currently being implemented to combat this universal problem. The most common method used to treat caries is to remove the decay and restore the tooth with a filling. Tooth restoratives are ideal because they improve the quality of a patient's oral health and return form and function to the tooth; however, restorative materials often fail. Failure can often result from dental plaque adhering to the surface of the tooth as well as the restorative material. Dental plaque is a biofilm of oral bacteria. Although there are many species of bacteria that are found in dental plaque, the most common that adhere to oral surfaces are Streptococcus mutans, Streptococcus sobrinus, and lactobacilli. In order to achieve long lasting tooth restoratives, it may be desirable that these restorative materials have antibacterial properties.

A component of polymer-based restorative materials is resin matrix. Producing durable as well as antibacterial dental polymers are imperative. Titanium dioxide nanoparticles have already exhibited improved mechanical properties as well as unique photoactivities. It is known that one of the unique photoactivities of titanium dioxide nanoparticles is that it has the ability to exhibit antibacterial and antiviral properties via the chemical energy that is released. Although there are some antibacterial properties of the titanium dioxide nanoparticles, further testing is needed in order to successfully develop a novel dental resin that contains titanium dioxide nanoparticles.

Our research tested various nanoparticle solutions for antibacterial properties. The nanoparticle solutions that were tested varied in concentrations of titanium dioxide, ethanol, and methylene blue. Some samples were pre-exposed to a visible light curing system and subsequently exposed to the same light prior to 48-hr incubation. Antibacterial properties were assessed by measuring the zone of inhibition via agar assays. The Kirby Bauer disk diffusion antibiotic sensitivity procedure was used to determine if the titanium dioxide samples exhibited zones of inhibition once exposed to S. mutans. To facilitate the testing for the antimicrobial properties, conditions had to first be optimized. Factors that were included while determining an optimal procedure were disk matrices, concentration of titanium dioxide samples, dry time (which were measured using percentages), as well as temperature. Once optimal conditions were established, we were able to accurately test the nanoparticle solutions for antibacterial properties.

Alfred University

A Molecular Dynamics (MD) Study of Surfactant Self-Assembly on Singled-Walled Carbon Nanotubes (SWCNTs)

Daniel Kutzik

Single-walled carbon nanotubes (SWCNTs) are rigid, hollow molecular carbon cylinders noted for their structural properties, as well as their varying electronic and chemical properties that make them appealing for a myriad of advanced technological applications. A practical barrier that stands in the way of greater technological adaptation of these materials is that SWCNT synthesis invariably results in mixtures that are highly heterogeneous with respect to size and chirality, the latter of which defines it as a distinct chemical species and gives it unique chemical properties. Ongoing research focusses on the process of surfactant-mediated dispersion. In solution, surfactants self-assemble around the hydrophobic nanotube core producing a mixture in which tubes are individually dispersed and contained in a surfactant shell. Determining the structure and properties of the SWCNT-surfactant complexes at the molecular level, and how this is affected by chirality, is the key to understanding their transport properties and solubility characteristics.

In this project, we used molecular dynamics (MD) simulations to study the self-assembly behavior of a variety of surfactants and co-surfactants on SWCNTs. We tested methods for building an accurate model to simulate SWCNT-surfactant systems for several bile salt surfactants and anionic co-surfactants, components widely used and important in experimental separation studies at NIST. An important factor in this study was choosing an interatomic potential, or force field. Two Class II force fields, TEAMFF and SciPCFF, were evaluated for their reliable parameterization of molecular forces in our simulation. We will present results for the simulated self-assembled behavior of the (6,5) SWCNT with the bile salt surfactant sodium deoxycholate (DOC), the anionic surfactant sodium dodecyl sulfate (SDS), as well as a DOC/SDS co-surfactant mixtures. The development of reliable protocols for simulating SWCNT/surfactant self-assembly processes paves the way for future work studying the transport properties and solubility behavior of these individual systems.

American University

Convergence of Magnus Integral Addition Theorems for Confluent Hypergeometric Functions in Terms of Bessel and Parabolic Cylinder Functions

Jessie Hirtenstein

In his 1946 publication, Wilhelm Magnus presented an elegant addition theorem for the Kummer confluent hypergeometric function of the second kind expressed as an integral of a simple product of two Kummer confluent hypergeometric functions of the second kind. We take advantage of asymptotics for the Kummer confluent hypergeometric function of the second kind to obtain precise convergence domains for Magnus' result. Recently obtained by Nico Temme, these asymptotics for the Kummer confluent hypergeometric function of the second kind are for the absolute value of the first complex parameter approaching infinity. Using well-known specializations of the Kummer confluent hypergeometric function of the second kind, we obtain integral addition theorems for Hankel $H_{\{0,1\}}^{(0,1)}$, Macdonald $K_{\{0,1\}}$, and respectively, Bessel functions of the first and second kinds $J_{\{0,1\}}$, $Y_{\{0,1\}}$. We also show how the integrands of these addition theorems can be given in terms of modified parabolic cylinder functions whose arguments lie on complex orthogonal straight line contours, $\pi/4$ radians off the real and imaginary axes.

Calculating Electrostatic Properties Using Lévy Flights

Mark Verdi

In molecular physics, the motion of a molecule can be modeled using random walks with steps whose lengths are determined by a normal distribution. However, these random walks are also useful in modeling a variety of other processes ranging from physics to finance. One notable example is using random walks to compute the self- capacitance and charge density of an arbitrarily shaped perfect conductor as implemented in the program ZENO [1]. Although random walks based on the normal distribution, also known as Gaussian random walks, are the most common type, they are not the only type. Generalized random walks known as Lévy flights, whose step lengths are determined by a particular heavy-tailed α-stable distribution, can be used to model other processes such as human mobility [2]. These distributions, whose most notable characteristic is their infinite variance, arise from a generalization of the Central Limit Theorem. We explore different ways of visualizing and understanding these distributions and use them to compute physical quantities. Specifically, we focus on the calculation of charge density and generalized α-capacitance and directly compare our results both to the ZENO method and to analytic results for the disk and sphere. We also discuss the challenges that arise in performing these simulations and the necessary steps for determining the α-capacitance of objects with general shape.

[1] web.stevens.edu/zeno
[2] I. Rhee et al. IEEE ACM T Network 19 630-643 (2011)

<u>Appalachian State University</u>

Electrical Measurements of Molecular Layers by Eutectic Gallium-Indium

Kayla Zimmerman

Organic molecules are appealing in electronic applications because they are cheap, abundant, and can be made so that they have specific properties. When using organic molecules in electronics, it is necessary to electrically connect them, without damaging them, to the outside world. Evaporation techniques cannot be used to make electrical contact with the molecular layers because the molecules used are organic and cannot withstand the high temperatures needed to evaporate metals without the molecules being damaged and/or creating an electrical short to the bottom contact. Instead of using conventional evaporation techniques, we used a soft, liquid metal as a non-destructive top contact to the molecular layer. We are developing a contact formation technique that uses eutectic gallium indium (E-GaIn) as a soft-metal contact probe to measure the electrical properties of molecular surfaces. The metal we used was a eutectic of gallium and indium because it is nonvolatile and nontoxic, and is easier to manipulate than other materials that are used as a top-electrode.

To ensure that the E-GaIn system was taking accurate electrical data, we fabricated Si/Au junctions and measured the direct current (DC) current-voltage (I-V) properties with the eutectic system and a

commercial probe station. We find that if the measurements are taken in the same contact configuration, the DC I-V measurements are nearly identical to each other. After this, we began working towards taking electrical measurements data of different molecular layers in a patterned-well substrate. The self-assembled monolayers (SAM) that were investigated are: octadecanethiol, hexadecanethiol, and tetradecanethiol. These three molecules all have the same head and tail groups, the number of methyl groups connecting the head and tail groups is the only thing that changes. The molecular quality was measured by Fourier Transform Infrared Spectroscopy (FTIR) to ensure that we had a dense, ordered SAM. This E-GaIn contact technique is a promising method to non-destructively electrically contact molecular layers.

<u>Arizona State University</u>

Process Optimization of Polymer Solar Cells
Joe Carpenter, III

Bulk heterojunction (BHJ) photovoltaic (PV) devices were produced from intermixed blends of donor (PBDTTT-C-T) and acceptor (P-NDI2OD-T2) polymers. The active layer of the devices was blade coated to simulate the large area slot-die coating technique utilized in manufacturing. Power conversion efficiencies (PCEs) of all-polymer devices were measured to be as high as 1.7%. High PCEs were achieved by altering the solution to contain 20%v/v chloronaphthalene, a slow drying solvent and 1%w/w DMDBS, a nucleating agent. Various blading speeds were attempted from 5 to 40 mm/s to obtain active layer films of around 100 nm. Thermal treatments were also attempted to increase drying speed. Initial characterization was performed with optical microscopy and ultraviolet-visible (UV-Vis) absorption spectroscopy. The electrical properties of the highest performing PV device were an open circuit voltage (V_{oc}) of 820 mV, a short circuit current density (J_{sc}) of 4.6 mA/cm^2, and a fill factor (FF) of 46%. Optimal processing conditions have been used in synchrotron diffraction measurements to correlate performance-processing relationships able to inform future formulations of devices.

Analysis of Fe V and Ni V Wavelength Standards in the Vacuum Ultraviolet
Jacob Ward

The recent publication *Limits on the Dependence of the Fine-Structure Constant on Gravitational Potential from White-Dwarf Spectra* by Berengut and Barrow suggests a potential variation in the fine-structure constant in the presence of high gravitational potential. The result of such variation would suggest new physics.

Given that the spectrum of white-dwarf stars is dominated by Fe V and Ni V, the proposed value for the fine-structure dependence upon gravitational potential was determined via observed shifts in the positions of Fe V and Ni V lines in the vacuum ultraviolet region (1100-2200 Angstroms).

Uncertainties for the wavelength standards of these species have been identified as the major source of uncertainty in the publication's presented value for gravitational dependence. Given the unique instrumentation available at NIST, an investigation of Fe V and Ni V spectra in the vacuum Ultraviolet region has been conducted to reduce the wavelength uncertainties currently limiting modern astrophysical studies.

The analyzed spectra were produced by a sliding-spark light source with invar (Fe/Ni alloy) electrodes at peak currents of 750-2000 amperes and processed via the NIST Normal Incidence Vacuum Spectrograph.

Calibration was done with Pt-II produced by a Platinum-Neon hollow cathode lamp utilized in the NIST Pt Atlas.

Augsburg College

Automated Live Cell Imaging of Stem Cells Expressing Green Fluorescent Protein
Elianna Bier

Fluorescence microscopy is a powerful tool for cell biology. Using fluorescence reporters (i.e., GFP), live cell imaging can monitor dynamic patterns of gene expression in complex and evolving cell populations. We have been developing imaging protocols that can be applied to pluripotent stem cell populations during expansion or self-renewal, and during differentiation. These important cells grow as colonies that can be much larger than a microscopic field of view. Thus, we have used computer control programs to optimize the image collection in order to image as many colonies as possible during a time lapse acquisition while non-perturbing growth conditions for the cells are maintained. Another important aspect of quantitative imaging is assuring that data is comparable between different experiments. We have also further enhanced existing procedures for assessing the performance of a fluorescence microscope. Taken together, this work has enabled the collection of large amounts of quantitative image data that can be used to derive a quantitative description of stem cell pluripotency.

Bates College

Raman and Infrared Studies of Few Layered $TaSe_2$
Andrew Briggs

Since the discovery of graphene in 2004, two-dimensional materials have been an important topic in physics. More recently different layered materials are being investigated for their semiconductive and superconductive properties. Of particular interest is the compound 2H-$TaSe_2$, on which this presentation will focus. Both sample production and spectral analysis will be highlighted. To obtain a few, atomically-think layers of $TaSe_2$, bulk crystals are exfoliated with a stamp of polydimethylsiloxane, a method similar to the "double sticky tape" method used to discover graphene. Choosing a substrate to support these layers is important as well, as it must be both easy to produce and provide a high optical contrast. Once produced, the samples are analyzed using two methods of vibrational spectroscopy. The first, Raman spectroscopy, is useful for rapid, reliable, and [sometimes] non-damaging identification of the layer number of 2H-$TaSe_2$. Raman spectroscopy depends on the scattering of laser light off of a sample due to vibrations between atoms. The second form of spectroscopy is called Fourier transform infrared spectroscopy (FTIR). At the heart of the FTIR is a Michelson interferometer which allows many wavelengths of light to interact with the sample in a single scan. Even collecting the FTIR of bulk 2H-$TaSe_2$ provides new data, although our plans include probing few layers as well. This research will shed light on the interesting optical properties and phenomenon of atomically thin 2H-$TaSe_2$.

Boise State University

Resilience: Planning for the Future
Andrew Adams

On average, natural and man-made disasters cause an estimated $57 billion in losses every year, with large single events such as Hurricane Katrina capable of inflicting costs over $100 billion. Current building design methods have focused specifically on the preservation of life safety when faced with a major hazard event, and have been successful in doing so. However infrastructure system interdependencies are not addressed and continued functionality of buildings and infrastructure post-event is often lost, requiring either demolition or lengthy repairs.

There has been a recent shift in thinking towards the idea of resilience and building with continued functionality and quick recovery in mind should a major hazard event occur. The work being done at NIST in the Disaster Resilience group is focusing on community resilience, defined as the ability of a community to absorb and recover from the effects of a community wide hazard event. A resilient community is therefore one that can withstand the impact of a hazard event and recover quickly enough to prevent significantly detrimental long term economic and social consequences.

The objective of my project was to compare and analyze existing metrics for resilience and identify possible strengths and weaknesses in order to help inform NIST's Disaster Resilience Framework, which is being developed as called out by The President's Climate Action Plan. Any proposed measurement needed to be flexible enough to apply to all-hazards, time-trackable pre-event and during recovery, actionable, objective, consistent, and simple. NIST's focus is on developing a resilient built environment as a foundation to support the social needs of a community. I was able to distinguish features from the different sets which align with NIST's objectives through the identification of critical elements desired in metrics for the Framework. The metrics which I examined were developed by the United Nations (UNISDR), San Francisco Planning and Urban and Research (SPUR), and the Community & Regional Resilience Institute (CARRI).

Modeling Materials for a Better Tomorrow: Computational Studies of Carbon Capture Materials MIL-53 and BPene

Eric Nelson

The rising level of atmospheric carbon dioxide is one of the largest concerns in our society today, for reasons both economic and health-centered. CO_2 emissions are produced predominately from the combustion of coal, oil and natural gases (ca. 80% of CO_2 emissions worldwide), and are projected to rapidly increase due to global economic development [S. Energy Policy 2007, 35, 5938]. In June 2009, the U.S. House of Representatives passed the American Clean Energy and Security Act, which proposes economy-wide CO_2 reduction goals of 83% below 2005's production levels by 2050. Capturing CO_2 at the source prevents damaging molecules from being released into the environment. Metal-organic framework (MOF) materials are a likely candidate for capturing CO_2 more efficiently than current technologies. Computational work that can accurately predict structure-property relationships in MOF materials would substantially reduce the development time for materials with desired properties. The focus of this study is to refine previous studies on MIL-53 and BPene, flexible nanoporous materials which flex when CO_2 or other gaseous molecules are adsorbed and desorbed. MIL-53 is a well-studied flexible MOF for adsorption and desorption properties; however, less is known about its behavior during changes between high and low temperature phases. Modeling MIL-53 and BPene provides information into the energetics of the phase transformation which establishes materials performance. The study uses density functional theory (DFT) calculations to study MIL-53 and BPene. The experimental structure and bandgap of the related material Cromium (III) Oxide were used as a test bed for optimizing DFT parameters and then applied to MIL-53. Preliminary results are encouraging, and suggest that the crystal structure and relative energies are in good agreement with experimental values. Final results from these findings are to be compared with experimental values and used as a benchmark for further theoretical studies.

Multi-Scale Characterization of Selective Sorbent Materials Through X-Ray Scattering Techniques

Meagan Papac

Recent developments in materials measurement techniques combine ultra-small angle X-ray scattering (USAXS), small-angle X-ray scattering (SAXS), and wide-angle X-ray scattering (WAXS), to provide multi-scale characterization of complex material structures. Scattering is characteristic of microstructural heterogeneities, while diffraction peaks found in SAXS and WAXS data provide structural information. In addition, a state-of-the-art sample chamber allows scattering and diffraction experimentation across a wide range of temperatures and pressures. Thus, environmental effects on structure and microstructure can be observed *in situ*, providing greater insight into material behavior in response to changing environmental conditions.

While this approach shows great promise for probing complex materials with microstructural heterogeneities and large atomic structures, it must be proven through comparative metrology. To evaluate the application of SAXS/WAXS data for phase identification and lattice parameter determinations, selective sorption materials (sodium aluminum silicate and bis(2-methylimidazolyl)-zinc, commonly NaY zeolite and ZIF-8) were employed to generate both SAXS/WAXS and conventional X-ray diffraction patterns for comparison. While differences exist between these patterns, their overall similarity suggests that, with appropriate data acquisition and analysis, combined SAXS/WAXS diffraction could be effectively used for material characterization.

To explore further usefulness of this method, SAXS/WAXS data of other selective gas sorption materials (Ni(1,2-bis(4-pyridyl)ethylene)[Ni(CN_4)] and catena-bis(dibenzoylmethanato)-(4,4'-bipyridyl)nickel(II), commonly Ni(bpene)[Ni(CN_4)] and NiDBM-Bpy) was analyzed across a CO_2 partial pressure range of 1 bar to 17 bar. Changes in peak positions and intensities as a function of CO_2 partial pressure were observed. A similar data set, involving the same materials and CO_2 partial pressures and including N_2 gas at equal partial pressures, was used to explore the effects of the second gas on the materials' adsorption behavior. The results indicate that further development of instrumentation, such as an extended q-range and more accurate intensity data, would facilitate the use of SAXS/WAXS diffraction peaks for structural characterization as well.

Optimization and Characterization of Perovskite Oxides as Potential Thermoelectric Materials

Kevin Talley

High energy cost, greenhouse gas emission, and climate change have increased interest in energy conversion materials. Thermoelectric materials produce an electric potential when exposed to a temperature gradient, enabling the recovery of lost energy, and energy efficiency improvement. The conversion efficiency of thermoelectric materials is related to the figure of merit *ZT*, $S^2 \sigma / \kappa$, where S is the Seebeck coefficient (voltage generated per degree of temperature difference), σ is the electrical conductivity, and κ is the thermal conductivity. Rare-earth cobalt perovskite oxides are being investigated as thermoelectric materials due to low thermal conductivity and high Seebeck coefficient values. Efforts have been made to increase the electrical conductivity by partial substitution of cobalt with various transition metals. In effort to optimize the conversion efficiency of these materials, two approaches were used to investigate the structure-property relationship.

First, a traditional method of solid state processing was used on the $RCo_{.75}M_{.25}O_3$ (R=La,Pr,Nd & M=Co,Ni,Fe,Mn,Cr) system. Subsequent X-ray and neutron powder diffraction were used in determination of the crystal structures, and TEM analysis was found to support the results. Magnetic susceptibility measurements showed the existence of various magnetic structures, and low temperature neutron studies were subsequently performed. Structural features were correlated to the Seebeck coefficient, resistivity, and thermal conductivity measurements.

Second, a high-throughput combinatorial technique was employed. In this approach a pulsed laser deposition technique was used to epitaxially grow a $LaCo_{(1-x)}Cr_xO_{3-z}$ combinatorial thin film library onto a single crystal $LaAlO_3$ substrate using $LaCoO_3$ and $LaCrO_3$ targets. X-ray diffraction was used to verify the existence of a single phase solid solution, and approximate the composition range (x) across the film library. Custom NIST screening metrology was used to screen the combinatorial film library for the Seebeck coefficient and resistivity values. Using this high-throughput technique we were able to identify potential compositions of interest for further investigation by bulk synthesis.

In this talk, a discussion will be presented on the structural features, and property measurements resulting from the serial, and high-throughput combinatorial method.

<u>Bowie State University</u>

Real-Time Access Control Rule Fault Detection Using a Simulated Logic Circuit
Skye Horbrook

Access Control (AC) restricts the users of a system to only have certain privileges. AC policies can be implemented based on different AC models, which are fundamentally composed of semantically independent AC rules in expressions of privilege assignments described by attributes of subjects/attributes, actions, objects/attributes, and environment variables of the protected systems. Incorrect implementations of AC policies result in faults that not only leak but also disable access of information, and faults in AC policies are difficult to detect without support of verification or automatic fault detection mechanisms.

This research proposes an automatic method through the construction of a simulated logic circuit that simulates AC rules in AC policies or models. The simulated logic circuit allows real-time detection of policy faults including conflicts of privilege assignments, leaks of information, and conflicts of interest assignments. Such detection is traditionally done by tools that perform verification or testing after all the rules of the policy/model are completed, and it provides no information about the source of verification errors. The real-time fault detecting capability proposed by this research allows a rule fault to be detected and fixed immediately before the next rule is added to the policy/model, thus requiring no later verification and saving a significant amount of fault fixing time. The implementation of the simulated logic circuit has been developed in JAVA.

CPCC: A Cyber Physical Cloud Computing Testbed
Paul Sabbagh

Cyber Physical Systems (CPSs) connect the "cyber and physical worlds by using sensors and actuators to bridge the computing domain to the physical domain" [NISTIR 7951]. The sensors monitor physical properties while actuators control the physical environment with computing elements in-between to process data. Adding cloud characteristics to CPS will allow components to be rapidly provisioned and de-provisioned for use in multiple virtual systems simultaneously, increasing efficiency, resiliency, and flexibility [NISTIR 7951] and encouraging innovation.

To validate the Cyber Physical Cloud Computing (CPCC) model and test component interoperability, a CPCC test bed was built upon which an industrial sous-vide system was implemented to demonstrate different aspects of the CPCC model.

Brown University

Maximizing the Spread of Information in Communication Networks
Sung-Ho Justin Oh

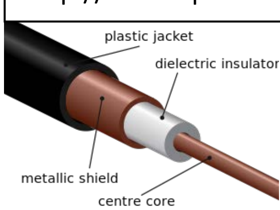
The first recipients of a message crucially determine whether information goes viral throughout a community or quickly dies down. Information is more likely to spread in a network if first given to the most influential members. We analyze how to determine the influential members of networks and network-like structures. Finding such members aids in making intelligent decisions in notifying communities of emergencies, advertising products, placing sensors in water main networks, and more. We model communication networks mathematically as a graph and mainly simulate the spread of information via random walks on the graph. Intuitively, a more influential node in a graph would have a shorter expected random walk length to other nodes of the graph. Thus our main goal is to find subsets of the graph nodes that minimize the time for random walks to first reach them. Calculating the expected time for a random walk to hit a certain node is easy to compute with linear algebra and Markov chain theory. Hence we present the following optimization problem: given a graph with n nodes, find a subset of k nodes that minimizes the objective function of mean hitting time. We show that such a problem is NP-Complete, however previous results show that greedy algorithms can approximate the optimal solution to within a certain guaranteed factor. We are working on developing new algorithms based on the geometry of the graph that will produce better approximations than the greedy approach.

Bryn Mawr College

Exploring the Electrical Properties of Carbon Nanotube Materials with Raman Spectroscopy
Noura Jaber

Single-wall carbon nanotubes (SWCNTs), which can be visualized as a rolled-up, two-dimensional carbon lattice (a.k.a graphene), have exciting physical properties such as low mass-to-length ratio and good thermal and electrical conductivity. As a result, SWCNTs hold great promise in many applications such as nanoelectronics and nanomedicine. Our study of SWCNTs examines two different applications. The first is substituting SWCNTs for copper in coaxial cables and the other is using SWCNTs on silicon wafers as field-effect transistors (FETs).

Figure 1: Coaxial Cable
http://en.wikipedia.org/wiki/Coaxial_cable



Coaxial cables, used to transmit radio and microwave frequency signals, are an established technological necessity. As seen in figure 1, the metallic shielding surrounding the dielectric protects the signal from noise and other disruptions such as lightning strikes. Because coax shields and cores are generally made of metals such as copper, their weight can be a significant obstacle when used on air and spacecraft. A potential alternative to copper is SWCNTs which could reduce the weight by 70%. The second application of SWCNTs examined was their potential use as FETs. Here SWCNTs were dispersed from different starting concentrations and chiral populations onto SiO_2/Si. These nanodevices are important in multiple fields and are being explored by industries and defense organizations.

The method used to probe the SWCNT materials in these applications was in situ Raman spectroscopy. Microwave or electronic signals were passed through the SWCNTs while Raman spectra were simultaneously collected. In Raman spectroscopy, inelastically scattered photons are collected which correlate to the vibrations between each atom in a sample. The Raman method was chosen because this type of vibrational spectroscopy provides a rich amount of information on SWCNTs' diameter, crystal structure, defect density, and more. By observing spectral changes as indicated by variations in Raman features such as the Radial Breathing Mode (RBM), D, G, and G′ peaks, we can identify the capabilities and limitations of SWCNT-based devices. SWCNT coax cables are illuminating the path to lighter, more fuel-efficient airplanes, jets and spacecraft—making flying less environmentally destructive and costly as well as enabling longer space missions and better astronomical research. SWCNT FETs are leading the way to better nanoelectronics which could benefit many industries and scientific fields.

Carnegie Mellon University

Simulation of an Ion Beamline for Isotopically Enriched Deposition
Christopher Addiego

Silicon based quantum computing technology is an attractive prospect because the current semiconductor industry has constructed a robust infrastructure focused on manufacturing silicon based devices. However, natural silicon is not suitable for such devices due to the presence of the silicon-29 (^{29}Si) isotope. The odd number of nucleons in the ^{29}Si nucleus means that each ^{29}Si atom has nuclear spin of 1/2 which can disrupt the coherent quantum states that must be maintained in a quantum computer. Therefore, it is necessary to enrich natural silicon to maximize the concentration of ^{28}Si and minimize the concentration of ^{29}Si if it is to be applied toward quantum computing.

The Quantum Processes and Metrology Group at NIST is developing a method for enriching silicon that uses a mass spectrometer to select only ^{28}Si from a beam of ionized silicon atoms which is generated from a natural silicon source. The enriched silicon is then deposited onto a silicon substrate. The goal of this project was to create a computer model of the apparatus using charged particle optics simulation software SIMION. Then, by optimizing the fluence of the simulated beam, we aimed to improve the fluence of the beam in the actual enrichment apparatus and increase deposition rates.

Case Western Reserve University

Calculation Hansen Solubility Parameters for Organic Solar Cells by the Cohesive Energy Density Method
Matthew Wade

In organic photovoltaic (OPV) solar cells, the conversion of photons to electricity is facilitated by a mixture of phase-separated polymers and functionalized nanoparticles. The power conversion efficiency of these solar cells is largely dependent on the initial morphology of the mixture. An indication of whether the morphology of a system is stable over a long period of time is the relative solubility of the compounds in the mixture. One possible way to represent this property is the Hansen and Hildebrand solubility parameters. For these values a smaller difference between the values for two different molecules indicates a greater likelihood that they will dissolve and form a solution. Physical measurement of these solubility parameters can be difficult, time-consuming, and require dedicated apparatuses. To avoid these issues, molecular dynamics simulations were conducted following the previously established cohesive energy density (CED) method of Goddard [1] to calculate the solubility parameters. Initial data indicate that minor changes to the setup of the simulation result in significant changes in the calculated values. To obtain accurate results, simulation setup parameters and partial atomic charges were taken from available literature. Later tests with these initial conditions indicated that the CED method accurately reflected solubility parameters from various databases. This method was then used to determine the solubility parameters for 3hexylthiphene-2,5diyl (P3HT) and phenyl-c61-butyric acid methyl ester (PCBM). Future work will examine a number of molecules to optimize the miscibility of compounds used in OPVs, and thus improve their longevity.

[1] M. Belmares, M. Blanco, W. A. Goddard, R. B. Ross, G. Caldwell, S. H. Chou, J/ Pham, P. M. Olfson, C. Thomas, *J. Comput. Chem.* **2004**, 25, 1814

Dynamic Properties of Metals Used in Additive Manufacturing
Calvin Zehnder

Selective metal sintering (SLS) is one of the few additive manufacturing methods that can 'print' metal into shapes unobtainable by conventional (subtractive) manufacturing methods. SLS uses metal powder that is spread onto a build plate, and then is melted and solidified in the desired shape by a computer controlled laser. This process repeats, layer by layer, until the required thickness is achieved. It is desirable to make an accurate computer simulation of the spreading of the powder onto the build plate so parts and build parameters can be modeled accurately and quickly, so the part can be 'built' several times without the waiting and the cost that is associated with physically making the part multiple times. In order to accomplish this, accurate physical property data must be known about the metal powder. To create a discrete element method simulation, the coefficient of restitution, stiffness, and damping coefficients must be known. To measure these, we used a set-up consisting of a high-speed camera with a microscope objective, and a custom built powder dropping mechanism, designed to accurately and reliably drop a very small volume of powder in front of the camera. This captures incoming and post-impact velocities which can be used to find the dynamic materials property data.

City University of New York

Designing Buildings for Wind Load
Zineb Bouizy

In the U.S., the design of buildings for wind is based on wind pressure coefficients listed in ASCE 7 "Minimum Design Loads for Buildings and other Structures" published by the American Society of Civil Engineers (ASCE). These coefficients are multiplied by the square of the wind velocity (obtained from wind maps) and other factors having to do with terrain, wind direction, etc. , to arrive at the design wind pressures for roofs and walls. These pressures are used in two different ways: 1) to design the Main Wind Force Resisting System, i.e., the building frame; and 2) to design the building cladding (envelope) and its components (C&C). For C&C, the spatial scale of the pressure coefficients must be taken into account because the coherence in time between peak pressures increases as the length scale decreases (wind is a randomly fluctuating phenomenon in time and space).

This project aims at updating the pressure coefficients for C&C. The current coefficients are based on a limited number of model tests performed in wind tunnels thirty years ago. Since then, more data have become available, some of which have been collected in a NIST database. More importantly, progress in electronic recording has allowed many more pressure sensors to be recorded simultaneously.

Pressure is assumed to be uniform over the tributary area of the sensor, and as the area of the cladding increases, more sensors become relevant. However, the pressures they record also lose coherence, with the resulting effect that area-averaged peak pressures decrease as the area of the cladding increases. This is indeed what was observed for one building analyzed this summer. Moreover, for this one building, wind pressure coefficients are significantly higher than currently specified. If these results hold for other buildings, pressure coefficients will need to be revised upward significantly, resulting in higher design wind loads.

It should be noted that the observed peak coefficient depends on the duration of the wind tunnel test. For consistency, statistical techniques for non-Gaussian time series were used to obtain the expected peak for a wind storm of one hour at full scale.

Development of an Efficient, Fiber-Coupled Quantum Dot Single Photon Source

Jing Chen

A single photon source is a light source which emits only one photon at a time. This source has many applications in quantum information processing and plays an important role in studying the fundamentals of quantum mechanics. For instance, a single photon source can be used in secure quantum communications protocols. In addition, this technology can be used to improve metrological accuracy and help standardize radiometry tools. Although single photon sources have much potential, there are many constraints on efficiently generating single photons.

One of the methods to generate single photons is optical excitation of a single quantum emitter like a quantum dot, in which a single photon is emitted when an excited-state electron returns to the ground state. In our research, we study single photon sources from quantum dots that are embedded in a high refractive index material, GaAs. When an incident laser hits a quantum dot, the emitted light radiates in all directions and is largely trapped in the GaAs material due to total internal reflection. This, combined with the low photon flux produced by working with just a single quantum dot, makes photon extraction efficiency paramount and is the main challenge of our research. The goal is to design a nanophotonic structure to funnel the maximum amount of single photons from the quantum dot to a single mode optical fiber.

A waveguide geometry with integrated grating out-coupler on one end and Bragg reflector mirror on the other end is one of the designs we are exploring to extract single photons from a quantum dot. When the quantum dot first emits preferentially into the waveguide, its emission goes equally into both forward and backward directions. Most of the light going in the forward direction of the waveguide is vertically out-coupled with a grating into an optical fiber. We incorporate a rear Bragg reflector end mirror so that light going in the backward direction in the waveguide gets reflected back to the grating and the majority of the quantum dot emission can be coupled out. The coupling efficiency we can achieve depends on several parameters of diffraction gratings such as grating period, etch depth and duty cycle. The optimization is done through simulation tools such as RODIS, CAMFR, and MEEP, each of which addresses part of the overall problem. The grating resonance of reflection and transmission of grating are found using RODIS. Moreover, reflectivity of the Bragg reflector and the coupling from the grating to the fiber are calculated using the mode expansion method from CAMFR. Finally, the finite-difference time-domain (FDTD) method is utilized in MEEP to simulate the whole system, enabling optimization of the output coupling efficiency.

Automating the Calibration of DMM Calibrators and Navigation Systems

James Fallon

My objectives as an intern in the Digital Multimeter and Phase Meter Calibration Laboratory are to facilitate the process of calibrating a digital multifunction calibrator, use optical character recognition to read a VHF Omnidirectional Range (VOR), and compress sensor data. The laboratory calibrates customer standard multimeters and phase meters using measurements of resistance, DC current, DC voltage, and the phase angle between signals. I performed measurements on a 1000:1 resistor divider bridge that is used to scale from a 10 volt reference to 1000 volts. My measurements agreed well with a more automated method. Resistors are used for calibrating the multifunction calibrator. Its calibration routine was adapted to control a new low thermal matrix scanner and give it the ability to select and use any resistor attached to the scanner. Wires were made for the scanner, but the updated program has not yet been tested.

The VOR lacks a GPIB or any computer interface. VOR calibration can be improved by creating a program which reads its display. The VOR is a radio navigation system that measures the phase difference between two signals. I made an existing program compatible with two webcams, to read two meters. To improve accuracy, the capability to use two fonts is being added. One font is created using webcam images and the other is very minimalistic. Characters will be read using a different metric for each font. The readings will be incorporated into the VOR calibration program at required time intervals.

Our measurements are influenced by temperature, so calibration or certification requires recording temperature data. Sensors collect data every minute, but that degree of temporal resolution is not needed. A summary of temperature and relative humidity data was created using a custom filter that eliminated data points at times when the data had low variance.

Developing New and More Efficient Ways to Solve the Time-Dependent Schrödinger Equation (TDSE)

Behnaz Ghouchani

In many interesting problems in the quantum theory of atoms and molecules, it is necessary to find the solution to the time-dependent Schrödinger equation (TDSE) where an atom or molecule is exposed to some external time-dependent perturbation. One specific example is an atom in a time-dependent laser field. One must propagate a known starting solution (say, the ground state of the system) at $T = 0$ to some final state at $T = t_{\text{final}}$. In general, this becomes a problem where one first discretizes the spatial degrees of freedom, for example, on a grid and then propagates in time using one of a number of different techniques. The main objective of this study is to compare different approaches as to accuracy and computational efficiency in performing the time propagation and to test a new approach, a variant of the exponential time differencing (ETD) method, that has not been seriously tried for the TDSE. The new approach has the merits that the time step that must be used in the propagation is governed by the intrinsic time variation of the laser field rather than the numerical stability of the propagation method. The model used for our study replaces the real atomic system by a one-dimensional model that has been widely used in the literature and which captures the essential features of the full 3D problem.

Discretizing the differential operators using known finite difference formula allows us to perform the propagation via the known approaches and to then compare them to the new method for both accuracy and efficiency. The study is aimed at understanding both the older time propagation approaches as well as the new approach. This has never been seriously examined before and even without ETD, is of great value. Results will be presented at the SURF symposium.

Data Mining Application in Web Services

Golnaz Ghouchani

Data mining is a growing field in computer science. It is the process of finding patterns or correlations among data sets by using various computational methods. Many data analytics (DA) engines have been developed for this purpose. The useful information retrieved from manufacturers' data mining could provide solutions on increasing companies' productivities and globally competitive advantages. In this research we proposed using web services for communicating data analytics information that is represented in Predictive Model Markup Language (PMML).

Web service (WS) is a method that provides communication between two systems through network connection. By using WS, manufacturing companies can easily communicate with the DA engines, send their data sets to the DA engines, and receive the mining results from the DA engines. WS has three major components: WS consumer, WS provider, and WS repository. Their interfaces are based on Web Service Description Language (WSDL), Simple Object Access Protocol (SOAP), and Universal Description, Discovery and Integration (UDDI).

The purpose of this research project was to design and implement a WS for supporting manufacturing data analytics. The approaches taken for this project include identifying WS consumer, WS provider, and WS repository; generating work flows among them using flowchart; and creating a sequence diagram and writing codes for the work flows.

Leveraging Web Development Infrastructure for 2D and 3D Visualizations

Mohamed Gueye

We demonstrate the use of web-based visualizations for computer security, human body measurement, and network research, all taking advantage of web development infrastructure. 2D and 3D visualizations displayed natively on web browsers without the use of plugins are presented. Our visualizations consist mainly of a 2D visualizations of the NVD (National Vulnerability Database) data feeds, and AnthroWeb3DMeasure (AW3DM), a 3D visualization of CAESAR[1] data set of laser scanned human bodies. The focal point here is to leverage web development infrastructure to integrate many types of visualizations, and to be able to distribute the results in a simple web page.

First, the NVD data feeds visualization is a filtering web application where users can navigate through yearly computer virus entries based on the NVD scoring metrics (e.g., Integrity-Impact, Confidentiality-Impact, Company, etc.). The user can then select how they want to visualize those entries (bullet chart, tree graph, scatter plot, and calendar view) using D3.js, a JavaScript library. Lastly, AW3DM uses X3DOM[2] and jQuery, JavaScript libraries, to present 3D visualizations of human bodies, a set of controls, and a tabular view of demographic data associated with each body. X3DOM is a 3D language that enables placement of graphical elements directly into the DOM (Document Object Model) of the web page.

D3.js, jQuery, and X3DOM provide a great deal of portability among modern browsers and system extensibility, as they do not rely on plugins.

Electronic Test Equipment Interface with LabVIEW for Charge Based Capacitance Measurement

Karla Parraga

As devices get smaller, especially the ones that are used as scientific tools, their characterization become more complicated, especially for measurement of capacitance. It is our goal to develop a reliable method for measuring capacitance at the attoFarad level (10^{-18}) in nanoelectronic devices. In order to make the measurement experience rather fast and user friendly, we have opted to interface the instruments we will be using with a powerful and well known software developed by National Instruments, LabVIEW. LabVIEW allows us to have everything we need in only one panel. From this panel, we want to be able to control the number of channels we will be using, choose the frequency we need and display graphs and data that will help us understand how close we are from achieving our goals.

To take the measurements needed in this experiment, we need to connect an arbitrary waveform generator with two power supplies, an oscilloscope and a source meter. Setting up all these instruments manually takes time and it is rather tedious, especially when multiple measurements are needed. Thus, interfacing these instruments with LabVIEW is important because it allows the user to take more measurements even faster while having all the commands needed from different instruments on the same control panel.
Even though LabVIEW is able to execute different parts of code at the same time or in parallel, the instruments we are using execute instructions in series and in a specific order; this imposes both a problem and a waste of resources. For example, if two channels are to be phase locked together, one as a master and the other one as a slave, the order of execution that the instrument expects is to assign the channel first, and then to turn the phase locking mode on. Otherwise done, the instrument will call an error. Furthermore, the assignment of the channels both master and slave could be done at the same time or execute in parallel; however, this would cause an error since the instrument only accepts instructions in series. Thus, even though LabVIEW offers the convenient feature of parallel code execution, the instrument has its own serial execution code limitations that need to be taken into account.

Clemson University

Could Fish Help Treat Cancer?

Jorge Hernandez Sanchez

Peptides are commonly found working along with other macromolecules to fulfill all kinds of functions as complexes, but in some cases they may be found acting alone. One group of peptides is the Piscidins: peptides with promising antimicrobial and possibly anti-carcinogenic activity. Piscidins constitute a family of cationic antimicrobial peptides that are widespread in teleost fish and have broad spectrum activity against a large number of Gram-positive and Gram-negative bacteria, including MRSA, viruses such as HIV-1, fungi, yeasts, and even cancer cells. Teleost (ray-finned) fish use the peptide as a mechanism of defense against infection. These peptides are electrostatically attracted to anionic bacterial membranes. Similar to other cationic peptides, piscidins, are unstructured in water, but become structured in the presence of lipid bilayers and exhibit membrane permeabilizing capability. In this study we investigate the ability of Piscidin-1 (P1) to form pores in lipid membranes. We employ several experimental structural techniques such as circular dichroism, X-ray and neutron diffraction. In particular, neutron diffraction may be used to observe the morphology of a peptide/lipid bilayer complex, the depth of insertion of the peptide in the lipid membrane, and the formation of pores, which would lead to cell lysis. In this work, I have observed that increasing the ratio of P1 to lipid results in gradual changes to the bilayer structure such as thinning of the bilayer and reorientation of the peptide with respect to the bilayer surface. These changes culminate, at high peptide concentrations, with an insertion of the peptide into the bilayer core, associated with formation of pores. Neutron diffraction and specific deuterium labeling is used to examine in detail the peptide conformation. Possible mechanisms for pore formation will be discussed.

College of New Jersey

Improvements in E-Mail Security: A DANE/OpenPGP Test System

Daniel Lessoff

Recently, there has been a trend of securing the initial exchange of asymmetric public keys via DNS instead of trusting certificate authorities. This method, known as DANE (DNS-based Authentication of Named Entities) completely cuts out the need for certificate authorities. This is a positive change, as certificate authorities are susceptible to attack. While most of the current focus has been on authentication for websites and related services, not much effort has been devoted to applying the same technique to email security. As a part of NIST's High Assurance Domain (HAD) project, our goal is to create a test system to facilitate the use of DANE for the OpenPGP email standard. The intention is to provide a system that will allow users to test easily whether they have properly uploaded an OpenPGP key correctly according to the provisions of the current version of the IETF draft concerning DANE and OpenPGP, and that they can use that key to properly encrypt, decrypt, sign, and verify the signatures of OpenPGP emails. Additionally, the test system will provide useful feedback if the test fails for any reason. The implementation is in Python, using the dnspython and python-gnupg modules for DNS lookups and the GnuPG implementation of the OpenPGP standard.

College of William and Mary

Three-Dimensional Structures for the NIST Chemistry WebBook: My Journey from Molecular Optimization to Self-Optimization

Sonia Dermer

The NIST Chemistry WebBook is a free online database of molecules used by researchers, engineers, and students worldwide. Currently, the WebBook contains information on over 110,000 structures, varying from chemical names to gas chromatograms. Our goal was to enhance the WebBook by optimizing 25,000 molecules and adding the optimized structures to the database. During this process, we also verified several forms of identification including International Union of Pure and Applied Chemistry (IUPAC) nomenclature, chemical formulae, and Chemical Abstract Services (CAS) numbers.

Using Gaussian09, a computer program for quantum chemistry, we calculated chemicals' optimized structures, thereby determining the atoms' 3-dimensional coordinates in each molecule. In order to compute optimized structures, we applied simple Newtonian ball-and-spring models (MMFF and MM2) and progressed to complex quantum mechanical theories (PM6 and B3LYP).

By the end of the summer, we hope to have computed comprehensive 3-dimensional data on every molecule in the WebBook. In the future, these structures can be used as bases for experimental or theoretical research. The net result is an enhanced WebBook containing more thorough, diverse, and reliable data.

Characterizing the First All-Biological Single Photon Source
Melissa Guidry

The reaction between luciferin and ATP with catalysis from the enzyme luciferase results in the emission of a single photon. It has been seen to exhibit low cytotoxicity, resulting in the development of biological probes for imaging. This is applicable to both cancer research and drug development, where the movement and quantification of molecules is needed. The bioluminescence process demonstrates many of the characteristics of an ideal single photon source, and is unique from other single-photon sources in that it does not require optical excitation. NIST's unique tools will prove the single-photon character of the source, as well as better detailing the kinetics of the reaction. The effects of different chemical or biological agents on the kinetics of emission may also be studied to help refine in vivo techniques.

My work involved designing, building, and testing the experimental setup that will eventually allow us to detect single photons from the reaction. Two specific components were designed: a specialized flow cell and a specialized optics system. The cell design allows the bottom microscope plate to be quickly replaced, essential because the luciferin must be immobilized and replaced once the reaction is finished. A virtual model was created, which may be 3D printed and aligned in the optics setup. Dr. Polyakov designed and assembled the optics system consisting of two lenses, one with a very high numerical aperture, and a second used to focus the light onto a fiber. Calculations were performed to determine optimum lens and fiber combination for detection. A 3D stage was assembled to allow the detector to move across the sample. A knife-edge technique was used to characterize the optics system. A silvered and nano-etched fiber was built to operate as a point source, which, once characterized with the optics, allowed for a better representation of the optical throughput of the setup. A liquid fluorophore solution was flowed through a cuvette to determine quantities of luciferin and luciferase which would be appropriate for the system.

Colorado School of Mines

Developing a System for Monitoring NCNR Fume Hood Radiation Levels
Spencer Connor

In a research facility such as the NIST Center for Neutron Research, fume hoods are commonly used when handling radioactive materials. A series of Geiger-Müeller tubes are positioned in the ductwork of the hoods to measure gamma radiation in the air or from any airborne particulates that may exist. The system monitoring these detectors must be secure, accessible to Health Physics personnel, and be capable of running for extended periods of time with little to no maintenance. This role is currently served by three co-dependent computers with a single user-interface. The NCNR Hood Monitor Project is designed to replace the data logging, trend analysis, and user-interface of the current system while retaining the original detectors and associated hardware. In order to maintain reliability and security, the data from each detector is logged and stored in an online database by a virtual server, which alerts Health Physics personnel of any abnormal changes in radiation levels. The NCNR Hood Monitor project also includes a desktop program to display current values, examine historical trends, and export data in several formats. By eliminating as many of the physical elements of the current system and allowing Health Physics to access the system from their desktop computers, the NCNR Hood Monitor maintains security while being adaptable and accessible.

Microscene Grave Detection via Hyperspectral Imaging
Austin Cummings

It has been demonstrated that mass grave sites produce distinct spectral signatures in a tropical moist forest environment and may be located via remote sensing (Kalcska 2009). I prepared six trials of four different "micro-scenes", both with and without buried proxy meat, to attempt to quantify the signature of a grave site versus a false grave. Dirt, grass, chia seed, and sand were chosen to reflect a wide range of environmental situations and germination rates. Using a standard hyperspectral imager, the mean and pure vegetation reflectance spectra for each scene were recorded over the course of several weeks, and compared using spectral angle methods. Additionally, a quarter-kilogram of proxy material was buried under several inches of soil, with grass seeds planted on top, to illustrate the inhibiting effect of decaying proxy meat on plant growth. Three reflectance standards were also analyzed to help associate an uncertainty with the imager used.

The spectral angle between a grave mean spectra and its corresponding false grave mean spectra was found to increase over time, indicating a growing difference between them. The spectral angle between vegetation grown in soil with proxy material and vegetation grown in soil without it did not have a definite trend with respect to time. For most mean spectra, the grave site was found to have lower reflectance values in both the visible region from 450nm to 650nm and in the near infra-red region from 800nm to 1100nm. This implies a distinct spectral signature resulting from chemical changes in soil and differences in the amount of vegetation grown in the soil, with a smaller impact due to changing plant chemistry. It was also observed that the grass grown above the quarter-kilo of proxy material was significantly more pale and shorter than the grass grown above pure soil. These results both present possible spectral indicators of buried proxy material and demonstrate the utility of developing micro-scenes in order to study the capability of locating mass graves using hyperspectral imaging in different environments.

Spectral Uniformity: The HIP Way
Logan Hillberry

An imaging spectrometer is a device that captures an image whereby each pixel is a high resolution spectrum. The spectra are captured by collecting images of the scene in discrete wavelength bands and combining them into a data cube. A hyperspectral image is one which is collected in enough bands to resolve the entire spectrum over a given wavelength range. Such an image is used in remote sensing with applications in environmental monitoring, defense, and homeland security. In an effort to better calibrate and test such imagers, the National Institute of Standards and Technology (NIST) has been developing a Hyperspectral Image Projector (HIP) capable of projecting dynamic scenes with an arbitrary programmable spectrum for each of its 1024x768 pixels. The HIP has a spectral engine, capable of generating an arbitrary spectrum, coupled to a spatial engine capable of projecting that spectrum into the correct location of the scene. This talk describes different configurations for coupling the spectral and spatial engines. The spectral uniformity of each is quantified by a spectral angle mapper (SAM) routine. The goal is a spectrally uniform and bright projected image. Using an integrating sphere provides the most spectrally uniform image, but at a great loss of light. Therefore, we explored more light efficient methods: a liquid light guide and a randomized fiber bundle. We present quantitative results comparing these methods.

Interfacing a Charge Based Capacitance Measurement Device with Atomic Force Microscopy

Tim Taylor

As Moore's law continues to prove itself correct, characterization of devices becomes more and more difficult. Smaller devices mean smaller characteristics such as capacitance. Normal methods of measuring capacitance via impedance do not have the resolution necessary, due to the parasitic capacitances associated with connection wires. Charge Based Capacitance Measurement (CBCM) is a new method of easily characterizing the capacitance of a device down to the atto-Farads by avoiding and nulling parasitic capacitances. This is done by measuring the average current by charging and discharging a device like a capacitor in parallel to a reference or control branch. The goal of this project is to prototype a modular CBCM device to interface with an Atomic Force Microscope (AFM) and an amplifier circuit. The AFM will allow for a tip, 10s of nms wide, to come in contact with a test device, and then CBCM will be used. The amplifier circuit will amplify a differential output to allow for easy and accurate measurements of capacitances of any nano-scale structure. To achieve this, simulations in SPICE were completed to arrive at a combination of a differential amplifier and an amplified integrator. To prototype, a printed circuit board was designed to allow for testing of the circuit performance. An overview of each step in the process will be discussed.

Cornell University

Water Consumption in Manufacturing Processes

Susan McGrattan

Water is rapidly becoming a scarce resource in many areas of the world and millions of people do not have access to adequate amounts of water for drinking and sanitation. Current supply levels may be unable to meet future demand from a growing population and economy, emphasizing the importance of conservation efforts. Since industry consumes a significant amount of water for cooling and production purposes, the need for sustainable water use practices is rising. A goal for sustainable manufacturing efforts is to reduce industry's consumption of water and other resources, such as energy and materials, while continuing to produce high quality products.

This project focuses on the water usage aspect of sustainable manufacturing. An extensive literature review was conducted to examine the water requirements and water use in a variety of manufacturing processes. Individual processes were selected at the unit manufacturing level and specific water consumption was determined for each. Process rate was used to normalize the data for comparison in order to identify water intensive processes. Water conservation efforts can be focused on these processes to reduce water consumption and provide potential savings. These figures will serve as a useful guide for future investigations into the impact of water usage on manufacturing.

Denison University

Ultra High Speed Electronics for Single-Photon Detection in Quantum Key Distribution

Kristina Dungan

The field of quantum information is very diverse in its physical implementations. It is highly advantageous when it comes to cryptography because coded information sent in this manner is inherently unbreakable. This security is due to the fact that when a quantum system is measured, it collapses into one specific state and detectable irregularities are produced (Monroe 1164). Meaning that if an eavesdropper were to look at the information, their actions can be detected, indicating that the information is not secure. This is formally known as Quantum Key Distribution. One common implementation of this field of Quantum Information uses polarized single photons, much like classical information except instead of electronic 0s and 1s, vertical and horizontal polarization states of single photons are used to encode information. This summer, my research focused on the detection of these photons to improve our ability to receive encoded messages.

To advance the performance of the above method, high efficiency single-photon detectors with precise timing resolution are necessary. Furthermore, not only is it necessary to know if a photon was detected, it is also necessary to record the precise arrival time of the photons. To accomplish this, we are creating a time-tagging system with 100 picosecond resolution that is capable of counting photons at rates above 500 MHz. Currently, this high resolution can be achieved using field programmable gate arrays (FPGAs), but this method becomes impractical as the count rate increases. So, we are now creating a high-speed circuit board with an input clock of 10 GHz to generate the highest resolution time tags, combined with an FPGA to keep track of the detection events over longer periods of time. The advantage of this approach is that the arrival time of the photon is encoded in four bits directly by the time tagger and so we only need four connections to the FPGA for each channel of the single photon detector. This will allow numerous channels counting at 100s of MHz with 100 picosecond resolution. To construct this new detector, we used EAGLE Layout Editor to design a printed circuit board that we will assemble and test.

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Eastern Kentucky University

The Application of Barrier Fabrics to Prevent Smoldering in Upholstered Furniture

Shane Leger

Barrier fabrics are textile materials, used in soft furnishings to prevent or delay the ignition of the cushioning materials in a piece of upholstered furniture. While being flame resistant is an important aspect of a barrier fabric, it cannot be the only factor taken into consideration when evaluating an effective barrier fabric. Smoldering is combustion without flame and a smoldering cigarette is a common ignition source of soft furnishing fires. Barrier fabrics could be a cheap and effective way for manufacturers to reduce the flammability of their products. Barrier fabrics could be used as individual components, laminated to the cover fabric, or laminated to the cushioning layer. In this study we have explored barrier fabrics laminated to cover fabrics. Earlier studies have shown that barrier fabrics that exhibit sufficient resistance to open flame do not necessarily offer smoldering resistance. The main objective of this study was to examine the effects of lamination.

El Camino Community College

Evaluation of a New Dosimeter for Industrial Radiation Processing
Freddy Cisneros

Radiation processing is widely used for the sterilization of health care products (e.g., syringes), to enhance the chemical structure of everyday products to improve their performance (e.g., wire insulation), to extend the shelf life of food, and many other useful applications. The most common type of ionizing radiation used in industry is gamma-ray photons from radioactive cobalt-60 sources.

In irradiation facilities bulk irradiation is commonly practiced where large amounts of products are exposed to ionizing radiation to maximize throughput. Due to the interaction of radiation with matter, one cannot simply assume that all the products in the bulk are uniformly irradiated. To assure that all the products in the bulk receive the necessary dose, dosimeters are placed in pre-established reference locations on the product containers. Upon the completion of the radiation process these dosimeters are measured prior to product release.

Alanine dosimeters are the most accurate and widely used dosimeters due to their high reproducibility and the broad range of dose. Two forms of alanine dosimeters are commonly used in industry, the film and pellet forms both of which have their pros and cons. The pellet form that used by NIST for their postal-based transfer dosimetry services is more accurate than the film form but small (4.8 mm in diameter, 3.0 mm in height) and non-labeled making it difficult to handle by the industrial irradiating facilities. The film form is less accurate but is barcoded and in the form of a long strip making it much easier to handle when irradiating in bulk and throughput is of essence.

To combine the best qualities of each type, alanine dosimeter manufacturers have begun making prototypes of a hybrid alanine dosimeter. These hybrid dosimeters consist of an alanine pellet packaged at the end of a barcoded plastic handle. This new form of dosimeter will be easy to use, more accurate than the film dosimeter, and will aid irradiating facilities in achieving a high throughput with high precision.

My research will analyze the properties of this new hybrid dosimeter compared to both the pellet and film dosimeters.

Elizabeth City State University

Measuring Three-Dimensional Angle of Through-Silicon via Using TSOM Method
Ama Agyapong

Copper-filled through-silicon via (TSVs) connect circuits located in different levels in an integrated circuit (IC) chip. Functioning of an IC chip is affected by proper formation of TSVs. TSVs are truly three-dimensional (3-D), high-aspect-ratio (HAR) targets. Non-destructively measuring 3-D shape, size and formation of the TSVs with high-throughput is a challenge using conventional tools.

In this work we present a NIST-developed through-focus scanning optical microscopy (TSOM) method for this application. The TSOM method uses standard bright-field compound microscopes to measure 3-D shape with nanoscale measurement sensitivity. The TSOM process takes multiple "out-of-focus" images, stacks them at the proper focal positions, and then extracts a vertical cross-sectional TSOM image. By making use of the useful characteristics of the TSOM images, 3-D shape of any nanoscale to microscale target can be extracted. In the current work we make use of the TSOM method to determine the angle of TSVs with respect to the surface. The TSOM method achieves this non-destructively with high-throughput, a distinct advantage compared to other conventional methods.

TSVs are expected to be normal (axis perpendicular) to the surface of the silicon wafer. However, during fabrication, the actual angle deviates from this desired angle and could lead to improper connectivity between circuits, jeopardizing proper functioning of products. By determining the behavior of TSVs across individual dies of the entire wafer, a solution can be created to solve problems caused or related to defects within TSVs.

Angles of TSV axes located in several dies across the wafer were measured using the TSOM method. Preliminary results indicate that the TSVs closer to the center of the wafer have near normal axes. Deviation of the TSV axis from normal increases as the die position reaches towards the edges. Overall behavior of the TSV angles across the wafer appears to be radial from the center of the wafer. The TSOM-evaluated measurements need to be confirmed using reference measurements.

Fayetteville State University

Evaluating Nanofilm Coatings to Prevent Flammability in Household Furniture

Sabrena Clayton

Three thousand people die every year in fires that started with household furniture. There is no fire retardant available that can prevent those fires. This summer we have tried to create a method to prevent the risk of fire from both open flame and smoldering. We utilized recipes previously tested on foam, and applied them to cotton fabric samples. These samples were then evaluated for their flammability using direct flame and smoldering tests.

Examining Electrical Cable Degradation in Nuclear Power Plants

Blake Thrift

In nuclear power plants, electrical cables perform critical tasks such as conveying power, facilitating communication functions, and monitoring the status of the reactor. As such, their performance is vital for the safe operation of a nuclear power plant. Electrical cables in nuclear power plants are often subjected to a variety of damaging conditions such as high temperatures and humidity, water and light exposure, and radiation. Premature electrical cable failures have been observed in nuclear power plants and have raised interest in investigating the service life of electrical cables. To this end, the polymer jackets and insulation of nine different types of cables commonly used in nuclear power plants were characterized by ATR-FTIR (Attenuated total reflection - Fourier transform infrared) spectroscopy, density, and indenter modulus. The electrical cables were then aged in three different environments: 55°C and 75% relative humidity, submerged in tap water at 75°C, or submerged in deionized water at 75°C. The effects of the elevated temperature and humidity or exposure to water were determined using the same characterization method described. Degraded cables showed little to no change in density, a decrease in indenter modulus, and an increase in carbonyl bonds.

Florida A & M University

Reactor Data at Your Desk V2.0
Alexander Hull

The NIST Center for Neutron Research, home to a 20MW research reactor, was approved for operation in 1967, and first reached criticality in December of that year. As technology advanced, much of the NCNR's facilities have been upgraded and improved, however much of the reactor's data has remained viewable only in the control room via consoles and analogue indicators. These indicators and historical logs for the reactor were only accessible to the reactor operators seated at the control console. Only recently has the data been made accessible remotely.

With a PC using labVIEW and an OPC server, the PC pushes all of the data points from the control room through a secure one-directional connection and onto the NIST network. A MySQL database has been setup to accept the current values and overwrite the old values with the new ones at a regular interval. A historical data table is created by pushing the values to a separate table that is appended, as opposed to overwritten. To make the data accessible to end users, the database was used to design a desktop application that would allow users to view the data points updating in real time as well as view trends by graphing the historical data; An internal website was also made, but with less functionality.

This project entailed improvement of the already existing programs with a focus on user-friendliness and functionality. Functionality was improved with additional features, such as the ability to export data as a CSV file for use with Microsoft Excel, while user-friendliness was improved with the addition of more intuitive aesthetics and error control for more ease of use.

Florida Institute of Technology

Data Preprocessing and Characterization for Manufacturing Power Data
Alejandra Dominguez

Demands for high quality, productivity, and sustainability are shifting the manufacturing industry toward the implementation of the Smart Manufacturing System (SMS). This includes the application of advanced technologies, data analytics, and their shared infrastructure in order to enable rapid optimization and control for agility, flexibility, and energy and resource efficiency. Data analytics, the science of analysis of data, is a key component in Smart Manufacturing Systems (SMS) for it enables the data set to be better represented and allows for clearer inferences to be made from the data. The first step in data analytics is to correctly preprocess the data and characterize it depending on its attributes. A well processed data set is important because the machine learning performances are dependent of the quality of the input dataset. Therefore it is crucial to correctly and accurately filter, reduce, and characterize the manufacturing data that has been acquired.

The purpose of this project is to develop a data preprocessing and characterization logic model for a machine's power consumption during metal cutting operations. The cores of the logic are to filter noise data, restore missing data, and characterize representative values from raw power data without losing any important information. A prototype has been implemented to validate the logic and measure the performance of the logic with use of the Matlab platform. The deliverable of this project can contribute to the development of a data preprocessor that creates a better input data set for reliable and efficient analytics modeling in manufacturing data analytics.

The Use of Discrete Event Simulation for Assuring the Performance of a Manufacturing System
Jordan Senatore

This research aims to demonstrate a method for optimizing performance based upon multiple Key Performance Indicators (KPIs) such as cost, energy consumption, carbon emission, and total production time. Often times these KPIs are conflicting and so a middle ground must be found that strikes a balance between the objectives. In current manufacturing systems industry experience is often used to minimize production time or cost; however, to factor in sustainability goals with competing objectives, a more objective tool is needed.

We use discrete event simulation as a method for assuring the performance of manufacturing systems in light of competing priorities. Simulation provides an objective method to quickly and accurately plan plant operations based upon a single objective or many competing objectives. Plant managers can quickly and easily explore many options at the beginning of each day or at the arrival of a new batch of orders. Simulation will allow for optimal configurations to be chosen that not only minimize cost or time, but also take sustainability goals into account. We constructed a model using Arena, a commercial simulation software package, of a machine shop with several machines that could each perform multiple processes. The manufacturing of a batch of parts was then simulated using the model while important KPIs were monitored. Machine settings (e.g. cutting speed, feed rate, depth of cut, etc.) were varied over a set range, thus allowing an optimal configuration to be found for each machine that leads to the highest performing system. Multiple scenarios were completed that test the ability of the system to find optimal settings ranging from a simple one part scenario with a predefined production plan to a much more complex system with multiple parts and no predefined production plan. The simulation model is used to determine optimal settings for each individual machine in the manufacturing system and then it is used to determine the optimal production plan to lead to the highest performing system.

The manufacturing industry is tending towards agile, more responsive plant designs and operations. This research will not only help optimize machine settings and configurations, but could also be used to explore the effects of disruptions and potential solutions. Disruptions can be internal (e.g. machine failure) or external (e.g. late material arrival or changed orders). The research will help improve overall industry efficiency, while opening up many possibilities for the future of Smart Manufacturing.

Geneva College

Extensional Flow-SANS of Wormlike Micelles
Bonnie Newman

Extensional flows are observed in many industrial applications including polymer extrusion as well as pharmaceutical consumer product processing and delivery, where safety, quality assurance, and marketability are crucial. Unfortunately, pure extensional flow is difficult to obtain and the associated properties can be challenging to measure. Micelles are structures which form in surfactant solutions at concentrations above the critical micelle concentration (CMC). Wormlike micelles are a specific type of high aspect ratio micelle with a micelle length that exceeds the persistence length. These solutions are good candidates for measurement with extensional flow-SANS because the structure and rheology of these systems have been studied extensively in shear flows, while limited extensional flow data exists. Additionally, previous studies have used micro-particle image velocimetry (µPIV) and optical birefringence measurements to characterize wormlike micelles in microfluidic cross-slots. Small angle neutron scattering (SANS), however, is a great technique to characterize wormlike micelles under flow, because the characteristic dimensions of the micelles are on the order of nanometers to hundreds of nanometers. In this work, we have begun to characterize the structure and rheology of cetylpyridinium chloride and sodium salicylate wormlike micelle solutions, using a specially designed cross-slot flow cell. This study explores the effects of channel depth and flow rate on the structural transitions of the wormlike micelles. Further, we measure the flow-induced alignment of the wormlike micelles and their subsequent relaxation during start-stop flow experiments. The results of this study will be used to help optimize the new cross-slot flow cell before it is used for experiments with more complex fluids.

Hamilton College

See You on the Flipped Side: The Construction and Optimization of RF Coils Used to Flip ^{3}He Polarization

Joelle Baer

^{3}He neutron spin filters (NSFs) are currently used at the NIST Center for Neutron Research (NCNR) to both polarize the incident neutron beam and analyze the neutrons scattered off of a sample. NSFs can polarize large beam areas, allowing for the integration of a spin flipper with the polarizing device. Therefore, it is important to be able to invert the spin state of the ^{3}He. For beamline use, the polarized ^{3}He cell is placed inside a cylindrical magnetically-uniform, magnetostatic cavity or shielded solenoid, and the ^{3}He nuclei align with the static magnetic field produced inside. A radio-frequency (RF) coil, placed around the cell inside, produces a field orthogonal to the holding field of the solenoid and can flip the polarization with negligible loss using the Adiabatic Fast Passage (AFP) nuclear magnetic resonance (NMR) technique. This project was based upon the construction and optimization of these RF coils. It is important to avoid material in the beam when designing RF coils, so a specially designed sin(θ) RF coil is used. Each coil was tested within the various solenoids to optimize the parameters that would flip the ^{3}He with the most efficiency. This efficiency is measured using Free Induction Decay (FID) NMR on a small portion of the cell's polarized gas, representative of the whole, using a small NMR coil. With the increase in beamline use, more RF coils are necessary to maximize the number of simultaneous experiments, and to simplify the solenoid use by pairing each one with its own coil.

Harvey Mudd College

Proposals for NIST Standards on Generation of Random Primes for Cryptography

Sarah Scheffler

Most modern cryptosystems rely on the generation of random prime numbers as part of the process used to create keys with which to encrypt and decrypt data. The generation of random, secret primes is at the heart of the security of all encrypted data. The National Institute of Standards and Technology (NIST) has standards for the process by which a cryptographic prime number is generated, which involves a Random Number Generator (RNG) and a test for primality. In this talk, I will discuss three adjustments to the prime generation process. I provide a way to customize the prime for users who wish to impose an additional constraint to their generated primes. I show that NIST's statistical test suite for RNGs is insufficient by itself to prove the security of that RNG. I also discuss modifications to the error bounds on the primality tests.

Hood College

BIRDS Residential: Measuring Sustainability
Tarang Hirani

Building stakeholders and investors need practical metrics, tools, and data to support investment choices and policymaking related to sustainable building designs, technologies, and regulations. The need for this is being addressed by extending the metrics and tools for sustainable building products, known as BEES, to whole buildings. This process involves the development of sustainability metrics that are based on extensions to Life-Cycle Assessment (LCA) and Life Cycle Costing (LCC) approaches involving building energy simulations.

Building Industry Reporting and Design for Sustainability (BIRDS) residential module applies the new sustainability measurement system to an extensive residential building performance database compiled by NIST. The database includes energy, environmental, and cost measurement for residential buildings in 229 cities across the U.S. The sustainability performance of buildings designed to meet current state energy codes can be compared to their performance when meeting four alternative building energy standard editions to determine the impact of energy efficiency on sustainability performance. BIRDS Residential focuses on entities such as federal agencies, state code officials, standards organizations, and the public to allow for high level analysis of energy efficiency.

My involvement in the project was to develop a web application for the BIRDS Residential database. The application relies on user-interaction to compare and contrast different energy, environmental and cost measurement constraints. Results are displayed as graphical representation of the impact of building location and investor's time horizon on sustainability performance.

Massive Virtualization and Its Effects on Software Entropy Sources
Robert Staples

Any data encryption method is only as secure as the key that is used in its encoding. Keys are often produced by pseudo-random number generators that use a truly random “seed” value. These seed values must be independent, secure, and preferably accessible on-demand. The sources of these seed values are known as “Entropy Sources,” because they are sources from which randomness, or “entropy,” is harvested.

In recent years, virtualization has exploded in popularity, as general-purpose computers have become powerful enough to run multiple “virtual” machines on the same hardware. What I wanted to know was whether virtualization had any effect, negatively or positively, on entropy sources. Given that a single piece of physical hardware underlies often hundreds of concurrently-running virtual machines, and often without the virtualized machine even being aware of it, is there any security vulnerability introduced there?

I used two methods to find any effects: the NIST SP 800-90B entropy estimation tests, and a cross-correlation test. I created a baseline set of data using multiple instances of the entropy sources running concurrently on the same machine; and I now plan to run multiple instances of identical virtual machines on the same hardware, and compare the results of the 90B and cross-correlation tests.

Through this research, NIST hopes to gain valuable insight into any possible security issues surrounding virtualization technology and the generation of cryptographic random numbers.

Jackson State University

Exploration of NSIT Mass Spectroscopy Data with D3
Ayotunde Olutade

We use two types of visualization to visualize mass spectrometer data. The first type of visualization is called Information Visualization. This consists of a variety of 2-Dimensional visualizations, which abstract the data in some way. We display these in web pages using the Data Driven Documents (D3) JavaScript library. We are using D3 because it is extremely fast, supports datasets of varying sizes, and facilitates interactivity. It also requires no browser plug-ins and works across different web browsers and operating systems. The second type of visualization is immersive 3D. We use the NIST Immersive Visualization software to display the mass spectrometer data as pure spectra. We developed visualizations of the libraries of pre-classified mono- and di-saccharides and a group of unknowns in order to classify the unknowns into one of the groups.

James Madison University

Computational Methods to Analyze Small Angle Scattering Data of Biological Molecules & Free Energy Calculations to Validate Structural Ensembles
Andy Heindel

Cardiomyopathy, the deterioration of the myocardium within the heart, is one of leading factors contributing to heart disease. Although cardiomyopathy can be acquired through post-natal mutation, many cases result from genetic abnormalities resulting in the mutation of a protein named Obscurin. Mutant Obscurin contains a single amino acid substitution, Arg4344Gln, within Ig58/59, two domains in Obscurin. This mutation lowers the affinity for two domains of Titan, Ig9/10. Titan serves as an adhesion template for contractile machinery in the sarcomere. When the binding affinity is lowered due the mutation within Obscurin, the passive elasticity within the muscle decreases. Although biological data supports this hypothesis, very little structural data has been collected. Consequently, small angle X-ray scattering (SAXS) was conducted to determine the low-resolution solution structure of Ig58/59 from Obscurin. Guinier analysis was then conducted and indicated Ig58/59 had a radius of gyration of 30.0Å. Theoretical structures were generated using Molecular Monte Carlo (MMC) and molecular dynamics (MD). Theoretical scattering curves were then predicted for the resulting structures. The theoretical scattering profiles spanned a region between ~18Å-~30Å. Solution structures were derived through comparisons between the theoretical scattering profiles and experimental SAXS data. Due to the computational complexity of MMC, however, generated structures are potentially energetically unfavorable. Consequently, a proof-of-concept study was conducted to determine the energetics of clustered MMC structures. Molecular mechanical energies and solvation free energies are being calculated and summed to determine the Gibb’s free energy (DG) of clustered structural ensembles. Further studies are being conducted to determine the feasibility of the generated structures. Preliminary SAXS data and other structural muscle proteins indicate an extended form, suggesting Ig58/59 is natively extended. With the use of SAXS data and Gibb's free energy data, a representative solution structure of Ig58/59 is likely feasible.

Gravimetry for the NIST-4 Watt Balance
Eric Leaman

The kilogram is the only SI unit to still be defined by a physical artifact, the International Prototype Kilogram (IPK). Currently, there is an international effort to redefine the kilogram in terms of the Planck Constant, h. One method of linking mass to h is through measurements made with a watt balance, an instrument that compares mechanical power to electrical power by moving a coil inside a magnetic field. Currently under construction is NIST's fourth generation watt balance, NIST-4, which will be optimized to realize mass once the value of h has been fixed. An inherent and direct source of uncertainty in watt balance measurements is the local acceleration due to gravity, g. During watt balance operation, the value of g at the position of the test mass must be predicted based on a model and measurements of gravity fluctuations throughout the laboratory. This value is then tied to an absolute reference point. During the summer of 2014, a three-dimensional model was created for the entire laboratory which allows for the vertical gradient of gravity at all vertical positions of the mass to be determined. The model was confirmed by comparison to horizontal mappings made using a portable relative gravimeter. Further measurements were made to create a tie between the position of a permanently-installed relative gravimeter and the horizontal-plane position of the mass. By combining model predictions and measurements, the absolute value of g at all possible mass positions can be determined accurately and with the low uncertainty demanded by such experiments of only a few parts in 109.

Rhodopsin/G-Protein Solution Studies via Nanodisc Lipid Bilayer
Matt Oehler

G-protein coupled receptors (GPCRs) are the largest and most diverse class of membrane receptors among eukaryotes. Their response to an extra-cellular agonist is coordinated with the activation of a cytoplasmic G-protein which, once activated, kick-starts an immense intracellular cascade. Because of their ubiquity and relevance in mediating an enormity of physiological functions, GCPRs are the target of a large percentage of pharmaceutical drugs. While there are GCPRs that respond to a diverse range of signals, here we aim to study the effect of light activation upon the GCPR, Rhodopsin using the light stable homologue of the species *Sepia officinalis*. Enveloping the Rhodopsin GCPRs in lipid-membrane nanodiscs will provide a native state bilayer that should offer a more accurate structural representation of rhodopsin in the cell compared to more common detergent methods. Solubilization of rhodopsin in nanodiscs can generate a monodisperse system in solution amenable to small angle neutron scattering experiments (SANS). This will allow us to observe, at low resolution, the particular configuration of rhodopsin within a nanodisc as a first step to understanding its interaction with the guanosine-nucleotide binding protein under the same parameters.

Juanita College

Describing the Quantum Character of Metallic Nanoparticle Plasmons
Alexander Debrecht

Nanoscale transmission of quantum excitations in quantum information technologies must preserve the quantum character of the information. One proposed realization for nanoscale quantum information transfer uses hybrid systems of metallic nanoparticles (MNPs) and semiconductor quantum dots, with plasmons in MNPs moving qubits from one quantum dot to another. A quantum description of the entire system treating the MNPs and quantum dots on an equal footing is needed to fully account for size quantization, quantized plasmons, coherent coupling, interparticle tunneling, and nonlocal and nonlinear response. To achieve this, a quantum description of the MNPs is needed.

A variety of studies have examined the nature of plasmonic excitations in metallic nanoparticles (MNPs). However, most of these studies have been done with time-dependent density functional theory, which can yield information on the nature of the excitations but not the quantum character, including whether the excitations are fermionic or bosonic and whether they are harmonic oscillator-like, as well as the charge densities for plasmonic states. Such quantum information is necessary to build accurate models for quantized plasmons in MNPs. To begin to address these issues, we have explored simple models for interacting electrons on a linear chain. For short chains, the eigenmodes of the interacting electrons are found exactly. As expected, the ground state shows a Mott transition as the hopping along the chain is varied. For the regime where the interacting ground state of the system is metallic, we discuss initial results that analyze the character of the excitations. The results are used to identify whether excitations are fermionic or bosonic, which excitations are collective, which are harmonic oscillator-like, and when nonlinear effects appear.

Magnetic Ground State of Industrial Sensors

Teresa Turmanian

Neutrons are a useful tool for exploring the microscopic nature of materials. Polarized Neutron Reflectometry (PNR) is used to determine the structural and magnetic depth profiles of thin films and multilayer structures. We have used PNR to study the magnetic ordering of giant magnetoresistive (GMR) sensors. The material used to sense the presence of an external magnetic field is a repeating structure of metallic thin films atop a substrate and several seed layers. The repeated structure is surrounded by Si, Si_3N_4, Ta, and NiFeCo layers below and a Ta cap above. The unit cell which, is repeated four times, consists of four thin (nm-scale) layers, namely Cu, NiFeCo, Cu, and CoFe. The ferromagnetic layers have magnetizations that, in the absence of a magnetic field, align antiparallel to one another. In the presence of a magnetic field, the layer magnetizations align with the field. The transition from anti-parallel to parallel alignment gives rise to a decrease in electrical resistance, allowing for the detection of the magnetic field. Consequently it is important to understand the magnetic ground state of the sensor when no field is applied. To perform a PNR experiment, a polychromatic neutron beam passes through a monochromator, polarizer, and spin flipper. After reflecting off the sample, the neutrons pass through another spin flipper, a supermirror analyzer, and finally into a detector. The sample is mounted on a stage which is rotated in unison with the detector in order to vary the neutron’s angle of incidence. The reflected intensity as a function of angle over time was measured on a wafer at room temperature in magnetic fields of strengths 20mT and 0.5 mT. The software program Refl1D was used to fit a model of the structural and magnetic scattering length density as a function of depth. The high field data is fit well by a model in which Cu is magnetized. This result was not expected since Cu is not ferromagnetic, implying that there is mixing of magnetic NiFeCo and CoFe layers and the non-magnetic Cu layers that separate them. The low field data was fit using the thickness and scattering length density values determined from high field data.

Lehigh University

FORC Measurements Using the Anomalous Hall Effect: A FeCuPtL1$_0$
Kyle Stritch

The first order reversal curve (FORC) method has been used for several years to understand the magnetic phenomena in various magnetic systems. The conventional method for taking FORC measurements involves the use of a vibrating sample magnetometer (VSM). However, it has recently been discovered that FORC measurements can also be acquired using a transport technique such as the anomalous Hall Effect (AHE). The FORCs generated from both of these methods reveal many similarities and key differences that need to be more fully explored and understood.

The FORCs of a series of five FeCuPt film samples, previously subjected to rapid thermal annealing (RTA) in the temperature range of 300^{o}C to 400^{o}C in 25^{o}C increments, were measured. Within this temperature range, the FeCuPt system transforms from the disordered A1 phase at 300^{o}C to the ordered L1$_0$ phase at 400^{o}C. Full interpretation of the FORCs are beyond the scope of this project, however, hypotheses can be made for the reasons behind the differences observed in the shape of the FORCs for the samples annealed at the five different temperatures. At a later time, the FORCs measured by the AHE method will ultimately be fully interpreted and compared to the conventional VSM measurements to better understand the similarities and differences between the two methods.

Louisiana State University and Agricultural land Mechanical College

Measurement of the Magnetocaloric Effect in Ni-Mn-Al Type Alloys
Daniel Lepkowski

Modern day refrigeration systems use environmentally harmful materials and inefficient compression and expansion cycles, providing a need for a new environmentally safe and efficient method for refrigeration. Magnetic refrigeration, utilizing the magnetocaloric effect (MCE), is much more environmentally friendly and theoretically can achieve higher efficiencies than the current system. This study looks at the Ni-Mn-Al type alloys because their structural and magnetic transformations are near room temperature which many believe to be indicative of a large MCE in the same temperature range. The specific alloys in atomic percent were $Ni_{45}Co_{5-X}Fe_XMn_{32}Al_{18}$ (x=0, 2.5, or 5). Co and Fe were used as additives in place of Ni in order to enhance the magnetic moment of a generally low moment material. This, in turn, is expected to enhance the MCE.

Samples were fabricated by arc melting high purity metals (>99.9% pure) in the correct stoichiometric ratios for the alloy. The maximum weight loss during melting was less than 1.1%. The as-cast samples were reasonably ductile, and the samples showed a dendritic microstructure which is indicative of composition variations. The samples were then annealed at 1050^{o}C for 72 hours in an argon atmosphere and quenched in an icy brine solution to ensure a single phase homogeneous material. The samples grew millimeter sized crystals and became much more brittle through the annealing process. Quantitative energy dispersive spectroscopy was used to verify the compositions of the annealed and as cast samples while differential scanning calorimetry (DSC) was used to locate the structural transitions for all of the materials. From the optical metallographic study, the X=0 (Co only) annealed sample appears to have a martensitic structure at room temperature while the other two samples appear to have a cubic structure. X-ray diffraction will be performed to confirm this result. Electron backscatter diffraction was used to map the surface of the sample and to find the orientations of the individual crystals. The X=5 (Fe only) sample was mapped to be a single crystal on the surface, while the X=2.5 (half Fe, half Co) sample showed approximately 14 crystals in various orientations. The MCE for each sample is calculated using Magnetization vs. Applied Magnetic Field data measured at successive temperatures. This data was integrated to determine a change in entropy vs. temperature curve for that sample. From that curve, the cooling capacity can be determined which is then corrected for the magnetic hysteresis work needed to cycle the magnetic field. The effect of the Fe and Co additives and the differing microstructures on the MCE of the alloys will be discussed.

Marquette University

The Role of Size and Crystallinity on Magnetic Nanoparticle Response
Hoan Henry Le

Magnetic nanoparticles have a variety of uses including MRI contrast, hypothermia cancer treatments, and biomedical tagging. However, the details of their magnetic response can greatly affect efficacy. First, we looked at the difference between 10 nm and 30 nm nanoparticles of Fe_3O_4 coated in a shell of oleic acid to protect them from oxidation. Compared to the 30 nm, the 10 nm nanoparticle-to-nanoparticle distance is closer, as expected. To fit the Small Angle Neutron Scattering (SANS) data, I used a hard sphere packing model, obtaining structural diameters of the two samples to be 10 nm +/- 1.4 and 30 nm +/- 0.4. Surprisingly, as determined by high angle x-ray diffraction, the 10 nm nanoparticles have crystallite domains of 6.84 nm, just slightly smaller than their structural size, while the 30 nm nanoparticles have domains of 7.55 nm, which is significantly smaller than their structural size. Interestingly, the nearly single crystal 10 nm nanoparticles were 78% as magnetic as bulk Fe_3O_4 at 1.2 T, while the 30 nm nanoparticles comprised of multiple crystalline domains were only 58% as magnetic as bulk.

Second, we set up two conditions to test the effect of spatial confinement: the original nanoparticles that were oriented randomly but held in place with oleic acid, and we created particles that were easier to rotate with the addition of a lubricating polyethylene glycol (PEG) solution. The net magnetization of the nanoparticles with PEG was slightly higher compared to the plain particles within error for both the 10 nm and 30 nm samples. Additionally we were able to extract an average canting angle between the magnetization of the nanoparticles and the applied field for a series of fields, to which we apply a Zeeman versus magnetocrystalline model.

Mary Baldwin College

Printing Drugs on Edible Substrates
Alana Rister

The purpose of the project is to determine a method of printing medications onto edible substrates. This research is important because it could be used to make medicine distribution systems that are inexpensive, accurate, and individualized. It will also provide medication for people who cannot swallow pills, which may be especially useful for the elderly and children. Inkjet printing has been shown to be a repeatable method for depositing small volumes of solution onto a variety of substrates [ref 1-3]. This project had three main focus areas: Ink formulation, substrates, and characterization. With Ink formulation, we worked with different medicines including Acetaminophen and Folic Acid to produce printable “inks” that we could use with a piezoelectric inkjet printer. This included experimenting with different solvents and concentrations to determine a suitable solution. Secondly, we worked with different types of substrates, from rice paper and icing sheets to gelatin molds, for identification of which substrates would work best to print onto. In addition, we were looking to see how many drops the substrate could hold, whether the ink would dissolve the substrate, and how well we could control the deposition on the substrate. Thirdly, we used various tools to characterize what was printed. We experimented with different ways to determine the concentration of what we were printing. In addition, we analyzed samples with several different microscopy methods that include SIMS, SEM, RAMAN, and FTIR- microscopy to view the crystallization of our printed medicines and to determine the spread the deposits on substrates. All in all, the research conducted through this project can contribute to most importantly being able to quantify what you are printing onto a substrate that would ultimately be taken as a medicine. Future research will investigate different substrates and new medicine-solvent mixtures to prepare different types of medicines.

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Massachusetts Institute of Technology

Metrology and Optimization of Additive Manufacturing and 3D Printing

Lourdes Bobbio

Additive manufacturing (AM) refers to an increasingly popular approach to manufacture products layer by layer from the ground up. This research project is the first step to help identify and address the limitations of the current generation of technology, as well as develop measurements tools and techniques to characterize and optimize these additive manufacturing instruments. The goal of this project was to identify the optimized operational characteristics and material limitations of several fused-deposition-modeling (FDM) type 3D printers using different filament materials.

In this research project, we used three commercially available FDM 3D printers and five different printing materials. Each of these printer-material combinations were tested under different printing constraints, such as extruder temperature (180-240°C), extruder speed (10-110 mm/s) and printed layer thickness (0.2-0.4 mm). In order to standardize the process and perform inter-comparison studies, a benchmark model was created that would identify different features used to determine the quality of the finished print job in terms of process capabilities and printer accuracy. We measured and compared how changing each parameter affected the final part with the goal of standardizing the parameters for each printer-material combination.

This talk will provide a brief overview of the diverse technologies used in 3D printing, and then go into detail about the design of the benchmark model, the various 3D printer machines used in this study, the measurement tools and techniques used to characterize the 3D printed parts. We hope that by the conclusion of this summer project, our findings will provide valuable reference data for the increasingly growing additive manufacturing and 3D printing community.

McLennan Community College

Virtual Fusion: Human Presence in Manufacturing Simulation
Victor Trujillo, Jr.

Virtual Reality has long since been a dream firmly entrenched in the psyche of any technology enthusiast. Until recently, Virtual Reality (VR) was a dream that seemed out of reach. The Oculus Rift is a VR consumer product that allows its users to immerse themselves in a virtual environment. The release of the Oculus Rift has opened up many windows for the use of Virtual Reality applications other than just for video games. Our focus is to combine the Oculus Rift and Microsoft's Kinect, to create an interactive virtual manufacturing environment for simulation and systems validation. Blender, which is a modeling and animation software tool, is used to design the environment in which the user will interact. The Unity game engine is used to incorporate both, the Oculus Rift and the Kinect with the models that are created in Blender. The Oculus Rift will display the environment, while tracking head movements by using a gyroscope, an accelerometer, and a magnetometer. The Kinect will track body motion and allow for relatively free movement in the environment. With the Oculus Rift and the Kinect running simultaneously, the user will be able to interact with the virtual environment as they would with the real.

Miami University of Ohio

Feedback Controlled Magnetic Field Zeroing for rare Earth Quantum Memory
Ethan Clements

In praseodymium-doped Y_2SiO_5, precision control of the magnetic field environment enables us to remove many of the decoherence mechanisms in the crystal. To control the magnetic fields we constructed Helmholtz coils oriented along 3 perpendicular axes. We also want to ensure that for long periods of time, our magnetic field zeroing remains stable and does not change due to alteration in the environment. To do this, we utilize a PI (Proportional, Integral) feedback loop so that our system responds to any changes in the environment. The system we constructed utilizes an Arduino Uno to measure and control feedback to the system. The Arduino measures the magnetic field using a triple axis magneto resistive digital magnetometer, compares with the desired magnetic field, then feeds this error value into the PI loop. The voltage output from the PI loop is sent to a transconductance amplifier which outputs a desired current proportional to the input voltage. This current passes through the Helmholtz coils generating a magnetic field. Due to our ability to accurately measure the magnetic field we are able to zero the local field or set it to a desired value. We designed our system to output up to 3 mT – so we can freeze out the nuclear spin flips. Our setup obtains a magnetic field control of .4 µT. This apparatus will aid in further experimentation with praseodymium-doped crystals as long lifetime quantum memories.

Middle Tennessee State University

MIX 13: A NIST Interlaboratory Study on the Present State of DNA Mixture Interpretation
Brooke Morgan

DNA evidence interpretation for single-source profiles-where single evidentiary profile matches the profile from the suspected perpetrator-are relatively easy to determine and report to a jury. For many cases the interpretation is not as straight-forward. In fact, one of the biggest obstacles faced in today's forensic laboratories is interpreting DNA mixtures, where two or more individuals are in the evidentiary profile. Historically there has been little guidance to assist the analyst in determining the components of the mixture. Peter Gill, a leader in the field of DNA typing once said, "If you show 10 colleagues a mixture, you will probably end up with 10 different answers"

In 2010, the Scientific Working Group on DNA Analysis Methods (SWGDAM) published guidelines to assist labs in mixture interpretation. Since then, many laboratories have improved their Standard Operating Procedures (SOPs) based upon the 2010 SWGDAM guidelines.

An interlaboratory study is a useful tool that allows laboratories to compare their analyses to other laboratories and determine if additional training is necessary. Previous NIST interlaboratory studies on mixture interpretation resulted in a wide range of variation within and between laboratories. In 2013, NIST conducted an interlaboratory study (MIX13) to examine the present state of DNA mixture interpretation in the U.S. after the implementation of the 2010 SWGDAM guidelines.

Here we present results from one of five MIX13 cases. A substantial amount of variation was found within and between labs when interpreting a two-person mixture of equal proportion. These findings can help the laboratory to identify potential limitations in their SOPs, provide resources for future training, and conduct research to improve mixture interpretation and reporting in the United States.

Millersville University

Evaluation of Development Technologies and Usability Design for Cross-Platform/Cross-Device Biometric Applications

Jared McAndrews

The standard protocol known as Web Services for Biometric Devices (WS-BD) was developed by the NIST Biometric Clients Lab, in response to the widespread shift towards mobile computing. WS-BD uses current web technologies to enable driver free and wireless communication between software running on nearly any platform and nearly any kind of biometric device. Web-Services for Acquiring Biometric Information (wsabi) 2.0 is an iOS-based application developed for the iPad to enable testing and demonstration of WS-BD devices. In order to address the growing popularity of smartphones, the design for wsabi 2.0 needs to be reevaluated for smaller form-factor devices. Additionally, new development should be done using cross-platform technologies. Some of the cross-platform development tools that we researched include Mosync, Apache Flex, Phonegap, and Google Web Toolkit (GWT). We began research and development of interface guidance for smartphone application, wsabi 3.0. After analysis of available tools and technologies, we decided to use GWT, and Phonegap. These tools facilitated the development of an application that leveraged and implemented web technologies available on every Internet-enabled device, particular smartphones. Both the Nexus 4, and the iPhone were used for development and testing. Detailed research on cross-platform development technologies, usability test results, and the current state of wsabi 3.0 will be presented.

Monmouth University

pH Dependence of Colloid Surface Interactions in Charged Depletion Systems
Nicole Famularo

Colloidal systems are a major component of our world, and can be observed in vastly different environments. From inanimate objects such as ink, cosmetics, milk, jelly, detergents, and aerosols, to biological materials such as blood, cells, proteins, and protoplasm. Because the majority biological systems are colloidal in nature, studying colloidal systems will lead to a better understanding of complex biological processes such as drug delivery, protein absorption, and cell membrane interactions. More specifically, the phenomena adsorption is critical to the aforementioned processes. A simpler colloidal system which is comprised of polystyrene colloid particles, depletants, and electrolytic solution, is being studied in order to the conditions that affect adsorption.

There are three prevalent forces in this system, gravity, electrostatic, and depletion forces. These forces constitute the potential energy of the system, which can be plotted to determine the particle's probable location relative to the interface.

Colloidal systems characteristically form potential wells near the interface. The particle is likely to spend the majority of its time in this well due to the large amount of energy it requires to exit. Hence, the particle is adsorbed onto the interface. The properties of the system determine how large the well and the potential barrier required to exit the well are salt concentration, pH, and depletant concentration. By adjusting these parameters, the ease at which a particle can adsorb to the interface or diffuse in the bulk solution can be controlled. Similar to digestion, the particles in the system being studied were subjected to acidic changes in pH which lessened the impact of the attractive depletion interaction, effectively weakening the tendency of the particles to adsorb. In order to counter this, the concentration of depletants was increased. The experimental data obtained via TIRF microscopy and MATLAB image processing was then compared to current theoretical models.

Montgomery College

Evaluate CO_2 Sorption Properties of Molecular Sieves with Distinct Pore Sizes and Extra-Framework Cations
Jarod Horn

Solvent-based technologies have traditionally been employed to capture CO2 from stationary sources. Yet, such technologies require significant energy for regeneration due to the large amount of water (70% by weight) present in the solution, which is required to minimize corrosion. Solid sorbent materials are being considered as a solvent-free alternative to reduce energy regeneration requirements and CO2 capture costs. To design new sorbent materials that meet such performance goals, we must have a detailed understanding of CO2/sorbent interactions. We have evaluated the CO2 sorption properties of octahedral molecular sieves (OMS) with manganese oxide framework in which the nanopores (prior to contact with CO2) appear to be of comparable size to the kinetic diameter of CO2. Experiments were performed in a high pressure gravimetric instrument and sorption data was corrected for buoyancy. OMS materials were used as model systems with one-dimensional (1D) pore geometry, which offer guest molecules within the 1D pores or tunnels limited degrees of freedom from which CO2 sorption mechanism can be easily drawn. In the spirit of working under a materials-by-design framework, the materials were carefully selected to represent a combination of extra-framework cations that [slowly] span the chemical space offered by the periodic table and test the effect of pore geometries.

Investigating the Influence of Temperature and Acid Matrix on the Determination of Arsenic in the Arsenic Speciation Reference Standards

My Duyen Le

Arsenic (As) is a toxic element and it has been listed as a carcinogen by the FDA. Arsenic appears in the ecosystem, in water and in our foods. Because of its toxicity, it is important to develop reference materials to determine the total concentration of arsenic. Arsenic exists in both organic and inorganic form. The toxicity level is dependent on the speciation of the element. NIST is currently in the process of developing and certifying the reference materials for the organic arsenic species: monomethylarsonic acid (MMA), dimethylarsinic acid (DMA), trimethylarsine oxide (TMAO), arsenobetaine (AB), and arsenocholine (AC).

In the certification of these materials, all As species need to be converted from the respective chemical form to As (V) to prevent sensitivity differences which could be observed using the inductively coupled plasma-optical emission spectrometer (ICP-OES) or mass spectrometer (ICP-MS). This conversion process generally requires high temperatures; however, other parameters (e.g. acid selection) have been explored to potentially streamline the process. In this study, results show hydrochloric acid is successful in completely converting all As species to As (V) under optimized digestion conditions. This will lead to the certification of the five new As speciation calibration standard reference materials.

Identifying the Sources of Error in Atmospheric Transport Gases

Dennis Ngo

There are many atmospheric transport models that study and analyze the behaviors of greenhouse gases; however, most models run into the potential of producing errors and uncertainties. The uncertainties will misguide modelers from predicting the outcome of meteorological conditions and concentration of greenhouse gases in the atmosphere. The purpose of this research was to evaluate the performances of the atmospheric transport model Weather Research and Forecasting (WRF). This will provide information for modelers to improve models by properly representing the errors and uncertainties from the atmospheric transport models.

By direct comparison of simulated data against field data collected during the controlled release experiment ETEX (European Tracer Experiment), we were able to quantify the uncertainties of different WRF configurations on the simulated concentrations, temperatures, and wind fields. The evaluation of all case studies revealed that the vertical and horizontal resolution affect the results significantly. However, the selection of the Planetary Boundary Layer (PBL) parameterization had by far the most significant impact on the simulation errors since it is controlling the vertical mixing. Overall, the simulations well-captured the plume dispersion in space and in time.

Data Acquisition and Reduction Software for Multi-Detector Prompt Gamma Neutron Activation Analysis System at NCNR

Martin Shetty

Neutron activation analysis is a non-destructive method for determining the elemental constituents of a sample. The precision of such measurements can be increased by creating a multi-detector system for the capture of gamma rays. One of the main limitations on such an instrument is the rate at which data can be collected and analyzed. My contribution to the development of this instrument is the development of software for the acquisition and reduction of data in real time.

As a sample is bombarded with neutrons, it produces gamma radiation characteristic to the nuclides present. Since certain nuclides emit multiple gamma rays, we may increase the certainty of their identification by detecting coincident gamma events with multiple detectors. In a prompt gamma application, a single detector may produce up to 100 GB of data per day. It is therefore advantageous to build spectra as events are detected. It is not enough to have spectra for each channel separately, since simultaneous events from different detectors must also be classified. Therefore, a robust and customizable piece of software is required.

Germanium detectors are aimed at a sample on the NG-D neutron beam line at NCNR. Captured gamma rays result in voltage peaks proportional to the energy of each event. Four such detectors are connected to a XIA Pixie-4 device, which digitizes the signals at 100Mhz and uses an FPGA chip to analyze and record the time and energy of each event into a buffer. New software written in C++ retrieves the buffered event data from the Pixie-4, parses it and builds spectra in real time. The necessary throughput is made possible by multithreading the various tasks of this process. A buffer acquisition thread commands the Pixie-4 to initiate runs and downloads the data when the external memory fills up. The retrieved data is placed on a thread-safe FIFO queue and a new run is initiated immediately to minimize dead time. A parallel worker thread waits for new buffers to arrive, parses them and passes events into another queue. Another worker thread is tasked with binning these events to generate spectra. The software is compiled for a Linux 64-bit environment for improved performance, stability and security. Further optimizations are envisioned to decrease acquisition dead time and provide novel representations of the gathered coincidence data. The software will also be augmented with tools dedicated to coincidence analysis.

<u>Morehouse College</u>

Fun in the Sun: Characterization and Analysis of Photodegraded Polyethylene

Paul Scott, II

Studies were conducted on the photodegradation of the common thermoplastic polymer polyethylene (PE), most commonly used in packaging, containers and piping. As expected exposure to extreme temperature fluctuations as well as UV irradiation causes photodegradation over the lifespan of these products. Lab based degradation or accelerated degradation, achieved through the use of a SPHERE (Simulated Photo degradation by High Energy Radiant Exposure) based ultraviolet radiation exposure chamber, was used to simulate prolonged exposure. Additional weathering data was obtained from samples exposed outdoors in Homestead Florida. A variety of analytical and spectroscopic techniques, including Attenuated Total Reflectance Fourier Transform Infrared Spectrometry, Differential Scanning Calorimetry, and Instron testing were used to determine baselines for polyethylene and compared to samples that had undergone accelerated and natural degradation. The mechanical properties and chemical degradation of the samples were correlated with exposure time and the correlations explored. Reciprocity parameters were also extracted from the correlations.

Mount Saint Mary's University

Interactive Data Analysis of Neutron Scattering Data
Joseph Lesniewski

This project concerned the creation of a software package for the automated refinement of crystal structure data collected from thermal neutron diffraction instruments which use Bragg's law. The software created is a rebuilt and extended version of the BLAND (Bumps Library for Analysis of Neutron Diffraction) project constructed using a more stable framework. BLAND couples the BUMPS library (Bayesian Uncertainty Modeling of Parametric Systems) developed by Paul Kienzle, which provides generalized automated fitting, with the CrysFML crystallographic library developed by Juan Rodríguez-Carvajal, which provides a wide range of neutron diffraction specific calculations. The DREAM algorithm, which uses a combination of Markov Chain, Monte Carlo, Differential Evolution, and Bayesian Analysis, is used to perform the automated fitting. This algorithm allows for a thorough and automatic exploration of the parameter space and minimizes the χ^2 value for the model fit. This avoids the need to painstakingly hand fit data as well as provides a method for quickly determining whether a data set fits a model at all (by attempting to fit the model in question and watching for parameter convergence). BLAND is designed to work both for data sets for materials containing non-magnetic atoms and materials containing magnetic atoms. These two cases were tested using diffraction data from Al_2O_3 and $LuFeO_3$ respectively.

North Carolina State University

Simulation of Cosmic and Background Radiation Through Detector Shielding
Jacob Lineberry

The PROSPECT experiment is a search for a sterile neutrino, a new type of particle whose existence is suggested by recent experiments close to reactors (short baseline). These short baseline experiments show a deficit of measured particles during neutrino mixing of the three types (electron, muon, tau neutrinos), suggesting there may exist another particle capable of mixing with neutrinos. The discovery of this theoretical particle would provide a strong candidate for dark matter and possibly explain the dominance of matter over antimatter. This search requires highly precise detectors, with sufficient shielding to limit background radiation, including gamma rays, muons, and neutrons. Utilizing Monte Carlo methods, simulations modelled various detector and shielding geometries, examining particle capture and creation. This simulation data explains various background radiation sources, including particle generation resulting from buildings, structures, and the shielding itself. Utilizing this data, the shielding and location of the detector may then be optimized to limit significant background radiation, allowing for the most efficient use of detector data.

Oberlin College

Creating a Color Preference Index
Mira Fein

Light sources for general white lighting can be created using a variety of light spectra. The spectrum of the illuminant has an effect on the color appearance of objects, including food, furniture, daily objects and skin tone. Some spectra show the colors of objects better than others. This effect is called color rendering. Achieving optimal color rendering is an important goal for general lighting products. In order to achieve this goal, light sources must produce a high quality light. To measure this, there is an international standard metric called Color Rendering Index (CRI), developed some 40 years ago. This metric measures "color fidelity," a quantitative measure of the ability of a light source to reveal the colors of various objects accurately in comparison with a reference illuminant. The reference illuminant is similar to incandescent lamps or daylight. This process functions on the assumption that the reference light is of the best achievable color quality. However, in reality, other lights and color ranges are often visually preferred. As a result, the CRI score does not often reflect visual evaluations. Therefore, we need a metric that compares the test lamp to a new reference light that is based on preferences determined by human perception, rather than a reference light based on theory. The two most important factors that affect the preference of a light are color saturation (intensity of color) and color temperature (the tone of white light from warm to cool color). The new metric will address these variations by creating a more generalized metric that can be applied to the general users of lighting.

The key purpose in developing the new metric is to identify the most satisfactory lighting for human color vision. To verify this hypothesis and determine the most preferred point of color saturation, along with the associated importance of said color, we have conducted a vision experiment with human subjects. Using the NIST Spectrally Tunable Lighting Facility, we have tested a wide array of color saturations and color temperatures in a natural and familiar setting. Our preliminary analysis of experimental data supports our hypothesis that actual preferred lights have higher level of color saturation than the traditional reference light. The findings of this study can be used as a basis for the development of a new standard that enables manufacturers to produce lighting products that are based on preferences established by people, rather than theoretical color fidelity.

Otterbein University

Neutron Powder Diffraction Experiments of Nitrogen and Oxygen Adsorption in Metal-Organic Frameworks to Estimate Adsorption Selectivity for Gas Separations
Stephanie Gnewuch

Metal-organic frameworks (MOFs) are materials composed of organic linkers connecting metal atoms or clusters to form porous structures. One of the many industrial applications under investigation for these materials is gas separation. MOFs exhibiting selective gas adsorption could be used in separation processes such as the fractionation of air into N_2 and O_2 as an alternative to using energy-intensive cryogenic distillation. Recent work at NIST has studied the adsorptive properties of the MOF-74 (M_2-2,5-dioxido-1,4-benzenedicarboxylate; M = Mg, Mn, Fe, Co, Ni, Cu, Zn) series of materials using neutron powder diffraction experiments to elucidate binding sites for gas molecules. Adsorption experiments on these materials reveal that they adsorb O_2 more strongly than N_2, making these potential candidates for use in the commercial separation of air. In this study, Mg and Ni analogs of MOF-74 were synthesized and activated to expose the strong binding sites located at an open coordination site on the metal atoms in the structure. The materials were then dosed with quantitative amounts of O_2, N_2, and a 79:21 N_2/O_2 mixture analogous to the composition of air. Neutron powder diffraction data were then collected for the dosed materials. Rietveld refinement and Fourier difference methods were used to determine the location of the gas binding sites and the orientation and fractional occupancy of the molecules at those sites. The single component diffraction data reveal both molecules bind at the same site but with different orientations. The mixture data can therefore be refined with both molecules occupying this site. Refinement of the fractional occupancies of each molecule at this site can give a molecular-level picture of gas separation mechanisms and potentially afford a means of better estimating adsorption selectivity values.

Pennsylvania State University

Looking Inside the Process of Additive Manufacturing with Ultrasonics

Nathan Brockett

The Additive Manufacturing (AM) community is interested in the details of what happens during the an AM build process, but currently there are very few examples of this kind of *in-situ* process monitoring. Having this kind of capability would allow for process optimization as well as real-time process monitoring and control, leading to higher quality parts. Previous work by NIST researchers has correlated ultrasonic longitudinal wave speed changes with changes in the porosity of the build part. This project works to measure the ultrasonic longitudinal wave speed changes during the build process by means of a contact transducer embedded into the build plate. During a build, a reference part is made above the transducer to allow for better readings of the time-of-flight between echoes. Changes in the porosity of the reference part may indicate changes in the internal structure of the part and provide one way of examining the stability of the build process. This project specifically developed the implementation of the system including the collection and analysis of the waveform data to find the time-of-flight of the ultrasonic longitudinal wave. For the collection, a customized Python program connects the computer to the oscilloscope, which is connected to the transducer. For the data analysis, Coiflet wavelet de-noising along with cross correlating the signal to one of the echoes finds the time-of-flight for the ultrasonic longitudinal wave between the echoes. One problem encountered was the effects of the temperature of the build chamber on the ultrasonic couplant. Experimentation showed that the heat hardened the couplant, which degraded the ultrasonic signal, therefore a heavier viscosity couplant was used and pliable rubber feet were added to provide positive pressure behind the contact transducer. This project's success will be an early way to, in real time, monitor the build process for an AM build.

Stress Development in Flowable Dental Resins Using a Cantilever Beam-Based Device

Komal Shaikh

The goal of this study is to measure polymerization shrinkage stress, degree of conversion, and change in temperature of a dental composite that is photocured with a tooth section (comprised of dentin). The light from the curing lamp reflects off of the surface of the tooth, and this may have an effect on conversion and temperature, consequently the shrinkage stress. High levels of shrinkage stress can restrict the use of certain dental composites, so it is important to determine the stress of the composites to see if they can be used in a clinical setting. In experiments, the dental composite is a 50:50 mass ratio solution of bisphenol A diglycidyl ether methacrylate (BisGMA) and triethyleneglycol dimethacrylate (TEGDMA), with 0.2 mass percent camphorquinone (CQ) and 0.8 mass percent ethyl 4-

dimethylaminobenzoate (4E) photoinitiators and varying glass filler contents (55, 65, and 75 percent). A cantilever beam based instrument (called tensometer) was used for the stress measurement and was complemented with a near infrared (NIR) spectrometer and thermocouple for measuring the conversion and temperature during the polymerization, respectively. The composite samples were cured in three sets of interface: 1. Composite/quartz rod interface, in which the rod was not silanized (the rod is used to transmit curing light), 2. Using quartz rods that were silanized, and 3. Using quartz rods with a tooth section attached that were both silanized. Attenuated total reflectance (ATR) was also completed on the sample 72 hours after it was cured. This allows us to compare the degree of conversion on the bottom and top surfaces of the sample. This study helps us determine which filler contents are suitable in a clinical environment, and whether a composite that is cured with a tooth, as compared to without one, has an effect on stress, conversion, and temperature during the polymerization process.

Purdue University

Mechanical Properties Characterization of Uniaxially Aligned Cellulose Nano-Crystal Films Utilizing Buckling Stabilities

John Epling

Cellulose is a polysaccharide-based biopolymer that serves as the structural framework of cell walls found in plants, trees, algae, tunicates, and a select number of bacterial species. These cellulose macromolecules organize into crystals which then arrange into lamellar fibrils with an axial stiffness of up to 130 GPa. Due to their durability and exceptional mechanical properties, cellulose nano-crystals (CNC), once abstracted from the fibril network, can be isolated for use in biodegradable nano-composites, organic electronic materials, and biomaterials applications. CNC thin films have been demonstrated as effective protective coatings due to their mechanical and optical properties. The mechanical properties of CNC thin films, specifically the Young's Modulus, can be enhanced by uniaxial alignment of the CNC crystals via shear casting from CNC-water suspensions. Uniaxial alignment of CNC within these films creates anisotropic mechanical properties that are shown to peak when measured in the shearing direction. However, a measurement technique still needs to be addressed to characterize the Young's

The Young's Modulus for oriented and randomly aligned CNC thin films was characterized using the strain-induced elastic buckling instability for mechanical measurement (SIEBIMM) technique. Sufficient adhesion and sub-micrometer film thickness values were crucial for proper buckling and mechanical characterization for both oriented and randomly aligned CNC thin films. Sample preparation for SIEBIMM involved affixing a sub-micrometer CNC thin film onto a thick, elastomeric polydimethylsiloxane (PDMS) substrate via spin coating and flow coating. Several key parameters were explored to optimize adhesion and minimize film thickness including CNC concentration in distilled water, water-ethanol co-solvent mixing ratios, spin speed, drawing rate, spin coating duration, and plasma treatment time. While applying compression, white light interferometry referred to as optical prolifometry, was employed to determine the wrinkle wavelength and film thickness. The elastic modulus of PDMS (measured independently) along with the calculated wrinkle wavelength and film thickness values were used to calculate Young's Modulus of the CNC thin film at different angles with respect to the shearing direction. Finally, experimentation showed that stiffness values were greater in the sheared axial direction as opposed to the transverse direction via flow coating. Proper implementation of anisotropic CNC thin films for electronic and coating applications requires a thorough understanding of the effects of microstructure morphology and its impact on mechanical properties and device performance.

Radford University

Modeling Grain Boundaries in Thin Film Photovoltaics
Joey Ashley

Solar energy is clean, abundant, and free, making it a very popular renewable energy source. Photovoltaic solar cells are made from semiconductor materials with an internal electrostatic field. Incident photons from the sun excite electrons in the material into more energetic states, leaving behind an empty lower energy state or a "hole". Ideally, the excited electron is then extracted as electrical current. Alternatively, however, the electron can relax into the initial equilibrium state, releasing the energy as heat or by re-emitting a photon (electron-hole pair recombination). The most common material used in solar cells currently is monocrystalline silicon, a very simple material consisting of a continuous crystalline lattice with very few defects and an efficiency of 21%. Thin film polycrystalline photovoltaics such as Cadmium Telluride (CdTe) are viable alternatives due to their inexpensive fabrication processes and reasonable efficiencies (of 13%). CdTe solar cells are more complex than their monocrystalline silicon counterparts in that the effects of their polycrystalline structure on overall device performance are not as well understood. In particular, polycrystalline structures contain grain boundaries, which are extended defects that separate crystallites with different orientations. These grain boundaries, are known to facilitate recombination of electron-hole pairs resulting in a loss in conversion efficiency. However, it has been found that grain boundaries also produce a space charge region which inhibits carrier recombination by separating the electrons and holes, and experiment finds more electron-hole pairs are collected in the grain boundary than in the bulk. By performing modelling simulations on experiments which measure the fraction of electron-hole pairs that are collected as a function of where they are created, we want to deduce the electronic properties of the grain boundary in order to more fully understand their effect on device efficiency.

Reed College

Three-Dimensional Structures for the NIST Chemistry WebBook: My Journey from Molecular Optimization to Self-Optimization
Ethan Ho

The NIST Chemistry WebBook is a free online database of molecules used by researchers, engineers, and students worldwide. Currently, the WebBook contains information on over 110,000 structures, varying from chemical names to gas chromatograms. Our goal was to enhance the WebBook by optimizing 25,000 molecules and adding the optimized structures to the database. During this process, we also verified several forms of identification including International Union of Pure and Applied Chemistry (IUPAC) nomenclature, chemical formulae, and Chemical Abstract Services (CAS) numbers.

Using Gaussian09, a computer program for quantum chemistry, we calculated chemicals' optimized structures, thereby determining the atoms' 3-dimensional coordinates in each molecule. In order to compute optimized structures, we applied simple Newtonian ball-and-spring models (MMFF and MM2) and progressed to complex quantum mechanical theories (PM6 and B3LYP).

By the end of the summer, we hope to have computed comprehensive 3-dimensional data on every molecule in the WebBook. In the future, these structures can be used as bases for experimental or theoretical research. The net result is an enhanced WebBook containing more thorough, diverse, and reliable data.

Rochester Institute of Technology

DNA-Controlled Purification of Carbon Nanotubes
Carolyn Krasniak

Sorting single-wall carbon nanotubes (SWCNTs) of different chiralities from a synthetic mixture provides a foundation for many fundamental studies and technological applications of SWCNTs. Several customized short DNA sequences were identified to show recognition abilities for specific SWCNT (n,m)species. This project focused on the purification of SWCNTs by DNA-controlled partition of nanotubes in polymer aqueous two-phase (ATP) systems. DNA sequences were explored and designed by the mutation of a particular sequence which showed the enrichment of specific SWCNT (n,m) species. Newly designed sequences were utilized to disperse SWCNTs in water by sonication. The resulting DNA-SWCNT dispersions were further subjected to purification by ATP separation method in order to screen designed DNA sequences with recognition abilities for a specific (n,m)species. In this ten week period, several single-chirality nanotube species were isolated using this unique approach including the rarely seen zigzag semiconducting (11,0) species.

Rowan University

Investigating Methods for Safe Vaccine Transportation
Jesse Kosior

The Centers for Disease Control and Prevention (CDC) distributes $3.6 billion worth of vaccine to low-income and under-insured children through its Vaccines for Children (VFC) program each year. Vaccines require strict temperature control throughout storage and transport to ensure they remain effective. Improperly-stored vaccines lose potency, resulting in waste, accidental administration of ineffective vaccines, and the risk of vaccine-preventable outbreaks. VFC providers may be required to transport vaccines in a variety of circumstances, including during emergencies like power outages, to distribute vaccines between satellite offices, and to deliver vaccines to field immunization clinics. Currently, the safety and effectiveness of commonly used vaccine transport materials is not known, and there is no practical method for determining vaccine potency upon arrival. For this reason, NIST has investigated methods for safe transport and temperature monitoring of vaccines. Real–life vaccine transport scenarios were simulated in tests using different containers, cold packs, refrigerant conditioning methods, and variable ambient conditions to observe the effects on contained vaccine temperature. T-Type thermocouples were immersed in vaccines and placed throughout the transport containers to monitor temperatures throughout testing. Temperature data logging devices recommended for use inside vaccine storage refrigerators were evaluated for their ability to track vaccine temperatures during transport. The results of this study will be used to develop improved, research-based transport guidelines for VFC providers, ensuring that vaccines remain safe and effective when delivered to the children who need them.

Micro- and Meso-Porous Structure Analysis of CO_2 Capture Materials Using Gas Sorption
Charles Scott

The expectation of possible CO_2 emissions regulation in the U.S. has naturally led to an increased interest in developing cost-efficient carbon capture materials to minimize environmental carbon dioxide pollution from stationary sources. The rational design and optimization of adsorbents for this application requires knowledge of the correlation between the CO_2 capture behavior and physicochemical characteristics of these materials. In this light, characterization of the micro- and meso-porous structure of candidate adsorbent materials (e.g., surface area, pore volume, and pore size distribution) using Argon sorption measurements at LAr temperature is an essential component of a materials-by-design approach. There are a wide variety of methods for the analysis of micro- and meso-pore structures based on gas sorption data such as DFT, BJH, HK, SF, etc. (most named after the initials of those scientists who developed them). The selection of the method is typically tied to the material chemistry and pore geometry of the sample being investigated. In this work, we reviewed the various methods available and selected the most suitable method for the characterization of a selected set of porous carbons and molecular sieves.

Cold Source Engineers: Maintenance and Operation of the PeeWee Cold Source

James Torres

A Cold Source Engineer has the responsibility of operating, maintaining, and upgrading the Cold Neutron Source (CNS) on the Neutron-Beam Split Core Reactor (NBSR). For the first project, reactor engineers do not have sufficient temperature control of helium affecting the thermosiphon at the small BT-9 cold source, nicknamed "PeeWee." A cold source, such as PeeWee at the NCNR, is a moderator providing "cold," or low energy, neutrons when placed near the reactor core. Low flow of cryogenic helium causes excess heat absorption for which a solution is the installation of a bypass with a programmable cryogenic valve supplying greater helium mass flow rate.

For the second project, manual operation of vacuum lines is needed when the Programmable Logic Controller (PLC)—the I/O device operating vacuum—is off (most likely during maintenance of BT-9). The PeeWee vacuum now has manual operation and awaits the installation of a new LD_2 source. Specifically, a proposed conversion of the NBSR to Low-Enriched Uranium (LEU) fuel will cause a 10% drop in neutron flux. To offset the loss, the cold source moderator will be switched from liquid hydrogen (LH_2) to liquid deuterium (LD_2). After this conversion, the vacuum lines will serve a few purposes including prevention of heat transfer from helium to LD_2 and prevention of flammable mixture of LD_2 and air. Contamination of vacuum will prevent reactor startup for several days, and so maintaining clean vacuum lines is essential at all times

Finally, in upgrading to new software, CNS alarms needed to be updated to be more intuitive for training and operation. The solution is to set, update, and check every alarm using the RS LOGIX 5000 ladder logic software.

Saint John's University

Comparing Different Approaches for Measuring Environmental Performance in the Manufacturing Industry

Andrew Bujarski

To improve industrial processes to become more sustainable, several approaches can be applied to identify and quantify the effects of the interactions between industry and the environment. The primary method for measuring the potential environmental impact of products is life cycle assessment (LCA). Traditional process based LCA measures a products environmental impact from "cradle-to- grave" covering the whole life span of a product from raw material acquisition to disposal. LCA can also be manipulated and altered into several variants and still achieve the overall purpose of identifying environmental performance. Economic input- output life cycle assessment (EIO-LCA) is one such variant where transactions between industries are converted using environmentally extended tables, in this case tables developed by NIST partners, into potential environmental impacts. Another variant of LCA worth analyzing is an ecological life cycle assessment (ECO-LCA) and the ECO-LCA model used in this project was developed by the Center for Resilience at Ohio State University. Unlike EIO-LCA where industry to industry interactions are measured, ECO- LCA catalogs industry's consumption of natural capital or goods and services derived from the environment. While LCA is the primary means to identify the environmental performance of an industry, it is not the only method. Measuring efficiency at different levels or stages of production is a different approach entirely that evaluates the utilization of resources and energy which could result in more informed decision making leading to an overall lower impact on the environment. This project analyzes, from cradle-to-gate, the manufacturing industries, as defined by North American Industry Classification System, at the three digit summary level and the six digit detailed level with a specific focus on the high technology manufacturing industries using the previously mentioned approaches. Analysis of the manufacturing industries will allow us to compare the impact different industries have on the environment based on a wide variety of criteria; at the same time comparing the approaches themselves as they evaluate the manufacturing industry.

Saint Mary's College of Maryland

Laser Interferometry for Radiation Dosimetry

Laura Andre

Current primary standards for quantifying the absorbed dose induced by radiation (energy deposited per unit mass) use thermistor probes to measure sub-milliKelvin changes in temperature in a sample. In medical physics, the irradiated material is usually water (considered tissue-equivalent for medical dosimetry), thus the probes themselves introduce perturbations and thermal gradients whose effects on measurements must be quantified and removed. Such effects, moreover, would make thermistor probes entirely inadequate for measuring dose distributions within water. The capability to image radiation dose fields within matter would be of immense benefit in industrial and medical applications, thus we are pursuing an alternative temperature probe that would use laser interferometry to reconstruct thermal distributions in tissue-equivalent materials. For the proposed system to be useful for medical dosimetry, it must be capable of measuring very small changes in the interference pattern, corresponding to minute changes in refractive index caused by sub-milliKelvin changes in temperature. Accordingly, we have attempted to use a cyclic interferometer to mitigate effects due to vibrational disturbances that are commonly observed with the classical Michelson interferometer. This allows for a more stable, sensitive setup that analytical estimates suggest would permit detection of temperature changes on the order of microKelvin, thus making it suitable for characterizing dose profiles of therapy-level ionizing radiation beams. The system is undergoing tests with glass and polymethylmethacrylate (PMMA) subjected to infrared heating, and plans are in place to test the system in a clinical radiation beam here at NIST.

Saint Olaf College

The Comet Assay: Methods for Quantitative Image Analysis and Reproducibility

Signe Braafladt

The Comet Assay, or Single Cell Gel Electrophoresis, is a sensitive and efficient technique for analyzing and quantifying, in single cells, DNA damage in the form of single and double strand breaks. DNA instability, from strand breaks, is associated with cancer and other health risks. The Comet Assay's increased use in a wide variety of applications emphasizes the importance of establishing standard assay protocols and understanding inherent sources of error and measurement variability. These sources of variability include the biovariability of the particular cells undergoing analysis, the assay protocol used to process the cells, the microscope system used to image the cells and the software used in the computerized analysis of these images. To determine the effect of these sources of variability on the measured percentage of damaged DNA (% DNA in tail), fixed preparations of mammalian cells with chemically and electrochemically induced DNA damage were analyzed for the effect of varying the microscope (Automated Olympus BH-2) and camera (Photometrics CoolSNAP HQ2) settings as well as image analysis parameters using Image J (NIH) and CometScore Pro (TriTek) software. Manual image analysis revealed large measurement variations due to microscope focus, camera exposure time and the software image intensity threshold. Automated image analysis revealed less variability, but within narrower limits of focus and exposure settings. The variations observed using both of these methods were highly dependent on the extent of DNA damage. Accounting for these sources of variability with determined optimal instrument settings allowed an accurate evaluation of the biological variability of the cells. The automated microscopy system is currently being used to determine reproducibility of the comet assay protocol used to process the cells. This will also be critical in obtaining the required statistical evaluation of various cell treatments, including the effects of cell treatment at fixed oxidative potential in the electrochemical environment.

Stem Cell Enumeration: Using Simulations to Inform Experimental Design

Mara Stutzman

Stem cells are used in basic scientific research, regenerating human or animal tissues, and cell therapy, where the cells are injected into a patient's body to facilitate recovery from disease or injury. Using the appropriate number of cells is crucial in both the development and application of new treatments. The current cell enumeration industry standard is the Hemocytometer, a manual counting method which has been used for over 100 years; this technique is time and labor intensive, and prone to human error and bias. Typically, new cell counting methods are tested for accuracy by comparing their results to those of the Hemocytometer. In this study, precision and relative accuracy of both the Hemocytometer and a new automated method, the NucleoCounter 200, were estimated in the absence of a reference measurement or ground truth cell count. For each method, stem cell concentrations were estimated using a series of known dilutions originating from a stock stem cell solution. The relative accuracy of each method was evaluated by examining the proportionality of the resulting cell concentrations to the known dilution fractions. Initial experimental data showed the NucleoCounter to be far more precise and no less relatively accurate than the Hemocytometer; however, these conclusions were weakened by the large uncertainties associated with the Hemocytometer results. A simulation study was conducted to illustrate the effect of alternative experimental designs, including measuring cell concentrations at additional dilution fractions or additional replicates at each dilution fraction. Based on these simulations, the cell enumeration experts will conduct a redesigned experiment while observing fiscal and time restraints.

Santa Clara University

AFM Applications of Optomechanical Transduction by a Microdisk Resonator

Maximiliano Silva-Feaver

A standard Atomic Force Microscope (AFM) uses a microscale cantilever with a nanoscale tip to scan a sample's surface. A laser is focused on the end of the cantilever and the reflected beam is captured in a quad detector used to detect beam deflection. To produce an image the tip is brought into contact with the surface and held at some set deflection as x and y stages move to scan an area of the sample. As the tip encounters surface topography or other forces induced by the tip-sample interaction the beam is deflected more or less than the setpoint. In response, a feedback loop moves a z stage up or down in response to the topography to create an image of surface topography or other detectable tip-sample forces.

Our group has designed an alternative way to sense cantilever deflection using near field optics instead of the traditional far field beam bouncing technique. Our design integrates a microdisk cavity resonator close to a nanoscale cantilever beam. As the beam is deflected it shifts the resonance of the cavity and by tracking the resonance shift we can detect tip motion. This configuration allows us to have nano-scale instead of micro-scale beams which increases the Q factor by greatly decreasing air damping. The decreased mass allows us to have very high resonant frequencies with much lower spring constants (k) than traditional micro-scale levers. These differences will allow us to scan faster, produce higher resolution images, and resolve softer samples better than a traditional AFM cantilever.

To demonstrate our transducer's increased performance in these areas we set up tests to compare our systems performance to commercially available tips. Tests include fast force curves, fast and high pixel count images, as well as Photothermal Induced Resonance (PTIR or AFM-IR) AFM. In addition we imaged samples with very small, atomic scale, features (Graphite) as well as very soft samples (teflon tape & DNA). Our results show that we are able to scan as fast as or faster than the fastest tips on the market and only seem to be limited by the hardware of commercial AFMs. In addition, we are able to achieve these fast scan rates with much less sample damage than commercially available tips scanning at the same rate.

Smith College

Measuring Sustainability in Commercial Buildings

Yadira Flores

What is the additional cost of constructing a building in a more energy efficient manner? How can changing the amount of insulation in the wall of a building impact the total annual energy cost? Will the energy cost savings pay for the additional construction costs over a course of twenty years? How does improving the energy efficiency of a building impact its environmental footprint? These are the type of questions that this project tries to answer.

This project aimed to create an extensive new commercial building sustainability database to support the BIRDS -Building Industry Reporting and Design for Sustainability- online interface. This database is comprised of 16 commercial building types, four building energy standard editions, 40 different investment time horizons, and 228 cities (about 14,592 unique cases). After running whole building energy simulations for each unique case, we calculated the initial building construction costs, annual operating energy costs, and future maintenance, repair, and replacement costs using the programming language Python. The environmental impacts associated with the construction and operation of each building is estimated using life-cycle assessment data. Indeed the economic and environmental impacts for each unique case differs as the building type, standard edition, investment time horizon and climate are varied.

In the end, this database can be used to the compare different types of building designs and how that would impact the cost and energy efficiency of new commercial buildings. Thus, making these life cycle cost analyses readily available and comparable could be invaluable to policymakers that set the state building requirements, building engineers, architects, and designers, and the general public.

Seasonal and Spatial Patterns in the Atmospheric Concentration of Greenhouse Gases

Maja Milosavljevic

Discrete measurements of the abundances of greenhouse gas made at various observatories worldwide serve to characterize the state of the atmosphere and help track changes over time that may be related to climate change. Time series of measurements of the atmospheric concentration of greenhouse gases provided by the National Oceanic and Atmospheric Administration (NOAA) at six observatories provide the raw materials to characterize the spatial and temporal aspects of the those patterns of variability. A key technical tool that I have employed for this purpose produces a decomposition of a time series into seasonal, trend, and remainder components. Then, comparisons between observatories and different gaseous species (carbon dioxide, carbon monoxide, methane, etc.) can be made for both the seasonal and trend components. In this presentation I will describe how these comparisons were done, and the corresponding results. The trend components show decreasing levels of carbon monoxide and methane gas as latitude decreases. Additionally, there are distinct seasonality patterns for all observed gases, and the concentrations in the northern and southern hemispheres are out of phase. In both hemispheres, greenhouse gas emissions are highest in the winter and lowest in the summer. Some of the observed patterns discussed in this presentation are supported by published literature, but others leave open questions of potential interest to atmospheric scientists and worthy of further study.

Correcting Temperature Records for Biases Unrelated to the Climate

Sara Stoudt

The series of daily surface temperature measurements recorded at a meteorological observing station may be affected by factors that are unrelated to climate: for example, changes in the physical location of the station, growth of nearby vegetation, or changes in land use in its surroundings, including urbanization and road construction. These factors bias the temperature record, and may mask any trend in temperature that may be an expression of climate change. Since these factors and the spurious effects they induce often are undocumented, there is a need for data analytic procedures to correct the temperature records, which is generally referred to as *homogenization*.

Several existing approaches to homogenization involve preliminary detection of change-points, which are the epochs at which spurious effects kick in. NIST statisticians have developed an algorithm that homogenizes surface temperature records without explicitly finding change-points first. This algorithm estimates the correction directly and also characterizes the uncertainty surrounding the homogenization using the statistical bootstrap.

During the recent SAMSI Workshop on the International Surface Temperature Initiative, which took place at the National Center for Atmospheric Research (Boulder, Colorado), a working group was organized to extend the range of applicability and improve this algorithm. An additional goal was to create an R package with the final product. I was a member of this group and my main contribution was to determine the form of bootstrapping that is more appropriate for the uncertainty quantification: parametric or non-parametric.

In my talk I will discuss the climate science motivation for this work, which falls under the scope of the NIST Program on Greenhouse Gases and Climate Science Measurements. I will also describe an example of the performance of the homogenization algorithm on a real-world surface temperature data set, with recorded change-points so that we can easily assess its accuracy, and compare the two alternative bootstrapping methods.

Stanford University

Smart and Synchronized! : Modeling the Effect of Time Offset in Power Flows Across the Smart Grid
Joseph Wu

The development of Smart Grid technology has provided several methods to enhance the conventional electric grid. One key improvement that is fundamental to the Smart Grid approach is the ability to gather and monitor information from the electric grid at unprecedented scale and granularity. In order to accurately measure and process the large volume of data from the grid, time measurements need to be synchronized across all sensors and actuators. In this project, a MATLAB dashboard will be developed to visualize real-time voltage and time data streamed directly from the NIST Smart Grid test bed. As each substation on the grid feeds live data to the dashboard, its voltage, time stamp, as well as time offset from a reference clock will be recorded and graphed.
The dashboard also allows the user to evaluate the impact of drift and variation of time keeping clocks on the fidelity of measurements. In order to present the impact of clock offset and jitter on measurements, a phasor representation of the sampled voltage measurement is displayed and continually updated on the GUI. Users can adjust parameters such as the sampling rate, reporting rate, preferred reference clock, etc. The completed GUI will be added to the NIST Smart Grid test bed to help process and present live data during experiments and demonstrations.

State University of New York Albany

Probe-Assisted Deterministic Doping
Chase Brisbois

Deterministic doping techniques use low through-put and expensive equipment to deliver a precise number of dopants to nanoscale regions on a semiconductor. We seek to introduce a cluster of dopant atoms into the surface of a silicon substrate by subjecting a dopant-containing thin film to various stimuli using an ordinary atomic force microscope (AFM) mounted with a diamond-coated tip. By using nanoindentation software along with a DC (direct current) pulse, we can apply large amounts of pressure and heat to nanoscale regions at the dopant-silicon interface. The DC pulse is triggered when the probe reaches maximum penetration depth. Currently, three "p-type," dopant-containing thin films are being investigated on lightly doped, n-type silicon: aluminum, polymer of 4-vinylphenylboronic acid and a self-assembled monolayer of allylboronic acid pinacol ester. These layers are characterized with AFM, FTIR or XPS and used in a probe-assisted doping process to introduce the dopants. The dopant film is then stripped off and the samples are probed for counter-doped regions by mapping surface potential and conductivity using KFM and TUNA.

Design and Characterization of Phase Shifting Photomasks for I-Line Projection Lithography

Benjamin Grisafe

Photolithography as a method for nanofabrication has limitations. Forming patterns smaller than the wavelength of light being used requires expensive immersion technology, superior lensing or specially fabricated photomasks capable of intensifying certain regions in the pattern. This type of mask, called a Phase Shifting Mask (PSM), has the ability to shift the phase of an incoming electromagnetic wave by 180° leading to beneficial destructive interference that ultimately enhances the intensity of exposed wafer regions. Increases in contrast and the captured 1st order enhance both the resolution of the features able to be patterned as well as the process latitude. This physical phenomenon allows for the patterning of features smaller than the wavelength of light being used.

This study presents methods for the design and fabrication of two types of PSMs on quartz to be used in an ASML I-line stepper: a Diffractive PSM and an Attenuating PSM. Design of an attenuating PSM requires a film capable of 5-15% transmission at this wavelength of light to achieve phase shifting. Chromium oxide (Cr_2O_3) exhibits this characteristic based upon the conditions of deposition and films were sputtered and characterized using ellipsometry. Diffractive PSMs, however, do not have a thin film causing phase shifts, but thickness differences in their place. A dry etch process was developed to isotropically etch quartz to desired depths. The process conditions of Heidelberg DWL 2000 laser writer was optimized to obtain precise control on the mask pattern dimensions. Finally, PSMs are used in the ASML I-line stepper and the critical dimension of the features patterned analyzed for proof of concept.

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

Non-Destructive Analysis of Thermal Stress in Copper Through-Silicon Via Using time Domain Reflectometry

Anil Adhikari

Electronics devices undergo continuous temperature fluctuation when in use. This continuous thermal cycling generates thermal stresses due to the different coefficient of thermal expansion (CTE) of materials of construction. These thermal stresses are known to be one of the major causes of failure in electronic devices, as they result in the formation of defects such as cracks, voids and delaminations, leading to shorts/opens in the integrated circuits. With the emergence of three-dimensional stacked integrated circuits (3D-SIC), as the microchip of the future, the concern for stress-related failures has increased. This is because the vertical electrical connections through the stacked chips are achieved with copper interconnects, called Through-Silicon Via (TSV), which are fabricated through the active silicon.

Unfortunately, the large mismatch in the CTE of Copper (17 X 10-6/ºC) and Silicon (2.3 X 10-6/ºC) leads to the generation of significant stresses.

In this work, radio-frequency (RF) based technique was used as a non-destructive fault-detection technique to analyze the impact of thermal cycling on the signal integrity of Cu TSVs. RF broadband (0-40 GHz) were passed through a test under device (DUT) comprised of a daisy chain containing 60 Cu TSVs. Using the vector network analyzer, the frequency and time domain characteristics of the DUT were determined as a function of the number of thermal cycles. From the frequency domain analysis, the reflection coefficient and the transmission coefficient were obtained. While in the time domain analysis, Time Domain Reflectrometry (TDR) was used to determine the defect location in the DUT non-destructively. If structure of the DUT is changed due to thermal stress, it results in the change in the TDR waveform. To locate the defect in daisy chain, the change in the waveform was monitored and the time taken by the wave to travel from one end of the DUT to the defect in the structure was calculated. The discontinuity of the waveform is marked by the formation of dip in the waveform due to increase in the impedance of the particular cross section of the DUT. As the thermal cycle increases, the change in the structure in DUT is more distinct and the impedance mismatched is prominent. In case of frequency domain analysis, scattering parameters were observed and compared at different thermo cycle. As the thermal cycles increased the loss in the magnitude of scattering parameters were distinct.

Micro-Viscometry of Reference mAB Protein Solution
Scott Anderson

Antibody therapy is already a sizeable medical field and is growing rapidly, including six of the top-ten-selling biologic drugs of 2012[1]. Many antibodies are currently under development, promising possible treatments for Alzheimer's disease, multiple sclerosis, and different types of cancers. Due to limits concerning the volume of fluid which can be injected intramuscularly, high protein concentrations may be necessary for some drug products. The need for these high-concentration solutions makes the viscosity of these solutions an important parameter, having an impact on the purification, fill/finish, and syringeability of the protein solutions.

A microliter capillary viscometer, developed at NIST, has the ability to measure the viscosity of very small samples of fluid (less than 10 µL). This particular study uses this viscometer to determine how the intrinsic viscosity and jamming concentration of protein solutions change when the sample is heat treated to induce aggregation. The NIST protein antibody, under development to be a reference material, is the primary protein solution considered in this study. These results will be used to test theoretical models of solution mixtures. Other protein solutions, such as α-chymotrypsinogen, are also tested.

Parallel Programming to Quickly Generate Libraries of Images for 3D SEM-Based Dimensional Measurements
Casey Levine

Integrated circuit (IC) manufacturers, such as Intel, IBM and AMD strive to create smaller and smaller transistors in an attempt to increase the capabilities of their ICs. Currently, transistors can be constructed effectively on the nanometer scale. To verify the quality of these incredibly small circuits, researchers are using scanning electron microscopy (SEM) and Monte Carlo simulations to generate

[1] Huggett, B. Public Biotech 2012 — the Numbers. *Nature Biotechnology*, 697-703. Retrieved July 14, 2014

realistic set or libraries of 3D images of these circuits on the nanometer scale. These simulations –using the CPU (central processing unit) and the current software implementation– could take up to several months to compute. In an attempt to speed up the simulation, parallel programing on a commercial graphics processing unit (GPU) using CUDA is being explored. In other types of Monte Carlo simulation implementations, GPUs have demonstrated up to a thousand times speed improvement over non-parallel implementations. A basic code to calculate electron trajectories in the simulation has been developed to evaluate the potential value of CUDA in the more sophisticated, complex simulation. The code has demonstrated noticeable speed improvements with little optimization, and should ultimately be capable of achieving a significant speed up compared to a non-parallel implementation.

Scanning Microwave Microscopy: A Promising Technique for 3D-IC Subsurface Metrology
Jonathan Michelson

Integrated circuit developers, in search of ever improving chip efficiencies, have shifted attention away from the standard, two-dimensional, planar designs towards a more promising build: the three-dimensional stacked integrated circuit (3D-IC, or 3D-SIC). Attracting tremendous research interest, these 3D-IC architectures indicate novel performance advancements – an enticing bit for the semiconductor and electronics industries. However, what would be beneficial in further developing this exciting technology's potential are robust techniques for the characterization & metrology of the subsurface "metallic forests" of electrical connections and devices buried in these multilayer 3D-ICs. The procedure of scanning microwave microscopy (SMM), with its non-invasive, high-resolution, subsurface imaging capabilities, appears to be a strong candidate for this task. SMM operates by sending microwave-frequency (1-20GHz) signals through a nanometer-scale conductive tip as it scans across a sample of interest, consequently detecting the changes in amplitude and phase of the reflected microwave signals (called S11-parameters) that are due to minute variation in tip-sample impedance. In other words, the SMM procedure can "map" S11-amplitude and -phase versus tip position, obtaining useful information about the amplitude-altering subsurface geometry. In this SURF project, the finite-element-analysis software COMSOL Multiphysics was employed to model a simplified SMM setup with various specific subsurface test structures. The S11 response for the simulations was obtained and compared with experimental S11 data. A good agreement between the COMSOL model data and experimental data was achieved, illustrating the effectiveness of the simulation approach as an investigative and predictive tool. This work helps interpret SMM subsurface results, and provides a functional platform for future subsurface imaging simulations of other test structures of interest. Continued refinement of these, and creation of other, software simulations for future SMM-metrology investigation is justified and encouraged by the results presented in this work.

High Resistance Characterization to 100 TΩ
Edward O'Brien

The primary goal of this research is to expand upon high resistance measurement techniques and standards. A 100 TΩ guarded Hamon transfer standard was designed which can be used to measure and calibrate other standard resistors and build-up to 100 TΩ from 1TΩ and 10 TΩ. This device was tested and characterized, its stability was determined based on its temperature coefficient, voltage coefficient, change in correction over time, RC time constant, and repeated transfers from parallel to series-parallel and series configurations. High resistance elements for new guarded Hamon transfer standards were also measured and characterized. A group of fifty 1 TΩ resistor elements were measured using a modified Wheatstone bridge. The elements, ranging between -20,000 μΩ/Ω and -40,000 μΩ/Ω, were then tested for voltage and temperature dependence. The elements with the smallest coefficients will be used to make multiple new Hamons which will have a build-up to 10 TΩ from 100 GΩ and 1 TΩ.

Software Defined Radio Development for Spectrum Monitoring
Paul Watrobski

Development of spectrum sensors is essential to monitoring the radio frequency spectrum. There are several reasons for spectrum monitoring: to inform policy makers, enable policy enforcement, and coordinate spectrum usage. The current spectrum sensor prototype developed at NIST requires both a software-defined radio (SDR) and host computer with a general purpose Central Processing Unit (CPU) to perform the digital signal processing (DSP), a majority of which is done on the CPU. There are several benefits to entirely offloading the DSP to the SDR. Portability is substantially improved with a single unit performing the DSP. In addition the monitoring bandwidth, previously limited by the CPU, can be increased.

The SDR used in this research contains a field programmable gate array (FPGA). The key benefit to using an FPGA is that it allows for inexpensive on-the-fly hardware development, allowing for dedicated DSP hardware to be created. Previous development for a related project used a fast Fourier transform to convert the signal to the frequency domain. This and several other DSP components from the related project are adapted to the current project. Additional processing, including time averaging and conversion to a logarithmic scale, is offloaded from the host to the FPGA. This new system is evaluated in comparison to the existing prototype in terms of accuracy, monitoring bandwidth, and CPU utilization. Because this system would be implemented on an embedded system containing a low-end processor there should be very little processing done on the CPU. Several of these embedded system spectrum sensors will be deployed and used to return spectrum occupancy data to a central database for storage and further analysis.

State University of New York Geneseo

Calibration of ^{22}Na Using the Sum-Peak Counting Method
Mollie Bienstock

A calibrated positron emitter, ^{22}Na, is needed for nuclear cross section measurements. The calibration of this source was performed using a self-calibrating sum-peak counting method which has the potential to replace calibrated sources for various other applications. The sum-peak method was used with three different detector setups: a single high purity germanium detector, a 4”x5” NaI well detector and the same NaI well detector paired with a 3”x3” NaI detector, obtaining a 4π-counting geometry. The ^{22}Na decays via positron emission mostly to an excited state of ^{22}Ne which promptly de-excites and emits a 1275 keV gamma ray. The 511 keV gamma ray produced from the positron annihilation sums with the 1275 keV gamma generating a 1786 keV peak in the observed spectra. The total counts in the three peaks as well as the total counts observed in the spectrum are used to calculate a value for the activity of the source. To get a better understanding of the source and the detector geometries, a simulation of the setups was generated using EGSnrc: software that uses Monte Carlo simulations to model radiation transport. Using this program, and subsequent Monte Carlo calculations, a model of the spectra produced from each setup was created and used to fit theory to data and get a more accurate number for the activity of the source. The results obtained from this experiment are being compared to independent measurements from HPGe gamma ray spectrometry and 4π NaI integral counting using calibrated detectors.

Swarthmore College

Automatic Ontologies: Standardized Terminology Generation for Document Comparison and Search

Jacob Collard

The generation of domain ontologies has seen increasing interest in information sciences for applications such as analysis of knowledge and standardization of terminology. We have developed a tool for the automatic generation of ontologies from text. With this tool, terminology can be extracted from natural language documents. The tool then standardizes the terminology, taking into account linguistic structure and creating a hierarchical set of classes.

Because ontology generation is automatic and unsupervised, this tool can be applied to any scientific field. The hierarchical structure allows for diverse search applications such as recommendations based on subclasses or superclasses.

The ontology can also be applied to document comparison. By comparing standardized terms instead of ambiguous natural language, the tool allows for semantic instead of purely lexical comparisons. Through document comparison, this tool can also generate conceptual as well as hierarchical links, which can be applied to more advanced searches and analyses.

Syracuse University

Improving Situational Awareness in Incident Responders Using Unmanned Aerial Systems

Stephen Cauffman

Incident response in the United States is largely governed by the National Incident Management System (NIMS), which is general framework developed by FEMA to standardize the approach to incident response. The framework calls for the selection of an Incident Commander (IC) who manages the various units involved and works to relay information between them. ICs must be aware of a large number of factors such as ground unit position, location of casualties, location of incoming resources, etc. The issue is that this information is normally relayed via radio communication, which can delay decision making. We focused on IC decision-making specifically and to understand this process we developed functional models of decision-making using a modeling language known as the Functional Resonance Analysis Method (FRAM). FRAM allowed us to view the process in a way that considers the system in terms of the various functions involved (not the components) and the normal variance in performance of these functions (functional resonance). It was determined that in order to effectively make decisions, it was important to have a sense of situational awareness, which is defined by Dr. Mica Endsley as the ability to take sensory information about a scenario and process it in order to develop predictions about how the scenario might evolve . To improve IC situational awareness, we propose a system using an unmanned aerial system (UAS) to gather information on a scenario involving a multi-car accident using video and radio sensors that can rapidly gather necessary information for the IC and present it in a way that can be processed easily and optimize decision making in incident response.

Tulane University

Residual Gas Effect on aCORN
William Byron

The degree of angular correlation between the beta electron and electron-antineutrino in neutron decay is denoted by the dimensionless parameter “a”. This value, in combination with other neutron decay parameters can be used to test the self-consistency of the Electroweak Standard Model. Previous experiments that measured “a” had systematic uncertainties on the order of 5%. The aCORN (a CORrelation in Neutron decay) experiment, which is designed to obtain a systematic uncertainty of less than 1%, is being carried out at the NIST Center for Neutron Research. The measured energy of the beta electron and time-of-flight between the beta and proton are used to determine the angular correlation between the electron and electron-antineutrino. In the experiment the proton travels several meters through a $1.33*10^{-5}$ Pa (10^{-7} Torr) vacuum before being detected. This work addresses a potentially important systematic uncertainty associated with the velocity dependent removal of protons by the residual gas. Initially it is assumed that the residual gas consists of pure molecular hydrogen. The effect is assessed with a Monte Carlo treatment that follows individual protons as they travel through the residual gas and weights them by their probability of interaction.

Adjustments and Additions to the OOF Software
Lucianna Kiffer

A time consuming process for many software developers is the maintenance of user error reports which generally come in the form of emails from users. These often lack necessary information and involve a lot of back and forth between the user and the developer. Part of my project involved creating an error reporting user interface that compiles all the information necessary for the developer to understand where the error is coming from, while also giving the user the opportunity to omit proprietary information or files. This error reporting code will be used in NIST's Finite Element Analysis of Microstructures software, Object Oriented Finite Elements (OOF). OOF is written in the languages Python and C++ and a second part of my project involved altering another software package called Simplified Wrapper and Interface Generator (SWIG) that OOF uses to generate wrapper code to translate between OOF's Python and C++ code. The version of SWIG used in OOF is an older stable version that was producing code that was being deprecated in modern compilers. These deprecations were producing warnings that could become problematic in newer compilers. For part of my project I cleaned up this version of SWIG to be distributed with OOF.

University of Alabama Tuscaloosa

Modeling Laser Pulsed Heat Conduction in Solids for All-Optical Ferromagnetic Resonance Spectroscopy
Sergei Wallace

The goal of this project is to develop an all-optical ferromagnetic resonance (FMR) spectrometer that enables: (1) higher frequency measurements (50 GHz to THz) on high-anisotropy materials (2) dynamic measurements of nm-thickness magnetic films through use of the magneto-optical Kerr effect (MOKE) (3) wafer-level, in-situ measurements during film growth due to non-contact instrumentation. Current FMR methods include time-resolved magneto-optic Kerr effect (TRMOKE) where strong “pump” laser pulses drive a material’s magnetization to procession while weaker, delayed “probe” pulses measure the magnetization through changes in polarization and intensity of the reflected light i.e. Kerr effect. Using a pulsed fiber microwave laser setup, our FMR technique will instead use multiple, rapid pulses from a single source to simultaneously pump and probe the magnetization up to once per magnetization precession period, approximately 10^2 to 10^4 times more often than the typical 80 MHz laser pulse repetition rate used for existing TRMOKE techniques. The material's oscillating temperature from the microwave pulses induces precession, so the benefits of this increased measurement rate may be limited if the temperature variations becomes too small to drive the magnetization. Therefore, it is necessary to model the material's temperature response to a range of laser pulse frequencies in order to know the pulse rate limits of our TRMOKE experiments. In this talk, I will present a model based on Fourier's classical heat conduction law for a semi-infinite solid with no convection and a sinusoidal pulsed, 2-dimensional (surface) Gaussian heat source. Results of the model for various magnetic systems of interest will be discussed.

University of California Berkeley

Super Sheet Metal Stressing: The Stimulating Design Process of Two Straining Devices

Scott Hallock

Automotive metal forming is somewhat of a trial-and-error process, as stamped sheet metals often spring back towards their original position and no longer fit within tolerances. American car companies lose up to $100 million a year on stamps/molds that create flawed parts. For this reason, data on mechanical properties of sheet metals is of particular interest to the automotive industry, where potentially large reductions in costs are expected from improvements in the predictability of forming outcomes. The basis of this project was the design of two novel devices that, when used with the NIST Center for Neutron Research's BT-8 Residual Stress Diffractometer, will provide new data on yield stresses as sheet metal samples are loaded *in situ*. The first device, named *Octo-strain*, is an eight-arm loading frame capable of generating any type of in-plane tensile loading, generating significant levels of bi-axial plastic strain, and the ability to define different strain paths. We expect that *Octo-strain* will significantly increase achievable strain levels when compared with typical cruciform straining devices. The second device is an *in-plane shear device* capable of generating both a significant shear force and a tensile force in the transverse direction. This device will enable measurements of the grain orientation-stress response which are of great value for crystal plasticity modeling, as well as the independent measurement of the principal stresses in shear deformation. Challenges in designing both devices come from the need to keep the design relatively modular, fit within certain size/weight boundaries, and create an entry/exit path for the neutron beam.

University of the District of Columbia

Advanced Plasma Etching for High-Aspect Ratio Nanometer Silicon (Si) Trenches

Collin Baker

Deep Si etching (DSE) is a critical process step in nano-fabrication. Alternating silicon (Si) surface coating and etching (Bosch) process has been developed to make high-aspect-ratio Si trenches. However, the sidewall of a fabricated trench using the Bosch process has scalloping roughness in the range of hundred nanometers which blocks its application in making nanometer scale Si trenches.

To reduce trench size and extend aspect-ratios is a challenge to the Bosch process because it requires the parameters to be optimized in opposite directions. In this study, new fast gas switch and pulsed plasma power supply will be used to improve the overall Bosch etching performance in making small, but high-aspect-ratio Si structures.

Based on our previous sidewall smoothness control study, Argon (Ar) gas will be introduced in this study to improve Si etching aspect ratio. Two approaches for adding Ar will be compared. One is to add Ar gas into the etching gases directly and another one is to add Ar gas as a separate etching step. Three major parameters will be optimized according to a Design of Experiment setup using the program Minitab. Analysis of the results will be performed by scanning electron microscopy and will focus on the Si aspect ratio, the etching rate, and the selectivity (etch rate of photoresist versus the etch rate of Si).

Test and Measurement of Emerging Border Gateway Protocol Security Mechanism

Kamala Mayo

The Border Gateway Protocol (BGP) is the glue that holds the Internet together. BGP routes data between the Internet's main components, Autonomous Systems (AS's), which are administrative domains that maintain their own local routing policies. BGP routes information among AS's and uses this information along with local routing policies to select the best route to a destination. BGP was originally conceived with no security. It is now vulnerable to malicious attacks and accidental misconfigurations, both of which can cause Internet outages that disrupt traffic flows. BGP vulnerabilities have been responsible for major security incidents such as Pakistan Telecom's attempt to censor YouTube in 2008, which knocked the site offline, and the China Telecom BGP hijack of 15 % of the entire Internet in 2010.

NIST has been working with the Internet industry and the Internet Engineering Task Force (IETF) to design and standardize new techniques to prevent BGP hijacks. One component of these techniques is a global Resource Public Key Infrastructure (RPKI) that provides cryptographically verifiable attestations about the ownership and use of Internet resources (e.g., IP Addresses and Autonomous System Numbers). In the early stages of deployment, there is industry concern about the robustness and interoperability of RPKI information. In this talk I will present information on NIST development test and measurement techniques designed characterize the completeness and correctness of the emerging global RPKI. In particular, I will focus on extensions I developed to the NIST measurement tools to enable continuous interoperability testing among two leading open source RPKI validation platforms, being developed by researchers in the U.S. and Europe.

<u>University of Florida</u>

Synthesis, Crystal Structures, and Phase Transitions in (Na,Li) (Nb,Ta)O_3 Ceramics

Jared Carter

Multilayer ceramic capacitors (MLCC) enable many electronic devices. MLCC commonly employ BaTiO3-based materials as dielectrics. The maximum operating temperature of these capacitors is limited to about 130°C, which corresponds to the temperature of paraelectric-to-ferroelectric phase transition in BaTiO3. However, many emerging applications, such as engine control units for automobile fuel efficiency and power inverters for operating motors on subway cars require capacitors to operate at higher temperatures. Thus, a search is under way for suitable dielectric materials.

(Na,Li)(Nb,Ta)O3 ceramics are among the candidates for high-temperature MLCC; yet, the crystal structures of these materials still remain uncertain. We used variable-temperature X-ray powder diffraction combined with transmission electron microscopy to evaluate crystal structures and phase transitions in the perovskite phase field of the NaNbO3-NaTaO3-LiNbO3-LiTaO3 quaternary system. The samples were prepared using solid-state synthesis both in air and reducing atmospheres. Our results revealed a complex interplay between ordering of polar cation displacements and octahedral rotations, which gives rise to a variety of perovskite-like superstructures.

University of Illinois Urbana-Champaign

Impact of Different Hose Stream Applications During Fire Suppression

Joseph Willi

A variety of hose streams and application techniques are used by firefighters to extinguish fires. The type of hose stream and the way it is applied during fire suppression has a significant impact on the cooling and movement of hot gases inside a structure. Thus, it is imperative for firefighters to have extensive knowledge of the effectiveness of different hose stream applications so the correct technique can be executed on the fireground.

This summer, researchers from the NIST Fire Fighting Technology Group conducted a variety of live-fire experiments at the Delaware County Emergency Services Training Center near Philadelphia, Pennsylvania. The main purpose of these experiments was to quantify the impact of different hose stream applications on the movement and cooling of gases in various fire scenarios. One set of the experiments specifically measured how different hose stream applications moved the air inside a structure without any fire involved. A second set of experiments illustrated how these differences affect the movement and cooling of hot gases in ventilation-limited fires. The data from these two sets of experiments can be used to evaluate and explain the impact of different hose stream applications during fire suppression. During this presentation, two specific types of hose streams, straight and fog, will be considered, and their impact on air movement and fire suppression will be discussed.

University of Maryland Baltimore County

R-Separation of Laplace's Equation in Rotationally-Invariant Cyclidic Coordinates

Brandon Alexander

There exist 17 conformally unique coordinate systems which admit harmonic solutions to the three-variable Laplace equation via separation of variables. Of these, four are determined by coordinate surfaces given by rotationally-invariant cyclides: bi-cyclide coordinates, flat-ring cyclide coordinates, flat-disk cyclide coordinates, and toroidal coordinates. With the exception of toroidal coordinates, these systems produce harmonics given by products of simply-periodic Lamé functions or Lamé-Wangerin functions and complex exponentials $e^{im\phi}$, where ϕ is the azimuthal coordinate, and m is the azimuthal quantum number.

We separate Laplace's equation for three versions of bi-cyclide coordinates: algebraic and Jacobian elliptic forms by Miller (1977) and a Jacobian elliptic form by Moon and Spencer (1961). In the process, we re-derive and correct past results, and quantify the connection between these bi-cyclide coordinates. We then present a generalized form for bi-cyclide, flat-ring cyclide, and flat-disk cyclide coordinates that is able to separate Laplace's equation simultaneously.

The long-term goal of this project is to produce expansions of a fundamental solution for Laplace's equation in terms of our derived harmonics.

Improvement of Systematic Uncertainties in Mass Calibration Using Robotic Comparators

Vignesh Dhanasekaran

The NIST Mass and Force Group is responsible for disseminating the unit of mass, the kilogram, to the U.S. Measurement System. This dissemination is accomplished through calibration of customer mass artifacts with NIST standards that are traceable to the International System of Units (SI). Working down from a 1 kg standard to submultiples typically involves manual placement of artifacts onto delicate mass comparators, introducing sources of uncertainty due to fluctuations in temperature, pressure, humidity and placement position. By automating the process with robotics, the human-induced uncertainties can be largely eliminated.

Traditional weighing designs used to calibrate masses from 1 kg to 1 mg require the placement of up to four masses on the weighing pan simultaneously. However, this type of design cannot be implemented on the NIST robotic comparators, as they are restricted to having a maximum of three masses on the weighing pan at any given time. To compensate for this restriction, it was necessary to develop new weighing designs that would allow the robots to calibrate the submultiples with no loss of accuracy or increase in uncertainty. The NIST Statistical Engineering Division developed a practical design that would meet these requirements; measurements were then performed with the robotic comparators to test the new weighing designs against results obtained by traditional manual mass comparators. Test results at the one kilogram level indicate that the robotic comparators differ from manual calibrations by less than 0.010 mg, which is the resolution of the balance. The standard deviations of the robotic measurements about their means were also less than 0.010 mg.

Analysis of Factors in Photovoltaic EVA Degradation

Gary Eurice

The use of photovoltaic (PV) products, such as solar panels, has experienced a tremendous growth in recent years. As a result, concern towards their reliability and safety has also risen. PV modules are often operated in harsh conditions, such as heat, moisture, and ultraviolet radiation, therefore, long-term reliability of PV modules remains one of the field's greatest challenges. Polymeric materials have become commonplace for use as an encapsulant in photovoltaic cells to provide mechanical, dielectric and moisture protection for the silicon component. One such material that is being abundantly used is ethylene vinyl acetate (EVA), a copolymer that is known for its cost effectiveness in the photovoltaic field. In service environments, the severe exposure conditions can cause the EVA material to degrade which also results in a yellowing effect. This degradation generally appears along with delamination, corrosion and a decrease in solar module efficiency, resulting in ultimate module failure. There are many different factors that can affect the degradation rate of EVA including UV light intensity, relative humidity, formulation type, oxygen diffusivity, and module geometry. In this project, the individual effects of these factors on model EVA modules were studied. Using the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure), these modules were subjected to UV exposure at service conditions. Three different EVA formulations, denoted A, B, and E, were examined as well as two different module geometries: a circular 19 mm diameter module and a 50 mm x 50 mm square shaped module. In addition, while exposure temperatures were kept constant at 80°C, exposure was performed at one of two relative humidity levels: 0% or 60%. Certain modules were also exposed to various levels of UV intensity. After each exposure, measurements were taken on a UV/Vis/NIR spectrometer to obtain quantitative estimates of discoloration. The Raman spectra were obtained on the same samples for complementary chemical information. Preliminary results have shown that formulation type and module geometry have a major effect on the EVA degradation rate while the effect of humidity was present but not as significant. In addition, evidence of photobleaching, an effect caused by oxygen diffusion that reverses the yellowing effect of EVA degradation, was observed on the edges of the square modules.

New Generation Dental Resin Composites

Abigail Jackson

In the USA alone, 122.7 million dental resin composite restorations were placed in 2006, an increase of about 40% from 1999 (ADA Health Resources Policy Survey). The current trend in clinical dentistry indicates that this number is likely to increase. Many if not most of the currently available materials and their accompanying instructions for use do not produce satisfactory durability and esthetics over time. The short average service life of these systems and concerns regarding leached unreacted monomers, and possibly bisphenol A (BPA), and degradation products from these systems are evincing a need for new, long lasting composite polymers, fillers and adhesive components to improve the dental and oral health of dental patients everywhere. Here, I present the concept of novel dental resins as sealants, resin matrix, and dental adhesives that are superior in properties and endurance to current BisGMA/TEGDMA resin systems. The durability of the new resins will be improved by replacing the hydrolyzable ester groups in BisGMA/TEGDMA systems with hydrolytically stable ether groups. New resin monomers that are not susceptible toward enzymatic or hydrolytic degradation were synthesized and characterized. In addition, new initiator systems were tested, and many combinations of different resin monomers were examined to achieve requirements for clinical practice.

Interfacial Shear Strength Measurements for Hybrid Nanocomposites Using Fiber "Push" Methods

Leonard Jacques

There are over 60,000 bridges in the United States currently considered "structurally deficient", it is important to discover ways to detect failures in structures before catastrophic events are allowed to occur. Hybrid composites reinforced with carbon nanotubes are a viable solution to this problem. Fiber composites are composed of a matrix that holds fibers oriented in their strongest direction. The interface between the fiber and the matrix is important to the overall strength of the composite, because failure in this region leads to composite failure. Hybrid fiber composites utilize carbon nanotubes, attached at the interface of the fiber, to enhance the interface strength and add conductivity to the material. The purpose of this project is to measure the change of the interfacial shear strength in carbon nanotube reinforced composites using "fiber push-out" and "fiber push-in" techniques. The "fiber push-out" technique involved the use of a Nanoindenter XP (MTS, USA) to push individual fibers, ~10 microns in diameter, out of a matrix of Epon 828 (Epoxy) cured with Ancamide 351A. The "fiber push-in" technique involves indenting the surface of the fiber to determine the interfacial shear strength. The test methods practiced have shown interfacial debonding between the matrix and the fiber. Ideally, measurement methods are simple, but are subject to many obstacles during implementation. Both techniques were employed to attempt to measure the interfacial shear strength of a bare fiber and a nanotube decorated fiber in the epoxy matrix.

Evaluating Dual Platforms for Bone and Vascular Regeneration
Caitlyn Maczka

The goal of this project was to evaluate various materials and methods available for creating bone scaffolding for dental tissue regeneration via airbrushing. The study examined the interactions between cells and their environment, as well as relationships between method of cell deposition and cellular viability. The study was divided into two research directions.

In the first, ability to deposit cells via a novel method of airbrushing was investigated. Cells were brushed onto tissue culture plates with different speeds of deposition, as well as with different airbrush nozzle designs, to determine optimum parameters for viable human bone marrow stromal cells (hBMSC). Various bioassays were implemented to obtain results, including PicoGreen assays, WST cell-proliferation assays, and live/dead imaging assays.

The second part of the project looked at the ability to coat synthesized polymer nanofibers with various bioactive proteins, specifically collagen 1 and fibrinogen. SEM imaging and Coomassie staining were used to examine protein adhesion to the nanofibers. Co-cultures consisting of hBMSC and human umbilical vascular endothelial cells (HUVEC) were used to verify cell response to these coated fibers networks.

Data indicates that of the two tested nozzle designs, one design shows higher levels of deposited cell viability than the other. As for the second part of the study, research indicates that polymer nanofibers made of poly-DL-lactide (PDLLA) and poly(lactic-co-glycolic acid) (PLGA) show the ability to be coated with tested proteins without any visible effect on nanofiber morphology. In vitro cell studies demonstrate that cells were able to recognize the bioactive protein coatings, as indicated by fluorescent imaging.

Identifying Distinct Regions in Multi-Material Microstructure Images with Clustering Algorithms
Jane Pan

Many fields of science and engineering rely on digital images for assessment, analysis and solutions, e.g. cell biology, meteorology, and diagnostic radiology. The image data that experts in these fields need to deal with are usually large and complex, and image processing algorithms become necessary to facilitate analysis and enable discovery. Image segmentation is a fundamental tool within image processing, in which our objective is to partition a given image into distinct regions representing different objects or entities, e.g. cells and materials. There are many methods to performing image segmentation, and one logical approach is through clustering. With clustering, we can treat the given noisy image as a large data set of scalar points, and our end goal would be to systematically categorize these points into groups—or clusters. A plethora of clustering algorithms have been used in the attempts of obtaining ideal clusters from noisy data sets, but a prominent issue many experts have struggled with is achieving consistency in the clusters that are formed and the number of clusters that are estimated. This brings us to the question of what defines a “good” cluster and whether there is a clustering method that ensures consistency. By analyzing a multitude of material images using simple clustering techniques, we were able to assess clustering methods using various clustering evaluation techniques and come up with effective algorithms to cluster multiphase material microstructure images.

Semantic Refinement Tool Development
Nasif Sikder

Systems integration is costly and time consuming. One of the reasons is that methods used to specify interface descriptions (how systems should communicate with each other) today are typically semantically imprecise. This issue is worsened in cloud based environments. Smart manufacturing systems are envisioned to be dynamically composed from software and hardware components provided by various vendors, some of which are cloud services; therefore, the ability to precisely specify interface descriptions is important for the success of the smart manufacturing vision. Today's interface descriptions rely on messaging standards delivered in XML schemas that are large and aggregate. Interfaces typically use only subsets of these schemas; however, software vendors have no way to precisely declare the subset used by a particular interface. In this research, we collaborate with the standard development organization, namely Open Applications Group (OAG), and industry partners such as Oracle, Infor, ADP, and Boeing to develop a method and tool to close the gap. The method is an adaption of the UN/CEFACT Core Component Specification (CCS also known as ISO 15000-5) and its context methodology. In this research, we align OAG standards with the CCS meta-model, implement the resulting model in the relational database (RDB) schema, import OAG standards into the database, and implement the context methodology in the semantic refinement tool. The OAG standards within the RDB are the syntax independent representation of the standards. Therefore, the semantic refinement tool allows the user to precisely specify a syntax independent interface description according to the needs of his/her information system, and export it not only in XML Schema syntax, but also in other syntaxes such JSON (which is important for integration with mobile systems). For my project, I am utilizing the CCS methodology and OAG standards in order to implement software which imports the standard into the RDB. One of the major challenges is to develop a method to validate the imported content with the original, as we deal with partially ordered content.

Application of Machine Learning Techniques for Manufacturing
Chelsea Vane

Although today's manufacturing companies are already efficient, data analytics could help drive them to the next step. Data analytics consists of computationally managing data to extract hidden patterns and to be able to predict the upcoming data states. The data analytics workflow is composed of different steps: data acquisition, data cleaning, data analysis, and data interpretation (including data visualization). In order to process and find knowledge in the data, data analysis is critical and involves, among others, machine learning. Machine learning, a branch of artificial intelligence, concerns the construction and study of systems that can learn from data. The goal of this project is to study how machine learning can be applied to predict power consumption in a turning process in manufacturing. We compare the efficiency of different techniques and software on a similar set of data. We also study the necessary set of features to generate a useful machine learning model that we could use to predict power consumption. The objective is to compare the output of this model with the theoretical power consumption in different scenarios and study what could improve the prediction quality.

<u>University of Maryland College Park</u>

Relating Quantitative Measurements to Human Assessment of Voting Ballot Mark Types

Andrea Bajcsy

The presence of marginal marks on voting ballots is a ubiquitous problem in voting systems and is a common source of dispute during large-scale, contested elections. Today, marginal marks are not clearly countable as a vote or as a non-vote by Optical Mark Scanners or Ballot Readers. There is a lack of quantitative measurements that would agree with human assessments of marginality and be unbiased in their classification of mark types.

We aim to establish quantitative measurements of marginal marks in order to provide an automated and objective classification of ballot-mark types. Utilizing 800 publicly-available ballot image scans from the 2009 Humboldt, California election, our contributions lie in (a) establishing a pipeline for extracting a set of unique image features that distinguish between votes, non-votes, and marginal mark types (check-mark, cross, partially-filled, etc.), (b) building a web-application for collecting semantic labels, and (c) relating image features with semantic labels by utilizing both unsupervised and supervised machine-learning methods.

The feature-extraction pipeline consists of the following steps: (1) registration of ballots to a common-coordinate system, (2) extraction of individual mark regions, and (3) computation of mark-region features. We correlate each mark to a baseline ideal vote and non-vote generated from example marks present on each ballot. The correlation to the baseline marks separates marginal marks from vote and non-vote marks at a very high level. Furthermore, the resulting correlations are used as a filter for selecting marks to be presented to human assessors via a developed web-application to collect marginal-mark types (6 semantic labels).

Next, we use the gathered semantic labels and the corresponding image features as our training data for the following supervised classification models: decision-tree model and probabilistic linear model. We report classification accuracy for multiple models and summarize the benefits and drawbacks of mark analysis at a larger scale.

D3 Spatial Decomposition Visualization Validation Tool for Cement Hydration

Luis Catacora

Concrete provides strength and structure to a large part of our world. The cement binder in concrete undergoes multiple interacting chemical and structural changes as it transforms from a liquid suspension to a solid mass. Understanding the nature of these transformations is important for building a sustainable civil infrastructure. The Inorganic Materials Group within EL/NIST is developing computational models capable of predicting the flow, hardening, and strength of cement.

To help understand and validate the models, we have developed an integrated interactive visualization and analysis environment for the model outputs. Our environment provides a variety of visual modes to enable precise quantitative measurements and visual information. We also combine 3D scientific data visualizations with information visualization using D3.js running in a web browser.

In this talk we will present the data produced from the computational modes, and show our findings and results from using our D3 Spatial Decomposition Visualization Validation tool.

Characterizing Transport Properties in Bilayer Membranes for Next-Generation Desalination Technology
Samuel Degraft

Multilayer membranes comprised of an ultrathin, selective polyamide layer atop porous, mechanical support layers are the state-of-the-art in water desalination. The fully-aromatic, dense polyamide layer is designed to achieve the highest salt rejection while minimizing resistance to hydraulic permeation. To develop future generations of desalination membranes, it is critical to understand the mechanisms which contribute to permeability and selectivity. From solution-diffusion theory, it is known that the performance depends on the transport and swelling properties of the polyamide membrane, therefore it is important to develop characterization techniques for these properties.

In this work, we use a quartz crystal microbalance with dissipation (QCM-D), a gravimetric technique, to measure water sorption behavior in model polyamide membranes. By characterizing these properties as a function of relative humidity, we are able to obtain information about the polymer network structure as well as develop an understanding of water diffusion within the membrane. Fully aromatic, model polyamide membranes were fabricated in the experiments using a novel molecular layer-by-layer (mLbL) technique. In this technique, highly crosslinked polymer networks are developed one molecular layer at a time through sequential and instantaneous reaction of two monomers solutions.

Using the QCM-D, we also study the effect of a hydroxyl-rich coating on the polyamide layer, a surface modification that is often used in commercial applications to mitigate the effects of fouling. The coating acts to increase hydrophilicity at the surface as well as prohibit bacterial growth. While surface modifications have been widely investigated for their anti-fouling properties, little work has been done to understand their effects on transport properties and overall membrane performance. We investigate the effect of a Polyvinyl Alcohol (PVA) coating on the transport and swelling behavior and quantitatively investigate the validity of a bilayer mass transport model.

Information Models for Sustainable Manufacturing
Nick Du

Current methods for assessing the sustainability performance of manufactured products do not account for manufacturing systems explicitly, and lack an effective method of comparing sustainability of different manufacturing processes. Characterizing a production process into a series of unit manufacturing processes (UMPs) is a methodology that allows for practical comparisons among different manufacturing processes. Corresponding UMP information models are then developed for individual unit manufacturing processes. These information models will, in turn, enable decision support for sustainable manufacturing.

To demonstrate the usefulness of such a methodology, a series of UMPs were developed to characterize a paper manufacturing facility and a powder metallurgy manufacturing process. Using a physics-based approach, a series of equations were used to model material transformations for individual UMPs within the facility. These equations describe the parameters involved in a given UMP as well as the minimum energy required for the material transformation. Further, IDEF0 (Integrated Computer Aided Manufacturing DEFinition for Function Modeling) models were created to simulate the powder metallurgy process and demonstrate the UMP methodology and information models for sustainable manufacturing.

Flammability Reduction in Upholstered Furniture
Evan Eisenberg

The foams and fabrics commonly used in upholstered furniture in the United States are very flammable and although only 4% of residential fires originate from upholstered furniture, these fires account for 25% of damages. To pass the current flammability tests, upholstered furniture now only needs to pass a fabric smoldering test. However, some of the current fabrics, like the thermal plastic olefin/polyester mix, behave very well in smolder tests but perform badly during open flame tests. The purpose of our research is to examine the fire spread rates in upholstered furniture with different combinations of outer fabrics, barrier materials, with and without polyester fiberfill wrap, and foams.

To study how the materials behaved when combined, real-scale mockups of the various material combinations were made by placing four cushions on a metal frame in the shape of a chair, which were then ignited by small flame. Videos of the tests were recorded from various directions. Using the recordings, the back cushion and the seat cushion were examined individually to study the fire spread's velocity. To do so, images were captured from the video at various times during the fire spread.

Using Photoshop, a grid was created to line up with the cushion being analyzed and standardize the images regardless of magnification and provide a consistent measurement of area. The images were edited to determine what portion of the cushion burned at that time. By inputting the edited images and the grid into a Mathematica program, the edited images were analyzed to determine the fire spread rate.

Although the project is still continuing, some conclusions have already been made. It is clear that cotton fabric's charring behavior causes it to be much more fire resistant than the olefin/polyester mix. Cushions with cotton fabric burn much slower and better protect the very flammable foam commonly used in upholstered furniture. The thermal plastic olefin/polyester fabric tends to peel away from the fire, exposing the filling materials foam, leading to a higher fire spread rate. It has also been found that Norfab barriers, a mixture of Kevlar and Basofil fibers, greatly inhibit fire spread as it prevents the flames and the heat from reaching the foam. However, nylon zippers that were used in the cushion are a very weak point. If the fire reached the zipper, it was observed to penetrate the barrier. In addition, it has been found that a type of foam manufactured in Great Britain, which has a more stringent furniture flammability regulation, contains a large amount of fire retardant which was considerably more effective in slowing the fire spread rate over both fabric types.

A New and Innovative Way to Conduct Uncertainty Analyses on HVAC&R Equipment!
Syed Elahi

In Heating Ventilation, Air Conditioning and Refrigeration (HVAC&R) field, heat pump and air conditioning equipment are rated according to Seasonal Energy Efficiency Ratio (SEER), which quantifies the energy consumed by the equipment while providing space conditioning. These performance evaluations are conducted through the methods described in the standards of the Air-conditioning, Heating, and Refrigeration Institute (AHRI). According to the AHRI standards, high quality test results are achieved by using uncertainty analyses for the selection of appropriate sensors to measure system temperatures, pressures, volumetric flow rates, and electrical energy consumptions. The SEER calculation and related uncertainty analyses can be time-consuming and expensive; therefore, NIST is developing a software tool that will assist the HVAC&R industry to perform these computations.

The SEER calculation uses both steady state and cyclic performance data for a particular piece of equipment. The steady state data describe the equipment capacity and efficiency at a specified set of operating conditions, where the equipment is given unlimited time to achieve steady operation. Conversely, the cyclic data capture transient performance of the system related to switching the equipment on and off. The cyclic performance is captured by a Cyclic Degradation Coefficient (C_D) that describes the reduction in system capacity during transient operation. The equations used to calculate C_D and SEER values are solved using the Engineering Equation Solver (EES) software package. The software is further used to compute the uncertainty in C_D and SEER, including metrics that identify the measurements that most significantly contribute to the overall uncertainty (i.e. which of the temperature, airflow, dew point, pressure measurements require high accuracy to achieve a low overall uncertainty in the SEER calculation). The uncertainties in C_D and SEER depend both on sensor uncertainty as well as test repeatability; part of this analysis will determine the relative importance of the two sources of uncertainty.

The deliverable from this project is a set of EES code that calculates C_D and SEER values and their respective uncertainties. These calculations and uncertainty results are then going to be added to other uncertainty analyses to complete the software tool. Finally, the complete software tool will be made available to the HVAC&R industry.

Toxicity of TiO_2 Nanoparticles in vitro and in vivo
Rachel Golan

Titanium Dioxide nanoparticles (TiO_2-NPs) are a common additive in food and commercial products. However, these particles can generate reactive species, which lead to subsequent DNA damage. In order to investigate the precise genotoxic mechanism of TiO_2-NPs *in vitro* and *in vivo*, the growth of human cells and model organism *Caenorhabditis elegans (C. elegans)* must be optimized and background DNA damage must be quantified in both models. Thus far, human hepatocarcinoma (HepG2) cells have been cultured and harvested, and nuclear and cytoplasmic proteins have been extracted for quantification of DNA repair enzymes. Several methods for nematode growth have also been investigated. Traditionally grown in agar, nematodes can also thrive in liquid cultures. Experiments were conducted to test which culture conditions (worm density, amount of feed and frequency of media renewal) produce the healthiest and largest number of worms in liquid cultures over several generations. A MATLAB program was designed to search through the *C. elegan* proteome for select repair protein fragments. The presence of a set threshold of fragments will enable quantification of DNA repair enzymes using mass spectrometric techniques. Progress has been made in each area of work. The HepG2 cells are growing well, but, the MCF10 cells are not yet proliferating efficiently. Results from the liquid culture experiments show that nematodes prefer a medium-feed *E. coli* environment, with an initial seeding density of 0.5 worms/ µL. According to the MATLAB program, seven *C. elegan* proteins contained four or more fragments from one human DNA repair protein, Nth-1, and these proteins will be further studied. In order to prepare for *C. elegans* DNA damage quantification, three potential DNA extraction protocols were tested: the Qiagen genome extraction kit, a mammalian cell high salt method, and a *C. elegan* method adapted to eliminate phenol and chloroform. The Qiagen kit may yield the largest quantity of DNA to be extracted from the *C. elegans*. These initial studies will establish a framework that will enable the lab to successfully investigate of the genotoxic effects of TiO_2-NPs.

Optical Calibration of Nanocalorimeter Chips Using Infrared Camera
Joshua Goldman

Nanocalorimetry is the measurement of thermodynamic properties of samples with microgram to nanogram mass. The measurement is based on a microfabricated sensor chip, so in order to derive temperature, we must relate it to resistance through *a priori* calibration. In this talk I describe a calibration method whereby an infrared thermal camera with a microscopic lens is used to measure the temperature of the heater on the sensor as it is heated with applied voltage. The resistance of the chip is simultaneously found by a four-wire measurement. We first determined the temperature-emissivity relationship for the sensor's platinum surface at the wavelengths used by the thermal camera. Using this data, temperature data from the thermal camera can be accurately corrected for emissivity. During a measurement, the temperature of the platinum heater is compared to a reference platinum surface which remains at room temperature (or another controlled temperature).

$$\frac{1}{T_{1_{corr}}} = \frac{1}{T_{1_{meas}}} + \frac{\lambda k_B}{hc}\ln\big(\varepsilon(T_1)\big)$$

$$\frac{1}{T_2} = \frac{1}{T_{2_{meas}}} + \frac{\lambda k_B}{hc}\ln\big(\varepsilon(T_2)\big)$$

This process is automated with a LabVIEW virtual instrument controlling a digital data acquisition system. We validated this method of calibration by measuring the melting point of an aluminum sample.

Hydro-Mechanical Response of Thin-Fil Polyelectrolyte Membrane Materials for Fuel Cells
Joshua Graybill

Perfluorosulfonic acid (PFSA) ionomers, particularly Nafion, are the most widely studied class of materials to be used as proton exchange membranes (PEM) in fuel cell applications. In an operating fuel cell the cycles of hydration and dehydration, and the mechanical response thereto, threaten the long-term mechanical stability of the PEM and, thus, performance and device lifetime. Therefore, it is critical that the water-dependent, mechanical response and properties of PEM materials for fuel cells be well understood. Despite the importance of the mechanical response of bulk PEMs to hydration cycles, which is critical to lifetime and durability, there is an increasing interest in thin film properties of these materials. This is due to the fact that often times PFSAs are used as a binder in the electrode layer where the material can be confined to films on the order of tens of nanometers thick. However, there are a lack of measurement techniques and platforms capable of measuring the mechanical properties of PEM films that are only tens of nanometers thick. Given this issue a relatively new measurement technique, which exploits the bending deflection induced from swelling strain in thin Nafion films on silicon substrates, was used to successfully measure and characterize the elastic cantilever bending stress over a wide range of relative humidity steps. Measuring the swelling strain of these same films allows the derivation of the modulus behavior as both a function of thickness and annealing. While the stress thickness shows a predictable elastic behavior for both thin and thick films that can be well quantified there is a distinct change in response upon annealing; namely the absence of a visco-plastic response that was previously observed in un-annealed Nafion films. Furthermore, there appears to be a residual background stress correlated to physical aging of the film after annealing that could provide insights into the humidity/time-dependent relaxation behavior of this material under thin film confinement.

Towards Robust, Universal Polymer Grafting
Ariel Isser

Polymer grafting, the process of tethering polymer chains to a substrate, is a common surface modification technique for synthesizing surfaces with unique physical and chemical properties. Many current grafting methods either require large amounts of polymer, unique polymer-solvent combinations, or complex synthetic steps. A simple method is presented here for grafting polymer chains with tether-points close enough to be considered "dilute brushes" using a variety of amino end-functionalized polymers, including polystyrene, poly(2-vinylpyridine), and poly(methyl methacrylate). Polymers were deposited from a dilute solution via spin-coating to the surface of a silicon wafer functionalized with 3-glycidoxypropyl-trimethoxysilane and then grafted through vapor-treatment in a chamber containing a reservoir of solvent. The films were characterized using ellipsometry to measure film thickness and atomic force microscopy to assess film topography and roughness. Preliminary results show that smooth, uniform films with thicknesses in the dilute brush regime were achieved for several of the polymers and conditions studied. The time- and solvent-dependence of brush formation were also evaluated. Current results suggest grafting kinetics depend on molecular weight and solvent quality.

Development of a High Resolution Photonic Spectrometer
Arec Jamgochian

We are developing the next generation of photonic sensors for applications in temperature and pressure metrology. This summer I was involved in executing critical tests for validating performance of a new high resolution tunable spectrometer. This spectrometer employs a C-band diode laser, a wavemeter, an InGaAs photo-detector, and a temperature bath to enable high resolution (0.1 pm resolution) investigation of photonic sensor's temperature response. We utilized single Fiber Bragg gratings and an array of 5 gratings in a single fiber to determine laser power dependence and temperature equilibration time. Furthermore, we successfully embedded Fiber Bragg gratings inside 3D-printed scaffolds. Our preliminary results indicate embedded FBG show significant changes in linewidth and temperature – dependent frequency response. This work lays the groundwork for future work in embedded sensors including the use of FBG in tissue engineering experiments.

Mayday! Mayday! : Investigating the Performance of Radio Cables in High Temperature Environments
Shelley Jin

Radios are lifesaving equipment that allows fire fighters to communicate with one another to coordinate firefighting operations. Therefore, it is essential that radios can operate in high temperature scenarios. There are no current standards regulating radio performance or testing; however the National Fire Protection Association (NFPA) is currently developing a code, NFPA1802, which will address radio performance. This project aims to make testing recommendations to the NFPA1802 committee.

In this experiment, investigators looked specifically at the cable that connects the radio to a speaker microphone. Earlier results indicate the cable might be the first component to fail in a fire. An in house fabricated device called a flow loop was used to subject these cables to varying amounts of convective heat stress. The flow loop contains a testing chamber equipped with a thermocouple tree, bi-directional velocity probes and heat flux gauges. Signals from these devices are recorded in a LabVIEW data file and are used to monitor the chamber to ensure consistent testing conditions.

Cables are isolated for testing by hanging them on a stand and then stretching them to so that the radio and speaker microphones are located outside the testing chamber during the test. Thermocouples are also arranged on the cable itself and the air in between the cable loops, in order to monitor temperatures on the equipment during the test. The radio is directly hooked up to a spectrum analyzer and the speaker microphone is routinely pressed to evaluate radio signal strength. The two main testing conditions are a 15 minute exposure at 160^{o}C, deemed a Thermal Class II fire situation, and a 5 minute exposure at 260^{o}C, deemed a Thermal Class III fire condition. Results showed that all cables tested managed to pass the Thermal Class II condition. Most failed when undergoing Thermal Class III, but some specified to be for “extreme” conditions survived. Based on this, the lab believes it would be prudent to recommend the NFPA1802 committee to require cables pass this criteria.

Uniaxial Orientation of Polymers: Fabrication of Anisotropic Organic Semiconductor Films
Maria Kaplan

Organic semiconductor films have the potential to enable sustainable manufacturing for printed electronics with low thermal budget, roll-to-roll processes. Unlike commonly used inorganic symmetric materials such as Silicon, organic films exhibit highly anisotropic local electrical properties. Anisotropy in organic thin films is important for semiconductor performance because typically only one direction in the unit cell will effectively transmit charge and have a high mobility. It is necessary to control polymer orientation and understand the material properties of printed films. This allows for optimization of the orientation of the active layer which will enhance device performance. The fabrication of anisotropic thin films can be accomplished using methods such as blade coating and drop casting. Film orientation by blade coating was studied by using two approaches: crystallization additives and nanogrooved substrates. Optical techniques such as ellipsometry, atomic force microscopy UV-vis absorption were used to quantify the film orientation on test substrates. Electrical testing of devices was performed on thin film transistors to determine anisotropic properties and mobility.

Large Image Visualization
Timothy Kim

Panoramic imaging in consumer digital cameras assembles a few partial images of a scene into a single coherent image. This occurs because the camera’s field of view is smaller than the scene being photographed. This phenomenon occurs on a much larger scale in Science: biologists generate very large images (100 000 pixels per side, for a file size of about 20 GB) when imaging plates with high-end optical microscopy; astronomers produce similarly large images in their sky surveys. These large images present two challenges: no display system (including display walls) can render them at full resolution; most workstations cannot load them into memory. These limitations leave us with a range of alternatives for viewing the image. At one extreme, the user can view a downsampled version of the image in order to fit the complete image on the display system. At the other end, the user can view only a partial section of the image at its highest resolution. I present a Java application programming interface (API) that is capable of querying regions of the image at a certain downsample level. Both the windowed region and the downsample level are specified by the user. This API allows for properly visualizing large images by generating the requested regions of the image (downsampled or not) on demand. This approach optimizes performance and system responsiveness by loading only the necessary portions of the image into memory. The API will be used in conjunction with a Graphical User Interface so that as the user zooms or pans across an image, the API will generate and display the correctly downsampled region in the view window.

Semantic Interpretation of Bayesian Inference in a Manufacturing Scenario
Gedaliah Knizhnik

Bayesian networks are a statistical tool that allows the modeling of deterministic and probabilistic relationships between variables in a system. Such relationships are prevalent in multitudes of industrial and manufacturing applications. Bayesian Networks provide a powerful and useful method of both computing the likelihood and analyzing the causes of failures. Understanding how this modelling methodology can be used in manufacturing is important to reducing costs and increasing efficiency by effectively managing and controlling failures.

Ontologies are formalized representations of information about concepts and their relationships. They encode information that humans understand inherently in a language that computers can understand and use to draw inferences. Ontologies thus provide a way to link real world information about a system with a computer's analytical tools.

In this project I studied existing literature on both Bayesian networks and ontologies in the realm of manufacturing and investigated the possibility and utility of a connection between the two; I used a Bayesian network to model a manufacturing scenario and an ontology to represent the semantics of the domain. The aim of the project is to show that the information in the Bayesian network can be mapped onto the ontology, and that the statistical inferences of the Bayesian network can be translated into specific semantic assertions and given meaning by way of the ontology. This is valuable because it can bridge the gap between numerical results and their relevance to the physical system by giving the conclusions specific meaning through semantic language.

Future goals of the research include the automation of this process, perhaps by means of the Java programming language.

Materials Informatics for the Materials Genome Initiative
Alexander Kordell

As announced by the White House in June 2011, the goal of the Materials Genome Initiative is to reduce the cost and duration of the materials development and deployment cycle by 50 percent. Acceleration of this magnitude requires accurate and efficient models for the calculation of phase-based material properties, including thermodynamic properties, diffusion mobilities, elastic constants, and thermal expansion coefficients. For a given phase, these models are expressed as functions of temperature, material composition, and pressure. Current access to phase-based property data is limited, as the needed experimental and computational data are often scattered across both real and virtual space. This problem makes it difficult to both locate and use data efficiently. Improving the access to of phase-based property data requires a new materials data infrastructure that incorporates flexible, platform independent XML-based data formats. Using XML-based data schemas will facilitate access to data repositories using existing and readily available tools, and will allow for easy data modification for future applications. This work will demonstrate the development of XML-based data schemas for thermal expansion and elasticity property data based on past experiments. The thermal expansion and elasticity data will be accessible in the NIST Materials Data Curator, the NIST Dspace repository, and the Granta MI interface within the ASM Structural Data Demonstration Project.

Machine Learning for Adaptive Robot Coordination

Gregory Krummel

In industrial applications with multiple robot collaboration, coordination of the individual robots' motions is critical for productivity and safety. When robots from multiple manufacturers and model lines are implemented together, the control dynamics for each system varies due to different hardware and software configurations. These differences vary even more due to environmental and operational changes such as temperature, load, wear, and updates to software and hardware. Coordination methods developed at NIST have been able to model multiple robots' transient behavior, but the models were estimated by the operator and were not adaptable to changing conditions. In addition, the transient behavior of each robot is non-linear, which complicates traditional methods for model estimation.

This talk will summarize the development of adaptive robot coordination using machine learning. The adaptive coordination automatically learns the models for the transient performance of each device. These models are applicable for a variety of coordination methods, including speed selection and delay estimation for each device. Automatically learning the behavior of each robotic device improves the time needed to adapt to a new device introduced to the manufacturing system, as well as adapt to environmental and operational changes. These automated methods were implemented on a Canonical Robot Command Language (CRCL), which is generalizable to control multiple heterogeneous devices. A KUKA LWR 4+ and a Robotiq 3-Finger Adaptive Robot Gripper were utilized for training, testing, and verification of the machine learning algorithms. These methods and metrics can be utilized in industrial applications with minimal input from the operator and minimal adjustment time.

MakerBot Round Robin Study: Manufacturing Plan Precision

Joshua Land

Additive manufacturing (AM) is one of the few technologies that will transform every sector in modern industry. Its application is virtually limitless provided that machines and process parameters are properly qualified. Yet, process qualification has not been conducted on a large scale. Instead, qualification has been an exclusively private endeavor with studies, tests, and respective results remaining proprietary. NIST intends to change this using Round Robin studies as means to assess various AM protocols, specifically in the realm of metal-based AM. Standardized protocols for Round Robin studies will facilitate the qualification of additive manufacturing processes and materials. Simpler fused deposition modeling (FDM) machines can be used to evaluate various study protocols before implementation with more advanced, direct metal laser sintering (DMLS) machines. This pilot study focuses on the manufacturing plan used to build test parts on several NIST-owned FDM machines, and measurements of dimensional accuracy. Results give an idea of how effective the manufacturing plan is at controlling variables associated with dimensional accuracy.

Making the Robot Think Twice: Improvements to an Ontology-Based Agility Framework for Manufacturing Robotics

Christopher Lawler

One area where it is clear that the increasing intelligence of robots can produce immediate gains is agile manufacturing, which aims to increase equipment flexibility, reduce changeover costs, and make smaller-scale production more economical. Companies want to install robots with cognitive and collaborative capabilities, but smaller manufacturers may not have the resources to develop them independently. To support agile manufacturing, the Intelligent Systems Division of the National Institute of Standards and Technology has a group building an open ontology-based framework, called Agility Performance of Robotics Systems (APRS).

In this project, multiple improvements to the evolving APRS framework were realized, making the system: responsive to real-time changes in its environment, standardized in the way in represents robot commands, less computationally expensive, and able to account for uncertainties.

Enabling responsiveness was achieved by writing a program that examines a Structured Query Language (SQL) database representing the current state of the world and outputs a Planning Domain Definition Language input file for the planner that decides what the controlled robot should do next. New syntax was developed and documented for compactly representing the location of scattered information in databases, so that the addition of new details to the world representation will not necessitate hard-coding mappings.

To ensure compatibility between all projects under the framework, the custom syntax that previously was used for canonical robot commands was replaced by an Extensible Markup Language (XML) schema. One parser that interprets such schema was also modified to leak less memory and be more object-oriented.

The representation of uncertainty throughout the framework was planned out and its implementation is ongoing. If sensor data is unclear beyond a learned threshold, the robot will re-evaluate the situation instead of executing a potentially incorrect action. To our knowledge, this is the first ontology-based robotics framework to incorporate non-binary truth values.

Augmented Reality for Smart Manufacturing: A Google Glass Exploratory Project

James Ledwell

Augmented reality consists of virtually enhancing real world physical elements with computer-generated elements, including a wide range of information: from texts and pictures to sounds, videos, 3D models, GPS information and more. The rapid spread of mobile devices, including the newly developed wearable sector is significantly contributing to this field.

To bring augmented reality to the manufacturing world is a challenge due to the complex physical environment of operation, the limited ergonomics of handheld devices, the lack of standardization in architecture for the development of mobile apps, the weak state of the art in the area of augmented reality for manufacturing, and the heterogeneity of possible use cases.

Our objective is to study the feasibility and explore the benefits of using Google Glass as a head-mounted device to augment the manufacturing reality by integrating digital virtual elements into the physical world. The project's goal is to establish reference architecture to support the development of manufacturing apps for head-mounted devices.

Our specific use case involves coalition based military activity. In coalition forces it is often far more efficient to share resources due to geographical and economic realities. This comes into play when requesting spare parts and maintenance in the event of equipment failure.   Our project consists of transmitting data about the malfunction collected through Google Glass's picture function and audio input to servers designed to simulate those of allied nations. The servers will respond and present users with a variety of options for obtaining a replacement part and receiving maintenance. The users will designate their choices and be notified upon the arrival of the services.

Augmented reality will lead to faster, safer and more accurate manufacturing processes. New commercial products like Google Glass can be used to further develop this field.

An Extraordinary Hall Effect Susceptometer for Fast Measurements of Magnetic Media

David Marin

As the magnetic recording industry continues to press the limits of hard disk drive capacity, there has arisen the great challenge of precisely controlling the material parameters of magnetic media. This is because the decrease in magnetic bit size needed for denser storage is accompanied by enhanced fluctuations between individual magnetic bits. In order to address this challenge, a better understanding of reversal in magnetic media must be undertaken through thorough investigations of magnetization reversal. We have developed a measurement apparatus to achieve fast characterization of thin film magnetic media using the extraordinary hall effect to probe the magnetization of the magnetic media. This apparatus is a type of susceptometer because it relies upon a small coil surrounding the magnetic media to probe the differential hall response ΔVHall to a small alternating excitation field ΔB.

We have generated 2D and 3D designs as well as 3D, scaled plastic facsimiles for the purpose of prototyping and evaluating the design. The susceptometer produces an alternating magnetic field up to 3.9 mT peak amplitude. After the sample is placed inside of the coil within the device, the susceptometer is attached to a track which allows for angular control, translation in and out of a larger electromagnet, and fast replacement of test samples. A digital switching circuit allows for multiple electrical configurations, including extraordinary hall effect and in-plane resistance measurements. For NIST to maintain a standard for the magnetization in hard drives, the standard deviation of coercivity must be decreased while simultaneously maintaining the desired mean coercivity within a reasonable cost range. By making quick, easy and accurate measurements, this susceptometer will help industry achieve faster turnaround on materials design and continue progress toward higher density hard drive storage.

Development of Low-Cost Data Acquisition Devices for Extreme Hazard Applications

Conor McCoy

Researchers collect data using different sensors to better understand the physical world. Data acquisition devices are a critical part of research because they interface sensors with computers for further analysis and data storage. Commercial data acquisition devices can cost thousands to tens of thousands of dollars, making their use in extremely hazardous environments where there exists a high risk of damage to the device, prohibitively expensive. Therefore, the development of a low-cost data acquisition system is necessary to overcome this financial barrier to research. A data acquisition device was designed and developed specifically for use in high temperature fire environments with the presence of low, medium, and high voltage hazards and served to log temperature measurements over time using a thermocouple.

This project sought to determine the components necessary in designing a data acquisition system and identify potential hazards to its performance for future consideration. The design of the data acquisition system was inspired by the use of the Arduino microcontroller found in previous designs. Similar hardware was employed, but our design is a stand-alone system unlike its predecessors, to ensure that it does not interface with a computer until hazardous conditions are over. Programming was done in a simplified C/C++ language. The final design is to be tested and validated by recording elevated temperatures.

It has been shown that microcontrollers are a reliable, accessible, customizable, and affordable option in developing a data acquisition system. Future considerations for this particular design include the measurement and assessment of the effects of Electrical Magnetic Interference and methods such as filtering to mitigate these effects. Field testing of this device will take place later in the year and will help to determine future improvements to the design.

Unidirectional Ballistic Resistant Laminates

Rohan Mittal

In the summer of 2003, a police officer's polybenzobisoxazole (PBO) armor was penetrated by a round the armor should have been able to withstand. This was the first time a ballistic-resistant body armor failed in the 30 year history of the National Institute of Justice (NIJ) Body Armor Standard. NIST led an investigation into the failure of this vest, and it was determined that hydrolytic degradation played a role in its failure. As a result, an environmental conditioning protocol was instated in the NIJ Body Armor Standard in 2008 to better screen armor for susceptibility to degradation due to hydrolysis. NIST continues to evaluate the armor service life through its long-term stability of high strength fibers research program.

The objective of my work is to research and develop a method to study unidirectional ballistic-resistant fabric laminates. While there are many different types of body armor, my work focuses on unidirectional (UD) laminates made with aramid and ultra-high molecular weight polyethylene (UHMWPE). The UD laminates consist of four nonwoven layers of fibers that are oriented in a 0°/90°/0°/90° pattern, bound with a resin, and are covered by a low density thin film of polyethylene on both sides. The challenge was to separate the body armor into their individual constituents, which include the fibers, films and resin. Once they are separated, it is possible to characterize their chemical and physical properties using techniques such as FTIR, DSC, TGA and tensile testing.

Body armor is subjected to mechanical degradation such as folds or abrasion during use that can potentially alter the performance of the armor. To simulate these situations, a sheet of armor was folded and placed under pressure, and then a tear test was performed to investigate changes in performance. These results will be further discussed in my presentation.

The Impact of Human-Robot Collaboration
Tom Oeste

The movement of manufacturing to countries featuring labor with low hourly wages over the last fifteen years has motivated the development of a new generation of industrial robots that can work side-by-side with human workers. This has created the new technology of Human-Collaborative Robotics, which combines the intelligence and dexterity of humans with the strength, repeatability and endurance of industrial robots. Since most robots are powerful moving machines, the safety of workers working around these robots has become a top priority for safety standards development that will provide guidance for the development of a comprehensive risk assessment of the robot arm, its tools, its controller, and the whole operating workspace where humans might be present. We are using biosimulant materials for the construction of disposable Human-Collaborative Robotics safety testing artifacts. These testing artifacts will make possible the measurement of damage when humans and robots come into contact and the severity of injuries caused by robot static and impact pressure. In order to test and calibrate these artifacts we have constructed a Dynamic Impact Testing and Calibration Instrument (DITCI). The subject of this project is the measurement of damage caused by simulated impacts. We apply varied impact forces and pressures in order to explore the range and severity of these injuries, using different impact tips to simulate robots equipped with a range of common tools (i.e. screwdrivers or circuit probes). Our testing artifacts currently consist of cowhide leather and ballistic gelatin, to simulate the human abdomen, but future work will investigate bone biosimulant materials as well. We have been developing novel methods for characterizing injury using high-speed video, which is complimented by force and acceleration data collected by the DITCI system. We also hope to embed pressure sensors within the artifacts themselves, so that localized injury data can be obtained. This technology could enable more manufacturers to implement Human-Collaborative Robotics by offering a simple, standardized safety testing system which requires little expertise to operate. The DITCI system can also serve as a test bed for further safety research, as a variety of impact environments can be simulated.

Molecular Cloning and Characterization of Adenylyl Cyclase Class II Secreted from Pseudomonas Aeruginsona
Swasha Rachuri

Background: Adenylyl Cyclase (AC) is an enzyme with key roles in cellular regulation. All classes of AC catalyze the conversion of Adenosine Tri-Phosphate (ATP) to cyclic AMP (cAMP). Four major classes of AC exist in nature. Class I AC's are of enteric bacterial origin and are regulated by sugar transport proteins. They occur in bacteria such as E. Coli. Class II AC's are virulent factors secreted by pathogenic bacteria such as *Bacillus Anthracis* (BA) and *Bordetella Pertussis* (BP). This class of AC is activated within the host cell by host-calmodulin and produces supra physiological concentration of cAMP, leading to host cell death. Class III AC's are of eukaryotic origin with some bacterial specie exceptions and are prominently regulated by guanine nucleotide binding proteins. Class IV AC's are only present in addition to another class of AC. Such is the case of *Yersinia Pestis,* a plague-causing bacterium containing Class IV AC in addition to Class I AC. Class IV AC's produce cAMP constantly, under unregulated conditions. This class is the smallest of all the AC's with no known regulation method.

Proposed Research: The human pathogen *Pseudomonas Aeruginosa* (PA) is an opportunistic, nosocomial pathogen that infects those with weakened immune function. Genome sequence analysis of PA revealed three genes within the genome that code for the expression of AC Class I, II and III. In this study, we aim clone the gene for Class II AC from PA (PAACII), and then overproduce and purify the resulting protein. Then, we can understand how it is regulated.

Accomplished Research: In order to study the regulation system, I first cloned the gene being studied via PCR amplification. Analysis of the gene sequence for restriction recognition revealed the presence of internal NDE1 and BAMH1 sites. These unique cloning sites are present in most of the protein expression vectors such as pET15B. Cloning was a two-step process: first, I cloned a NDE1 to BAMH1 fragment and then I cloned the BAMH1 to BAMH1 fragment. I designed primers with appropriate restriction recognition sequences, NDE1 and BAMH1 for PCR amplification of two-thirds of the gene. The resulting PCR fragment was then cloned into the same sites present in pET15b, creating a unique BAMH1 site. The remaining one-third of the gene was amplified with primers having BAMH1 sites at both ends. This fragment was then cloned into the unique BAMH1 site present in the pET15b recombinant. However, this fragment has the potential to become ligated in the two possible orientations. To find the fragment in the correct orientation, we analyzed numerous final recombinants for an insert that was approximately 900 base pairs in size. Then, a final recombinant in the correct orientation was selected for DNA sequencing and protein expression. E. Coli BL21(DE3) cells were transformed with the recombinant and PAACII was overproduced by induction with IPTG (inducer). The overproduced protein contains amino terminal Histidine tags, coded by the vector sequence, allowed recognition of Nickel-affinity resin. Therefore, purification was achieved in a single step. Crystallization of the protein will be pursued next to study the molecule in detail.

Viewing Stem Cells in Three Dimensions on a Large Scale

Jacob Siegel

With the current capabilities of confocal laser scanning microscopes, a large number of 3D images can be acquired rapidly. Biologists have been leveraging these rapid microscopy imaging capabilities to study shape properties of stem cells placed on various scaffolds. While the large number of cells provides statistical significance to biological studies, there are missing tools to visually inspect a large number of cells simultaneously and collaboratively.

To address the gap in studying cell-scaffold interactions from a large number of 3D images, we have created a tool called the Mass Stem Cell 3D Web Viewer. The design of the viewer allows biologists to compare cell shapes in three dimensions at multiple resolutions, identify unique and discriminating shape characteristics for 10 scaffold types and about 100+ cells per scaffold, and share all acquired and processed cells among geographically distributed cell biologists.

Mass Stem Cell 3D Web Viewer is a client-server system that consists of a multi-resolution pyramid of cells on a server side from which data are retrieved and rendered on a client side in a web browser. The pyramid on a server side is built using Java and the ImageJ 3D library. The client side is written in HTML5/JavaScript and uses the XTK library for rendering 3D content. Due to the limited display screen size in pixels and the amount of RAM to load 3D images on a client side, a down-sampled version of each cell is retrieved from the pyramid. The pyramid level is determined based on the number of cells requested to be displayed on a screen and the available RAM. Using this approach, if the user only chooses to display one cell then a cell is displayed at full resolution otherwise a cell is shown at a lower resolution. Furthermore, the 3D volumetric multi-resolution representation of each cell is converted to a mesh representation consisting of vertices and faces which lowers the memory requirements as well. The current prototype has been deployed on one of the NIST internal servers and is being evaluated by biologists.

Enzymatic Biodegradation of Traditional and Novel Restorative Dental Resins
Christopher Wong

Polymer based composites have widely replaced mercury amalgam as dental restorations with decreased toxicity and increased aesthetics. However, esterase enzymes found in both saliva and cariogenic bacteria such as *Streptococcus mutans* have been found to cleave ester bonds found in the traditionally used bisphenolglycidyl dimethacrylate (bisGMA) and triethylene glycol dimethacrylate (TEGDMA) based resins, resulting in restoration degradation and failure in the long term. A novel dental monomer without ester bonds, triethylene glycol divinylbenzylether (TEGDVBE), has been synthesized in order to circumvent esterase degradation. Using model enzymes cholesterol esterase (CE) and pseudocholinesterase (PCE), as well as *S. mutans* cultures, this study aims to compare degradation of both monomeric and polymeric forms of the traditional and novel resins. High performance liquid chromatography is used to isolate and quantify degradation products after incubation with enzyme or bacteria. In addition, surface roughness of polymer pellets before and after degradation is characterized by atomic force microscopy. In the presence of CE, PCE, and *S. mutans*, the novel TEGDVBE is expected to release no degradation products and exhibit no increase in surface roughness compared to the control. The traditional resin is expected to degrade into methacrylic acid (MA), triethylene glycol (TEG), and 2,2-bis[4phenyl]propane (bisHPPP) and increase in surface roughness. If *S. mutans* is able to degrade TEGDVBE, future studies will need to be performed to isolate and identify non-esterase enzymes capable of involved in the degradation.

Seeing is Believing: Visual Data Analytics for Smart Manufacturing
Bowen Zhi

Visualizing data –transcribing data into graphical forms – is a useful tool for presenting, analyzing, and mining data. As old as the method is however, data visualization is often used poorly; visualizing a dataset effectively in an intuitive, meaningful, and aesthetically appealing way can be deceptively difficult. In recent years, the sheer amount of data collected has increased, and thus the difficulty of visualizing this data effectively has likewise increased.

In the manufacturing industry, improvements and optimizations to factory floor production systems require the analysis of large volumes of data with complex structure, which in turn require effective data visualization methods. These methods would need to handle various types of data: raw numeric sensor data from each factory machine (about power consumption, waste, humidity, temperature, noise levels, and so on), categorical and numeric data on the materials being imported to the factory, as well as more abstract data such as machine specifications, mathematical models, algorithm results, and business goals. In this project, we evaluate various data visualization techniques for their usefulness in visualizing this multidimensional, multilayered data, while also taking into account computation complexity and algorithm structure. We then formulate some specific data visualizations for potential use in data analytics for manufacturing, with the goal to then develop an interface to implement these visualizations.

University of Massachusetts Amherst

Towards Developing Composability in Modeling and Simulation of Additive Manufacturing Processes

Andrew Dodd

Additive Manufacturing (AM) is emerging as a viable solution for the creation of net shape, complex parts with a significantly shorter lead time. Cutting out the need for highly specialized manufacturing tools, dies, and molds, AM Computer Aided Design (CAD) tools allow us to easily make design changes in manufactured parts with little to no increase in cost or lead time. While AM processes are poised to revolutionize manufacturing in aerospace, medical, dental and many other industries, there is still much to be understood about the underlying physics involved in these processes.

The focus of this project was on the metal powder bed fusion process, specifically that of Selective Laser Melting (SLM). Despite the existence of many different models and simulations of the laser heating, melting and cooling process, none of them accurately simulate the SLM process in its entirety from powder material properties (as well as laser, scanning, and environmental control parameters) all the way to final material properties and deformations. That is not to say that many simulations are not coming close, but no model accurately represents every facet and physical phenomenon of the highly complex, heating, melting, and solidification processes. In order to address this issue and to develop more adaptable multiscale models, the research topic of composability has been proposed. To demonstrate that two or more models can be composable, or integratable and interchangeable, was the main goal of this research. This is being achieved by reviewing and analyzing currently available models of SLM and searching for links between their constraints, inputs, and outputs in the hope of identifying complementary models. Ideally, identifying areas of composability will lead to the development of more highly integrated, accurate, and reusable models.

University of Michigan Ann Arbor

Advancing Manufacturing Process Diagnostics and Prognostics by Leveraging Supply Chain Strategies

Gianluca Capraro

The global economy is dependent upon many key contributors: distributors, suppliers, manufacturers, and customers which facilitate the distribution, production, and purchasing of goods and services around the world. These interconnected entities make up the supply chain. The success of the supply chain depends on the efficiency, reliability, and productivity of its various components, one of which are manufacturers. If a manufacturing process declines or fails altogether, production is disrupted, distribution is disrupted, and the supply chain is also disrupted through the chain of events. Any form of disruption to supply chain operations can lead to devastating effects that are felt on a global scale. To maintain a successful supply chain, it is not only necessary to address supply chain logistics, but it is also critical to understand the manufacturing processes that are driving product generation.

The vast complexity of supply chains implies that they are subject to a multitude of risks, ranging from minimal to severe in impact and infrequent to common in occurrence. The presence of risk in supply chains necessitates strategies and methods to predict, mitigate, or respond to disruptions. These supply chain strategies have been heavily researched. However, less research has been performed on the subject of risk and disruption, prediction, prevention, and reaction within the manufacturing process domains. The similarities in goals, functions, and designs between supply chains and manufacturing processes suggest that strategies used in mitigating or responding to supply chain disruptions can yield promising results if applied to manufacturing processes. I present current supply chain mitigation and contingency strategies as well as the available diagnostic and prognostic techniques applied to manufacturing processes. A comparison between supply chain strategies and manufacturing diagnostic and prognostic techniques will be presented. I propose implementing successful and/or promising supply chain strategies to enhance manufacturing process diagnostics and prognostics and build more resilient processes. The proposals made in my research provide a new perspective on the subject of risk in manufacturing and manufacturing process diagnostics and prognostics.

The Effects of Shim Arm Depletion and Xenon Buildup on Estimated Critical Positions in NBSR for New- and Mid-Cycle Startups

Bryan Eyers

The NCNR laboratory at NIST hosts over 2500 guest researchers and scientists each year to utilize the NSBR reactor and attached facilities. Thus, small miscalculations of startup reactivity can result in significant financial and temporal costs to both NIST and its guests. The goal of this project was to develop a more reliable procedure that allows operators to quickly and accurately assess startup reactivity requirements over a wide range of core conditions through historical data analysis and by exploiting recently improved computer simulations of the NBSR.

In conventional nuclear reactors, reactor criticality is determined by the concentration of neutron emitters and neutron poisons in the core. In the NBSR, the primary neutron emitter is fission in the U-235 fuel, and its major poisons are four movable reactor shim arms and the in-core concentration of Xe-135, an isotope commonly produced by fission. Understanding the depletion or buildup rate of each factor is crucial – both in determining whether the reactor is capable of starting up, and when estimating the critical position of the shim arms required to do so. For example, as Xe-135 builds up after a reactor shutdown, it can prevent the restart of NBSR at any shim angle for 24-36 hrs until sufficiently removed by radioactive decay ($t_{1/2}$ ~ 9.1 h).

The reactivity depletion of the U-235 fuel was evaluated in a Monte Carlo neutron transport program called MCNP using depletion data provided by Brookhaven National Laboratory; a pattern was determined in the depletion rate of the shim arms by evaluating the most recent 15 years of operational logs; and the time-dependent Xe-135 concentration was solved analytically and verified by an iterative method. A procedure was developed to estimate critical shim positions based on the cycle number, unconventional fuel loading, the core inlet temperature, the position of the regulating rod, and the time since shutdown. It was verified using over 100 historical startups with an average shim position error of 0.44 degrees, and a standard deviation of 0.30 degrees, over a 41 degree range.

University of New Haven

Impact of Convective Heat on Firefighter Turnout Gear

Scott Wiercinski

In 2012 there were 31,490 reported firefighter injuries on the fire ground and 22 firefighters were killed during fire ground operations. Firefighter turnout gear (jacket and pants) are a main component to the firefighter's personal protective equipment (PPE). NFPA 1971, the standard on protective ensembles for structural firefighting and proximity firefighting, provides guidelines for testing how well the turnout gear will protect skin from second degree burns called the thermal protective performance test. The three layers of the turnout gear are placed above a radiant heat source and a convective flame; above the layers is a sensor that detects the temperature that the firefighter's skin would be feeling. The test gives a good scope on the convective heat transfer over time (through the turnout gear) and how it would affect a firefighter's skin in flashover conditions.

Firefighter turnout gear is comprised of three different layers: the outer shell, the moisture barrier and the thermal liner. The outer shell is designed as the first layer of defense and provides minimal amounts of the thermal protection. Along with thermal protection, the outer shell provides cut and abrasion resistance and minimal water repellency. The moisture barrier, located beneath the outer shell, provides resistance to water, chemicals and viral agents. This barrier is also the most delicate and prone to damage. The last layer is the thermal liner which is where the majority of thermal protection comes from within turnout gear. The thermal liner traps air between layers of nonwoven material that is attached to a face material. Air is an excellent insulator; however moisture and compression can greatly influence the effectiveness of the thermal layer. Moisture is an excellent conductor of heat and displaces the air, while compression eliminates air allowing an unimpeded conduction of heat through the turnout gear.

This project focused on the impact of convective heat transfer through turnout gear, using experimental data from fire experiments that resulted in an exhaust flow path exposure, to determine the impact on the firefighter's turnout gear. Both bench scale and full scale experiments examining the heating of the turnout gear were conducted. Also, firefighter line of duty deaths were examined and compared to the experimental data.

University of Oklahoma

A Comparative Assessment of the LPB Algorithm for Materials Science Keyword Extraction

Adam Dachowicz

Keyword extraction from large bodies of text is useful in the early stages of building databases and ontologies over the domain the text covers. Many methods for keyword extraction are built on natural language processing (NLP), which allows for programmer-aided computer extraction. In this project, the Limited Paradigmatic Variability (LPV) NLP keyword extraction method is evaluated to determine if it will be effective in generating preliminary keywords contained in a large materials science corpus. The terms extracted can then be vetted by domain experts during the early stages of ontology construction. The quality of the keyword extraction, then, is of particular interest. A superior method will produce more relevant keywords, making the job of field experts easier and improving the quality of the final ontology. The efficiency of the method is also important, since a more efficient method will reduce the time (and cost) of the preliminary steps in ontology construction.

For this project, we work with a corpus of several thousand materials science papers, containing about 20 million words, and aim to extract terms useful for an ontology relevant to the Materials Genome Initiative (MGI). In particular, we evaluate the LPV method by comparing results to the widely used term frequency-inverse document frequency (TF-IDF) method, taking "gold standard" terms produced by domain experts to be examples of "true" keywords. Other metrics like term length and total number of occurrences in the corpus are also considered with LPV and TF-IDF scores while performing classification with the Weka machine learning software to see if this improves correct keyword identification. This analysis is carried out on two separate document lists: the full corpus, and concordances built around different word stems.

Large-Eddy Simulation of Flow Over a Backward Facing Step

Benjamin Toms

Large-eddy simulation (LES) of turbulent flow over a backward facing step is studied using the Fire Dynamics Simulator (FDS). FDS is a NIST in-house Computational Fluid Dynamics (CFD) model that utilizes LES to model low-Mach number flows driven by combustion heat release and buoyancy forces. LES efficiently simulates turbulent flow by directly representing the large-scale turbulent motions, while modeling smaller scale motions with eddy viscosity models. Recently, FDS has been applied to urban canopy modeling and wind engineering. As such, it is important to study geometrically influenced flows, including the appropriate specification of boundary conditions and resultant downstream flow evolution.

For the present study, a set of cases is designed to test the influence of grid resolution, inlet turbulence, wall boundary treatments, and eddy viscosity models. The computational results are validated with experimental data. A grid resolution of $h/\delta x = 10$ adequately modeled the flow, although a doubling of resolution resulted in the realization of smaller scale kinematic features. The inlet turbulence conditions were determined to be the most significant contributor to downstream flow evolution. Reattachment length was found to be directly related to the magnitude of RMS velocity in injected turbulence. The choice of eddy viscosity model was found to have negligible influence, while the no-slip condition and an LES log-law-based wall function performed similarly for the given flow.

University of Pittsburgh

Application of Laser-Cooled Lithium Ion Source Focused Ion Beam Technology for Materials Analysis and Processing

Eric Marksz

Focused ion beams (FIBs) are widely used tools in many industries, due to their invaluable ability to mill away material, implant ions deep into a material, and provide imaging capability with different information compared to SEM and TEM images, all at high resolutions. NIST has developed a one-of-a-kind ion beam source, using lithium in place of the traditional gallium. Using lightweight Li^+ ions at energies of 1-4 kV reduces sputtering yield and penetration depth. I used this unique system to explore opportunities for a Li^+-FIB for analyzing and processing new materials, including materials for Li-S battery technology, MWCNT-epoxy composites, nitrogen-vacancy (NV) centers in diamond, as well as biological samples and graphene electrodes.

Sulfur-copolymer composites were made by NIST researchers for application as cathodes with improved cycle lifetime compared to current materials for Li-S batteries, considered a possible next step in battery technology for electric vehicles. The Li^+-FIB was used to controllably implant lithium into regions of this material as a method to better understand how lithium interacts and functions in the material during battery discharge.

The negatively charged NV^- center in diamond is highly regarded for its potential application in magnetometry sensing and quantum information processing, due to a long-lived ground-state coherence. Near-surface NV^- centers are needed to facilitate coupling and enhance sensitivity. The Li^+-FIB was used to induce lattice damage in diamond single crystals with [N] < 1 ppm, followed by a recrystallization heat treatment, promoting diffusion of vacancies and nitrogen impurities to form desirable NV^- centers. Due to the shallow implantation depth (<100 nm) of the lithium beam, these NV^- centers are believed to remain more near the surface than other treatments penetrating to depths of several microns.

The Li^+-FIB was also used to image MWCNT-epoxy composite materials, following timed exposures of these materials to UV lasers. UV light degrades the epoxy matrix, leaving behind a compact and highly conductive surface layer of MWCNTs. Surface wires with possible self-healing properties were created on the composites by patterning the UV laser exposures. The Li^+ FIB was used to clearly image the location of the MWCNTs within the composite, taking advantage of the high charging contrast available with an ion microscope.

<u>University of Puerto Rico</u>

Utilizing ANSI/ASHRAE Standard 37 for Volumetric Airflow Uncertainty

Nathaniel Barrios Fuentes

As part of promoting U.S. innovation and industrial competitiveness, the HVAC&R Equipment Performance Group has a project in which an advance in measurement science is made for the improvement on life quality. This is the Fault Detection and Diagnostic (FDD) for Air-Conditioning and Heat Pumps project. A project that consists of developing effective FDD algorithms by stating a standardized procedure for the classification on different commercial FDD products based on their capacities, so as to avoid the performance degradations and increased energy consumptions of the system. This talk will show a part of the FDD project, a Heat Pump Modified Airflow Measurement Apparatus constructed with the specifications of ANSI/ASHRAE Standard 37-2009.

As stated on the standard, the method is an option for obtaining airflow rate. The energy balance of the system, with the thermodynamic properties of this air that is passing right through this apparatus, will give the volumetric airflow. The commissioning process of the apparatus and the LabVIEW virtual instrument (VI) used for acquiring data will be shown. A VI monitors the temperature sensors (thermocouples), calculates and plots the temperature changes on the system, and produces data that are also used for the acquisition of volumetric airflow. This airflow is also plotted, analyzed, and used for the acquisition of uncertainty on the equipment. The uncertainty calculations will demonstrate the values to use as standards for devices that comply with this ANSI/ASHRAE Standard.

Real-Time Analysis of Route Origin Validation of Border Gateway Update Stream
Manuel Ortiz

The Border Gateway Protocol (BGP) is considered to be the glue that binds together the different networks within the Internet. This control protocol is responsible for exchanging the routing information between the BGP routers of different autonomous systems (AS's). It helps in determining how the Internet traffic should be routed. Based on information in BGP messages or updates, BGP routers construct routing tables that enable forwarding of the data packets from their origination point, through a sequence of AS's, and finally to the destination address.

The original design of BGP did not contain any security features, and hence BGP is vulnerable to address hijacking, eavesdropping and other attacks. NIST has been working with the Internet Engineering Task Force (IETF) to secure the BGP protocol using cryptographic methods. The Resource Public Key Infrastructure (RPKI) enables the creation of cryptographically signed objects called Route Origin Authorizations (ROAs). The ROAs can be used to validate route originations and prevent prefix hijacking. The next step that NIST and others are working on is the BGPSec protocol, which is an enhancement of BGP that would further add AS path validation to BGP.

I have developed a tool using Wireshark that enables visualization of the validation state of BGP updates. My tool specifically extracts the prefix and the origin AS pair information from updates, feeds the same to RIPE's online update validator and obtains a validation result. Using this tool, a network operator or researcher can identify and visualize in real-time any anomalies in BGP updates seen on the wire. Then the user can specifically investigate the underlying causes for those anomalies. I will be extending the tool to extract and display the BGP extended community information also which is used by BGPSec routers within an AS to convey validation results internally.

Testing an Electrical Power Frequency Disturbance Recorder (FDR) Device
Jennifer Sandoval Casas

Among the smart grid programs that since 2009 have been sponsored by the U.S. Department of Energy (DOE), different sectors of the electric utility industry have been installing Phasor Measurement Units (PMUs) and deploying technologies to modernize and monitor in a proper way the conditions along the electric grid. These PMU devices are placed at the transmission level and send data regarding the instantaneous voltage, current and frequency. Pursuing that same objective, a Frequency Monitoring Network (FNET) was deployed by the University of Tennessee by developing Frequency Disturbance Recorders (FDRs) and placing them at the distribution level of the power grid. The FDR works as a sensing device that monitors the real-time, GPS time-stamped, single-phase voltage phasor and the frequency out of a 120V electrical outlet. The FNET measures and checks the deviation of frequency from the nominal 60Hz value, which indicates the stability between the electric generation and the load, and sends data to FNET servers. This data is used by the North American Electric Reliability Corporation (NERC) for event analysis and predictions of the grid instability. The research project is focused on comparing the FDR's phasor information with the IEEE Std. C37.118.1-2011 (IEEE Standard for Synchrophasor Measurements for Power Systems). A series of tests in steady and dynamic state are made to the FDR, comparing the Total Vector Error (TVE) and the Frequency Error (FE) of the data streams from the device with the requirements of the standard. Such limits are that the TVE remains under 1% and the FE below 0.005Hz or 0.025Hz (depending on the test). The results will provide details on the accuracy of a sample FDR and on its correlation with the IEEE Std. C37.118.1-2011.

Fabrication and Electrical Characterization of Rubrene Single – Crystal
William Serrano-Garcia

Organic semiconductors are attractive for realizing flexible and novel electronic-based solutions to nontraditional, non-silicon centric problems. Electronic devices such as light emitting diodes (OLEDs), transistors (OTFTs), sensors and solar cells (OPVs) have all been demonstrated by using organic semiconductors, and OLEDs are already present in high volume commercial electronic applications like cell phones pointing to the tremendous commercial opportunities. OTFTs have yet to find similar wide adoption in existing technologies and fundamental physical understanding remains limited. Importantly, charge transport and trapping mechanisms differ in organic transistors as compared to inorganic transistors, and as a result commonly used analogies of organic semiconductors to inorganic band transport theory can break down. This is especially apparent in their response to small signal stimulus and at high frequencies required for some analog circuit applications. In this study, we perform detailed electrical characterization on organic field effect transistors (OFET) made using single crystal rubrene, a conjugated organic semiconducting material grown by physical vapor transport and laminated onto thermally oxidized silicon wafers. We study the AC behavior of single crystal organic transistors using impedance spectroscopy to investigate "ideal" electronic behavior in organic transistors. Impedance measurements permit us access to small signal, high frequency behavior and allow us more nuanced investigation of the small signal response trapped vs. mobile charge, and the determination of the low field mobility and threshold voltage. For some OFET test structures we modified the silicon dioxide gate insulator interface with a self-assembled monolayer, octadecyltrichlorosilane (OSTS), to the probe trapping at the insulator-rubrene interface where charge accumulation and transport occurs. Using a transmission line model to fit the AC impedance of the transistor channel coupled with a parallel resistor-capacitor model of the contact impedance, we gain insight into charge transport in the channel while discriminating the effects due to contact impedance. We compare mobility, threshold voltage, and characteristic transistor channel response determined by impedance measurements to values found through more widely employed DC characterization of transistors to verify the effectiveness of DC measurements to predict AC performance limits.

University of Rochester

Creating a Fast Piezo-Actuated Mirror for the Elimination of Fiber Noise
Ananya Sitaram

When a dilute gas of bosons is cooled to temperatures close to absolute zero, Bose-Einstein condensation and superfluidity occur. Our lab investigates superfluidity and the characteristics of toroidal Bose-Einstein condensates (BECs). The torioidal BECs are studied after first creating a current and then applying a “barrier” to a portion of the ring. The barrier is a focused laser beam and creates a repulsive potential. The goal is to create a small enough potential barrier (< 1 micron) so that tunneling behavior can occur in the BEC. In order to create a sufficiently small barrier, the diffraction limit of the optics being used to focus the laser must be overcome. One way to go about this is to use a different type of barrier that uses two laser beams instead of one. One problem that arises in this setup is that the detuning between the two beams of light must be precisely controlled.

To solve this issue, a closed feedback loop was designed and built using a proportional-integral-derivative (PID) circuit, which locks the frequency of one beam of light onto the set frequency of the other beam of light. This way, if the phase of one beam changes, the other varies directly with it, and the two beams of light will be phase locked. In addition to the feedback loop circuit, a piezo-electric mirror with a bandwidth of ~100 kHz was built. When installed in an interferometer, the piezo actuated mirror can be controlled by the feedback loop circuit to minutely adjust the path length and the phase of the beams of light.

University of South Carolina

An Analysis of the Effects of Simulation Parameters on CFD Aeordyamic Bluff Body Simulations Using Experimental Design Technique

Rachel Kuprenas

In the field of structural engineering, the only acceptable way of obtaining wind pressure data for structural design has been through wind tunnel testing. This is problematic in that full scale models can rarely be tested, running a simulation is expensive, and the results tend to vary as much as 50% between tests among several laboratories. Recently, computational fluid dynamics (CFD) simulations have been considered as an alternative. However, CFD simulations without a proper verification procedure can result in very poor wind effect data. Therefore, it is necessary to develop a systematic approach for reduction of numerical errors associated with simulation parameters while maintaining manageable computational resource requirement.

To address this issue, this study develops an approach for estimating the sensitivity of CFD aerodynamic bluff body simulations to the values of the simulation parameters. The approach is based on an experimental design technique by which the maximum amount of information on the relationship between input factors and output responses can be obtained from a specified, manageable number of simulations. A CFD program called OpenFOAM is employed to simulate flow around a square cylinder in two dimensions to reduce the total run time of the simulations in this study; however, additional 3-D simulations are required for adjusting parameters associated with the span wise direction and comparing with experimental test data the numerical results of characteristics of velocity around the cylinder and pressure on the cylinder surface. The use of this study can results in large reduction of computational resources required for a simulation with minimal loss of accuracy in the simulation results.

University of South Florida

Examination of a 3D Printed Biocompatible Polymer for Stents

Laura Byrnes-Blanco

Three-dimensional (3D) printers have become a key resource for biomedical and bioengineering fields because of their abilities to print complex geometries and use numerous printing styles and materials that range from metals to biologics. For example, 3D printers have allowed for the successful creation of custom, implantable devices and artificial tissues. Here we examined the topographical and nanomechanical properties of a biocompatible polymer that was created with fused deposition modeling. This polymer will be used to create stents: devices that can be temporarily or permanently implanted into a blood vessel or other bodily passage to help facilitate proper fluid flow. We imaged the surface structure of this polymer and determined if the Shear and Young's Moduli change significantly across the extruded beads and their fusion sites. This analysis will allow for the characterization of the effects the 3D printing process has on the polymer and its viability for stents and other uses.

All of the topographical and force spectroscopy data needed for analysis was collected by atomic force microscopy (AFM), which probes samples with micro-fabricated cantilevers. AFM data accuracy is directly related to the accuracy of the cantilevers' specified spring constants – which are typically defined with ±50% accuracy by manufacturers. To promote the most accurate measurements possible, a Laser Doppler Vibrometer was used to find all cantilever spring constants with approximately ±1% accuracy.

University of Texas Austin

Quasi-Elastic Neutron Scattering of Methanol Aggregates
Jeffrey Self

It is well known that liquid alcohols form supermolecular aggregates because of their hydrogen bonding tendency. However, the resultant structuring of even the simplest alcohol—methanol—is not yet fully understood. The associative properties of simple alcohols in the liquid states have been investigated mostly from the structural point of view using static neutron and x-ray scattering as well as computer simulations. We performed QuasiElastic Neutron Scattering (QENS) to observe experimentally the dynamics of these supermolecular formations over molecular length- and time-scales. The use of polarized neutrons and isotopic substitution allowed for the static and dynamical characterization of structures with a typical lengthscale of ≈5 Å. I will report results on the lifetime of these structures investigated as a function of temperature. A molecular dynamic simulation was also conducted and analyzed to gain a better understanding of the obtained data.

The Characterization of Relative Hydrogen-Bonding Strengths in AB Block Copolymer/C Homopolymer Blends
Ying-Heng Tein

Directed self-assembly (DSA) of block copolymers has been extensively studied as an advanced patterning method for electronic devices. A key challenge remaining before DSA can be implemented is reducing the patterning pitch length, while also decreasing the line-edge roughness (LER). One approach to forming smaller features and decreasing LER is to use pre-existing materials to produce an AB block copolymer/C homopolymer blend that has selective hydrogen-bonding interactions. The objective of this project is to quantitatively characterize the relative hydrogen-bonding strengths of polymer blends via fourier transform infrared spectroscopy (FTIR) and to find the Flory-Huggins interaction parameter (χ), of an AB block copolymer/C homopolymer blend via small-angle neutron scattering (SANS).

Various compositions of polystyrene-*block*-poly(methyl methacrylate) (PS-*b*-PMMA) with poly(4-vinylphenol) (PVPh) were quantitatively characterized by relative hydrogen-bonding strengths. PS-*b*-PMMA is a widely accessible block copolymer that has a weak segregation strength; however, by adding PVPh in the blend, the PMMA block can selectively associate with PVPh via hydrogen bonding. Based on previous studies of different polymer blends, it's hypothesized that through the selective association of a low molecular weight homopolymer with one block of the block copolymer, the addition of the homopolymer can order a disordered block copolymer to form smaller pitches in DSA.

Using FTIR, the relative hydrogen-bonding strengths are studied as a function of temperature and are quantitatively characterized by finding the fraction of hydrogen-bonded carbonyls in the polymer blend. The same samples were examined with SANS to calculate the χ parameter for a given blend composition. The correlation between fraction of hydrogen bonds and change in the interaction parameter will be examined.

University of Texas Dallas

Developing a Domain Specific Model Library and Supporting Tools for Manufacturing Modeling and Optimization

Ryan Miller

There are many existing applications available for analyzing manufacturing processes. However, the learning curves for most of these applications are steep and require extensive programing and/or mathematical knowledge. Process engineers are currently missing an intuitive and easy method to model, simulate, and optimize their manufacturing problems. With a manufacturing domain model library, a domain user such as a process engineer could model manufacturing processes using a Modelica Graphical User Interface (GUI). These modeled processes can be simulated to perform what-if analysis for decision support. The same manufacturing process models can also be optimized with regard to specific parameters and metrics. For this purpose, the Modelica models will be translated to the Sustainable Process Analytics Formalism (SPAF) models, an application-independent format, which can then be compiled to a standard optimization model and executed using optimization solvers such as CPLEX to derive optimal results. These results will be provided to the users through the Modelica GUI as actionable recommendations.

In this project, an extendable manufacturing domain model library is created using the Modelica modeling language and environment. Reusable manufacturing models and components are developed. More model components can be added as needed. A translator is developed using Java to translate Modelica models to SPAF models and instantiate optimal results through the Modelica GUI.

The Authentication Equation: Visualizing the Convergence of Security and Usability of System-Generated Passwords

Cathryn Ploehn

Password management is the ubiquitous struggle of the modern human. However, despite usability factors playing a vital role in authentication, password policies and requirements focus solely on the security without regard to human components. In fact, password policies and usability needs are often in contention.

Until an improved authentication method beyond character input is developed and implemented on a large scale, developing methodologies for comprehending and balancing these competing requirements is vital. These methodologies are critical in informing new requirements, increasing overall cybersecurity of the large enterprises that implement them. The development of these methodologies will improve the ability of NIST to inform how to improve the government's overall cybersecurity posture. In particular, a visualization tool will aid in pragmatically exploring of the convergence of security and usability in password components.

This research project culminated in building such a data visualization tool to explore different password usability and security metrics. The visualization tool integrates various metrics (such as entropy or predicted difficulty), enabling the exploration of the intersection of usability and security in password generation. The tool integrates findings from previous NIST password usability studies and leverages web technologies in order to flexibly display datasets automatically generated from sets of passwords.

High-level and low-level trends in password datasets of varying sizes can be explored dynamically. The tool provides three levels of granularity to view password metrics. The data can be filtered and sorted by various password characteristics including: length, number of keystrokes required based on device (traditional desktop computer, iOS, and Android mobile devices), linguistic and phonological difficulty, entropy, and other factors. The tool is designed in a way to provide flexible analysis of data, providing groundwork to more thoroughly study the interaction of security and usability in the generation and management of passwords.

University of Virginia

Understanding the Additive Manufacturing Digital Thread
David Chu

Additive manufacturing (AM), the process of building objects layer by layer, has grown increasingly popular as it provides a more efficient alternative for producing complex parts than conventional processes. There are several different AM processes that are currently in use, including direct metal laser sintering (DMLS) and fused deposition modeling (FDM). Each process involves many different factors (e.g. the type of material that is used and machine control parameters) that interact with each other and give rise to variability in AM processes. This variability makes it difficult to achieve traceability and repeatability in part production.

To control variability, it is necessary to understand the flow and management of information, referred to as the "digital thread," within an AM process. With this concept in mind, the objective of this project was to identify the key information used in part development by different AM processes, specifically DMLS and FDM. Understanding the critical parameters associated with each process will lead to more efficient information management, facilitating traceability and therefore helping to control variability in AM processes. Industry and lab visits were used to gather information about the steps of each AM process and the important parameters involved in each step.

The results of this project will help manufacturers to more efficiently manage AM process information. The insight gained will enable them to reproduce parts more accurately, make more informed process selections, and improve their manufacturing processes.

Critical Geometries in Additive Manufacturing
Kevin Zeng

Imagine the day when you can fabricate an engine block or wing from metal powder in your own garage using additive manufacturing. Currently, additive manufacturing is making strides to become widespread and standardized. One of the roadblocks that is hindering the standardization of additive manufacturing is that the realization of critical geometries such as internal features and lattices through additive manufacturing has yet to be completely understood.

The objective of this project is to design and build a test artifact containing internal features and structures that cannot be measured with post process external techniques (e.g., by coordinate measuring machine). A test artifact, named the Modular Artifact for Measuring Internal Features

(MAMIF), was prototyped on the Makerbot Replicator and Objet stereolithography 3D printer, and produced on the EOSINT M270 Direct Metal Laser Sintering (DMLS) machine. Non-destructive techniques such as ultrasonic testing were utilized to measure and characterize the dimensional accuracy in building such features. The results of this project will be used to develop methods using NDE (non-destructive examination) techniques to qualify and measure these critical geometries in metal-based additive manufacturing.

University of Washington

Exploring the Structure of Surfactants with Rheo-SANS in Two Dimensions

Aaron West

Micellar phases created by surfactant self-assembly have been studied for their breadth uses in scientific research and industrial applications. The wide use of these micellar formations motivates the study of the structural evolution in dynamical systems present in industrial processes. Undulation stabilized lamellar phases have been predicted to collapse at high shear rates due to loss of pressure between bilayers. Small angle neutron scattering data has been collected at various shear rates and viscosities, showing evidence of a transition to this collapsed structure and a previously unknown metastable structure. In order to properly characterize this structure and understand the mechanism of formation, new analysis using recent advances in 2-dimensional data fitting procedures is required. Through visual observation of the 2D data, a series of scattering models will be applied to 1-dimensional cuts of the 2D data to find the best possible descriptions of different aspects of the scattering profile, which can then be used as starting values for 2D fitting. The complex mixed systems present in this structural evolution process will be the major focus of this work.

Utah State University

Two-Dimensional Electron Gases at the Surface of Potassium Tantalate

Benjamin Pound

Transistors are the work horse of modern electronics, and as such the electronics industry is being driven to make transistors smaller, faster, more durable, and more efficient to meet ever-increasing computational demands. The three main parts of a transistor are the source, drain, and gate. When a voltage is applied to the gate of a field effect transistor (FET), a thin layer of semiconductor material beneath the gate becomes electrically conductive and allows current to pass between the source and drain. The usefulness of FETs in electronics comes from their ability to be “turned on” or “turned off” by changing the gate voltage.

Because of limits inherent to traditional transistor design and materials, however, innovations in transistor technology will soon not be sufficient to satisfy society’s computational needs. Recently it was found that many members of a versatile class of materials – perovskites – also support thin conducting channels, called two-dimensional electron gases (2DEGs).

Several key advancements in this field include the ability to engineer high precision, high mobility interfaces of perovskites on silicon – a necessary step for integration with current technologies - and the fabrication of a single transistor with a 1.5 nanometer feature size. This feature size is far smaller than current industry standards, highlighting the potential of the perovskite class of materials in future transistor technology. In addition, there is a hope that the diverse physical properties of perovskites -

including magnetism, piezoelectricity, and superconductivity – can be accessed in novel electronic devices.

This research focuses on understanding the 2DEG found at gated surfaces of the perovskite potassium tantalate ($KTaO_3$). We have developed a simplified portable model for the electronic structure of this 2DEG that takes its input from bulk experimental information. This model will be described with particular emphasis on differences between the 2DEG in $KTaO_3$ and conventional technologies.

Vanderbilt University

Automating the Culture of Microbial Biofilms
Megan Madonna

The introduction of automation in biological protocols can increase experimental throughput, decrease user errors, and potentially improve experimental reproducibility. One application for such automation is the culture of bacterial biofilms. Bacterial biofilms are complex, micro-ecosystems that form spontaneously on surfaces throughout nature. In particular, biofilms representative of the oral environment (e.g. dental plaque) are useful for studying therapies important in human health and disease.

In the current work we validated automated liquid handling operations for the generation and analysis of cultures of *Streptococus mutans*, a common oral microbe. Both 96-channel and 8-channel parallel pipetting steps were validated using a BioMek FX automated liquid handler. Automated fluid manipulation was highly reproducible and allowed the routine generation of *S. mutans* cultures 10-25 times faster than manual preparations. Toxicity assays performed on the microbial cultures to study mouthwash ingredients showcased the utility of automated procedures to accelerated routine analysis. The high-throughput of automation enabled rapid evaluation of a variety of assay parameters and culture conditions. Overall, automated liquid handling accelerated research investigations using microbial biofilms.

Virginia Polytechnic Institute and State University

Standard Testing Method for Density of Hydraulic Cement
Michelle Helsel

The density of hydraulic cement is critical in calculating the fineness of cement powder and has an essential role in the determination of concrete mixture proportions. Consequently, density has the ability to affect strength, hydration, and permeability of concrete. The current standard by ASTM is the "Test Method for Density of Hydraulic Cements" (ASTM C188), which utilizes a liquid displacement method to measure the volume of the powder cement. The experiment originated in 1944, and both the materials and procedure have undergone little change over the past seventy years. Impositions associated with the current standard have forced the construction industry to cease routine density testing, causing problems with cement volume ratios. Therefore, the industry requires a readily available method to promote frequent density testing and diminish concrete failures.

As the industry seeks new practical methods for testing density of hydraulic cement, other approaches are being explored. The present research will examine the apparent interest of potential alcohol substitutions into the standard procedure. In addition, recent computer technology embraces gas-comparison pycnometry as a possible alternative to the current standard method. The described methods will be compared to determine the most consistently accurate method for which to test density of hydraulic cements.

Reproduction and Characterization of Commercial Cu-Ni-Zn Alloys
David Lichtman

The alloys in the copper-nickel-zinc ternary system can be used in musical instruments, keys, marine equipment, and other applications. Materials design techniques can be used to create alloy compositions and heat treatment processes that use a percentage of zinc while retaining the properties of more expensive Cu-Ni binary alloys, thereby greatly reducing production costs. An important step in the alloy development process is understanding the relationships between thermo-mechanical processing techniques and the physical properties of the designed alloys. Analogs based on the compositions of commercial ternary alloys were cast and different thermo-mechanical processing techniques were applied. Some of these techniques included cold rolling, warm rolling, annealing, oil quenching, water quenching, and furnace cooling. The order in which the processing steps were applied can also be a variable. Samples were characterized through energy dispersive x-ray spectroscopy (EDS), Vickers micro-hardness testing, optical metallography, and conductivity testing. Characterization data were incorporated into predictive models to determine the next step in the alloy development process. The results from the characterization as they relate to the design process and the development of thermo-mechanical processing techniques will be presented and discussed.

RM for Strain Measurements in SEM
Chris Reynolds

High resolution electron back-scatter diffraction (HR-EBSD) is an evolving technique for measuring lattice strains and rotations in crystalline materials in the Scanning Electron Microscope (SEM). There is not currently a strain measurement standard that can be used to verify the accuracy of experimental setup or analysis method. As a result the need for a reference material (RM) with known strain was established to improve the accuracy of strain measurements. One application for this RM is band gap engineering in the microelectronics industry. SiGe and Si are common semiconducting materials which are being investigated for reference material development. Thin films of SiGe were deposited epitaxially onto Si wafers by commercial vendors. In order to be suitable for EBSD analysis, structures were etched into the SiGe films using the NIST nanofabrication facility. A parametric study of strain measurements using the HR-EBSD technique was performed for evaluation of strain measurements on the SiGe structures. Because Si and Ge have a difference in crystal lattice size, strain is measured using the shifts of the EBSD patterns. These shifts are used to measure strain in the CrossCourt 3 strain measurement software by cross-correlating the Si and SiGe EBSD patterns. This experiment investigated the effects of SEM parameters on the calculated strain. Consistency of calculated strain should be observed in similar features of the samples at different working distances and various EBSD pattern processing parameters. However this was not always the case and this presentation will provide some insight for why different values and trends were observed in this experiment. Results will contribute to a RM standard for industry to select the proper parameters to calibrate EBSD equipment.

Wake Forest University

Residual Additive in Organic Photovoltaics
Derek Fogel

We report on the effects of residual 1,8-diiodooctane (DIO) on the electrical performance of poly(3-hexylthiophene-2,5-diyl) (P3HT): phenyl-C71-butyric acid methyl ester (PC[71]BM) bulk heterojunction (BHJ) photovoltaic cells. DIO is widely used throughout the field of organic photovoltaics as a processing additive which is theorized to increase the efficiency of cells by controlling the morphology of the active layer, but little is known about the effects or quantity of DIO which remains after fabrication. We performed detailed analysis of the electrical properties for device test structures with DIO additive and dried for different times. Our devices were fabricated by spinning a 30 mg/ml solution of 5:4 P3HT:PC[71]BM in 1,2-dichlorobenzene with 2% DIO by volume over a layer of PEDOT:PSS on a glass substrate with pre-patterned ITO contacts. The PEDOT:PSS layer was spun in a chemical hood at room temperature, and dried under Ar ambient at 140°C for 10 min. The active layer was spun and dried for 5 minutes at room temperature under an Ar ambient and then baked for different times at 60°C under an Ar ambient. To complete the electronic test structures, we deposited Ca/AL contacts in high vacuum (10^{-7} mbar) with a total time in vacuum of approximately 45 minutes. We optimized this procedure for efficiency at an active layer thickness of approximately 220 nm, and all devices were processed nearly in parallel to minimize unintentional variations between test structures. We then measured the current-voltage (J-V) characteristics under one sun equivalent illumination intensity. We found that the efficiency, fill factor, and short circuit current of the cells increased with drying time and plateaued at 20 minutes. This suggests that there is some residual DIO in the film, which evaporates slowly but is nearly absent after 20 minutes. We are awaiting Fourier Transform Infrared Spectroscopy results to confirm and quantify the presence of the residual additive. We also found a similar trend in 15 mg/ml cells with 2% DIO which were optimized for fill factor. We then used impedance spectroscopy data to determine the underlying mechanism through which the residual additive decreases efficiency, fill factor, and short circuit current. The impedance spectroscopy data allowed us to extrapolate the number of deep level traps in the film from the recombination rate and carrier density vs voltage, and we found that there is no correlation between drying time and number of deep level traps, which indicates that the residual DIO is not introducing these deep traps into our films. We also examined plots of conductance vs frequency and found that the cells with the most additive showed hallmarks of ionic transport, which may explain the decrease in efficiency. Further analysis on the impedance data will lead to a more definitive determination of the dominant mechanism for the relationship between residual additive and decreased efficiency, fill factor, and short circuit current.

West Virginia Wesleyan College

CT Imaging of the Lungs and Investigation of Dual Energy CT
Lauren Cronise

Computed tomography (CT) machines are widely used in clinical settings to diagnose and plan treatment for medical issues, and accurate methods for analyzing the images are crucial for proper diagnosis. Lung tissue remains a difficult tissue for standardization due to lung's changing density, and the CT scanner variations have created a significant barrier for assessing disease progression in a clinical setting. Therefore, having an accurate standard TEM (tissue equivalent material) is essential. To test NIST's new lung reference standard, SRM 2088 (Levine and Chen-Mayer, 2013), we ran CT scans of the material in a anthropomorphic phantom, 3D printed from the Walter Reed Army Medical Center, to measure the alteration of HU (Hounsfield Unit) in a phantom that simulates scattering compared to the values measured in air. This phantom was created from a process that involves creating a density mask from reconstructed CT images in software similar to SCAN IP (Simpleware), which segments the material in each mask relative to the Hounsfield Unit range desired to simulate bone and various tissues. This data can be used by radiologists and researchers to better calibrate their machines and improve diagnosis accuracy in areas such as emphysema and lung cancer. Such an effort requires quantification of the scanner spectral dependence of the Hounsfield Unit. We are investigating the dual energy CT (DECT) approach in the post reconstruction imaging space, by first calibrating the NIST scanner (Philips Brilliance 16) using materials of known composition, by implementing a method published by Yohannes *et al* (2011, 2012). Once the energy dependent parameters are determined experimentally for each spectrum, DECT may be employed to solve the unknown materials by the decomposition method. Materials that have different elemental compositions or mass densities can have the same photon attenuation; we can recover the underlying information about the material through a different energy scan (Hünemohr *et all 2014*). We are working on this by back calculating a known material in a scan to test the accuracy of reconstruction with data from DECT.

Yale University

Measuring the Concentration of Specific Metallic Ions in Solution Through Induced Nanoparticle Aggregation

Tanya Shi

The detection of biological and chemical agents plays a fundamental role in a vast variety of scientific fields. Engineered gold nanoparticles (AuNPs) are emerging as a powerful tool for the measurement of these small molecules, particularly in environmental and biological systems. They possess unique physical and chemical properties, such as tunability, biocompatibility with many ligands, and a high surface-to-volume ratio, which make them excellent platforms for the fabrication of chemical and biological sensors. In addition, functionalized AuNPs can be made to aggregate in the presence of certain reagents and a specific metallic ion in solution.

The goal of this project was to selectively quantify iron (III) ions in solution by measuring induced gold nanoparticle aggregation. In order to do so, the gold nanoparticles had to first be functionalized, meaning the surface chemistry altered, in such a way that the iron ions would cross link the functional groups on the particle surface and result in aggregation. In this project, dopamine was used as the complexing agent for ferric ions. Several physicochemical reaction schemes were designed and tested with the goal of creating bonds between iron (III) and the AuNPs, but also of preventing aggregation prior to the introduction of ferric ions.

In addition to using ultraviolet-visible (UV-vis) spectroscopy and dynamic light scattering (DLS) to characterize the AuNP samples, a new technique called single particle inductively coupled plasma mass spectrometry (spICP-MS) was employed to measure the size distribution of AuNPs and quantitate the degree of aggregation. Operating in single particle mode and utilizing a high-temperature plasma discharge to ionize the sample, the ICP-MS was used to determine the number concentration and particle size of dilute nanoparticle suspensions. The project also explored the effect of varying the ligand coating thickness, gold concentration, dopamine loading, and buffer composition (pH) on the detection of ferric ions. In the future, the goal is to use this method to enable selective and sensitive measurements of metallic ions in environmental samples.

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2014

SURF STUDENTS BY

ACADEMIC INSTITUTION

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UNIVERSITY	STUDENT	TITLE OF TALK	OU
Alabama State University	Duncan, Shayla	Development of a Standard Toxicity Assay for Nanomaterials Using *Caenorhabditis elegans*	MML/NCNR ChemBio
Alabama State University	Stewart, Shakeria	Assessing Antibacterial Properties of Novel Dental Resins Containing Titanium Nanoparticles	MML/NCNR MatSci
Alfred University	Kutzik, Daniel	A Molecular Dynamics (MD) Study of Surfactant Self-Assembly on Single-Walled Carbon Nanotubes (SWCNTs)	MML/NCNR MatSci
American University	Hirtenstein, Jessie	Convergence of Magnus Integral Addition Theorems for Confluent Hypergeometric Functions in Terms of Bessel and Parabolic Cylinder Functions	ITL
American University	Verdi, Mark	Calculating Electrostatic Properties Using Lévy Flights	MML/NCNR MatSci
Appalachian State University	Zimmerman, Kayla	Electrical Measurements of Molecular Layers by Eutectic Gallium-Indium	PML/ElecEng
Arizona State University	Carpenter III, Joe	Process Optimization of Polymer Solar Cells	MML/NCNR MatSci
Arizona State University	Ward, Jacob	Analysis of Fe V and Ni V Wavelength Standards in the Vacuum Ultraviolet	PML/Physics
Augsburg College	Bier, Elianna	Automated Live Cell Imaging of Stem Cells Expressing Green Fluorescent Protein	MML/NCNR ChemBio
Bates College	Briggs, Andrew	Raman and Infrared Studies of Few Layered $TaSe_2$	PML/ElecEng
Boise State University	Adams, Andrew	Resilience: Planning for the Future	EL
Boise State University	Nelson, Eric	Modeling Materials for a Better Tomorrow: Computational Studies of Carbon Capture Materials MIL-53 and BPene	MML/NCNR MatSci
Boise State University	Papac, Meagan	Multi-Scale Characterization of Selective Sorbent Materials Through X-Ray Scattering Techniques	MML/NCNR MatSci
Boise State University	Talley, Kevin	Optimization and Characterization of Perovskite Oxides as Potential Thermoelectric Materials	MML/NCNR MatSci
Bowie State University	Horbrook, Skye	Real-Time Access Control Rule Fault Detection Using a Simulated Logic Circuit	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Bowie State University	Sabbagh, Paul	CPCC: A Cyber Physical Cloud Computing Testbed	ITL
Brown University	Oh, Sung-Ho	Maximizing the Spread of Information in Communication Networks	ITL
Bryn Mawr College	Jaber, Noura	Exploring the Electrical Properties of Carbon Nanotube Materials with Raman Spectroscopy	PML/Physics
Carnegie Mellon University	Addiego, Christopher	Simulation of an Ion Beamline for Isotopically Enriched Silicon Deposition	PML/Physics
Case Western Reserve University	Wade, Matthew	Calculation Hansen Solubility Parameters for Organic Solar Cells by the Cohesive Energy Density Method	MML/NCNR MatSci
Case Western Reserve University	Zehnder, Calvin	Dynamic Properties of Metals Used in Additive Manufacturing	EL
City University of New York	Bouizy, Zineb	Designing Buildings for Wind Load	EL
City University of New York	Bravo Parraga, Karla	Electronic Test Equipment Interface with LabVIEW for Charge Based Capacitance	PML/ElecEng
City University of New York	Chen, Jing	Development of an Efficient, Fiber-Coupled Quantum Dot Single Photon Source	CNST
City University of New York	Fallon, James	Automating the Calibration of DMM Calibrators and Navigation Systems	PML/ElecEng
City University of New York	Ghouchani, Behnaz	Developing New and More Efficient Ways to Solve the Time-Dependent Schrödinger Equation (TDSE)	ITL
City University of New York	Ghouchani, Golnaz	Data Mining Application in Web Services	EL
City University of New York	Gueye, Mohamed	Leveraging Web Development Infrastructure for 2D and 3D Visualizations	ITL
Clemson University	Hernandez Sanchez, Jorge	Could Fish Help Treat Cancer?	MML/NCNR MatSci
College of New Jersey	Lessoff, Daniel	Improvements in E-Mail Security: A DANE/Open PGP Test System	ITL
College of William and Mary	Dermer, Sonia	3-Dimensional Structures for the NIST Chemistry WebBook: My Journey from Molecular Optimization to Self-Optimization	MML/NCNR ChemBio
College of William and Mary	Guidry, Melissa	Characterizing the First All-Biological Single Photon Source	PML/Physics

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Colorado School of Mines	Connor, Spencer	Developing a System for Monitoring NCNR Fume Hood Radiation Levels	MML/NCNR MatSci
Colorado School of Mines	Cummings, Austin	Microscene Grave Detection via Hyperspectral Imaging	PML/Physics
Colorado School of Mines	Hillberry, Logan	Spectral Unifority: The HIP Way	PML/Physics
Colorado School of Mines	Taylor, Timothy	Interfacing a Charge Based Capacitance Measurement Device with Atomic Force Microscopy	PML/ElecEng
Cornell University	McGrattan, Susan	Water Consumption in Manufacturing Processes	EL
Denison University	Dungan, Kristina	Ultra High Speed Electronics for Single-Photon Detection in Quantum Key Distribution	PML/Physics
Eastern Kentucky University	Leger, Shane	The Application of Barrier Fabrics to Prevent Smoldering in Upholstered Furniture	EL
El Camino Community College	Cisneros, Freddy	Evaluation of a New Dosimeter for Industrial Radiation Processing	PML/Physics
Elizabeth City State University	Agyapong, Ama	Measuring Three-Dimensional Angle of Through-Silicon via Using TSOM Method	PML/Physics
Fayetteville State University	Clayton, Sabrena	Evaluating Nanofilm Coatings to Prevent Flammability in Household Furniture	EL
Fayetteville State University	Thrift, Blake	Examining Electrical Cable Degradation in Nuclear Power Plants	EL
Florida A&M University	Hull, Alexander	Reactor Data at Your Desk V2.0	MML/NCNR MatSci
Florida Institute of Technology	Dominguez, Alejandra	Data Preprocessing and Characterization for Manufacturing Power Data	EL
Florida Institute of Technology	Senatore, Jordan	The Use of Discrete Event Simulation for Assuring the Performance of a Manufacturing System	EL
Geneva College	Newman, Bonnie	Extensional Flow-SANS of Worklike Micelles	MML/NCNR MatSci
Hamilton College	Baer, Joelle	See You on the Flipped Side: The Construction and Optimization of RF Coils Used to Flip ^{3}He Polarization	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Harvey Mudd College	Scheffler, Sarah	Proposals for NIST Standards on Generation of Random Primes for Cryptography	ITL
Hood College	Hirani, Tarang	BIRDS Residential: Measuring Sustainability	EL
Hood College	Staples III, Robert	Massive Virtualization and Its Effects on Software Entropy Sources	ITL
Jackson State University	Olutade, Ayotunde	Exploration of NIST Mass Spectroscopy Data with D3	ITL
James Madison University	Heindel, Andrew	Computational Methods to Analyze Small Angle Scattering Data of Biological Molecules & Free Energy Calculations to Validate Structural Ensembles	MML/NCNR MatSci
James Madison University	Leaman, Eric	Gravimetry for the NIST-4 Watt Balance	PML/ElecEng
James Madison University	Oehler, Matthew	Rhodopsin/G-Protein Solution Studies via Nanodisc Lipid Bilayer	MML/NCNR MatSci
Juniata College	Debrecht, Alexander	Describing the Quantum Character of Metallic Nanoparticle Plasmons	PML/Physics
Juniata College	Turmanian, Teresa	Magnetic Ground State of Industrial Sensors	MML/NCNR MatSci
Lehigh University	Stritch, Kyle	FORC Measurements Using the Anomalous Hall Effect: A FeCuPt$L1_0$ Case Study	MML/NCNR MatSci
Louisiana State University and A&M College	Lepkowski, Daniel	Measurement of the Magnetocaloric Effect in Ni-Mn-Al Type Alloys	MML/NCNR MatSci
Marquette University	Le, Hoan	The Role of Size and Crystallinity on Magnetic Nanoparticle Response	MML/NCNR MatSci
Mary Baldwin College	Rister, Alana	Printing Drugs on Edible Substrates	MML/NCNR ChemBio
Massachusetts Institute of Technology	Bobbio, Lourdes	Metrology and Optimization of Additive Manufacturing and 3D Printing	MML/NCNR ChemBio
McLennan Community College	Trujillo, Jr., Victor	Virtual Fusion: Human Presence in Manufacturing Simulation	EL
Miami University of Ohio	Clements, Ethan	Feedback Controlled Magnetic Field Zeroing for Rare Earth Quantum Memory	PML/Physics
Middle Tennessee State University	Morgan, Brooke	MIX 13: A NIST Interlaboratory Study on the Present State of DNA Mixture Interpretation	MML/NCNR ChemBio

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Millersville University of Pennsylvania	McAndrews, Jared	Evaluation of Development Technologies and Usability Design for Cross-Platform/Cross-Device Biometric Applications	ITL
Monmouth University	Famularo, Nicole	pH Dependence of Colloid Surface Interactions in Charged Depletion Systems	MML/NCNR MatSci
Montgomery College	Degraft-Amanfu, Samuel	Characterizing Transport Properties in Bilayer Membranes for Next-Generation Desalination Technology	MML/NCNR MatSci
Montgomery College	Horn, Jarod	Evaluation CO_2 Sorption Properties of Molecular Sieves with Distinct Pore Sizes and Extra-Framework Cations	MML/NCNR MatSci
Montgomery College	Le, My Duyen	Investigating the Influence of Temperature and Acid Matrix on the Determination of Arsenic in the Arsenic Speciation Reference Standards	MML/NCNR ChemBio
Montgomery College	Ngo, Dennis	Identifying the Sources of Error in Atmospheric Transport Gases	EL
Montgomery College	Shetty, Martin	Data Acquisition and Reduction Software for Multi-Detector Prompt Gamma Neutron Activation Analysis System at NCNR	MML/NCNR ChemBio
Morehouse College	Scott II, Paul	Fun in the Sun: Characterization and Analysis of Photodegraded Polyethylene	EL
Mount Saint Mary's University	Lesniewski, Joseph	Interactive Data Analysis of Neutron Scattering Data	MML/NCNR MatSci
North Carolina State University	Lineberry, Jacob	Simulation of Cosmic and Background Radiation Through Detector Shielding	PML/Physics
Oberlin College	Fein, Mira	Creating a Color Preference Index	PML/Physics
Otterbein University	Gnewuch, Stephanie	Neutron Powder Diffraction Experiments of Nitrogen and Oxygen Adsorption in Metal-Organic Frameworks to Estimate Adsorption Selectivity for Gas Separations	MML/NCNR MatSci
Pennsylvania State University	Brockett, Nathan	Looking Inside the Process of Additive Manufacturing with Ultrasonics	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Pennsylvania State University York	Shaikh, Komal	Stress Development in Flowable Dental Resins Using a Cantilever Beam-Based Device	MML/NCNR MatSci
Purdue University	Epling, John	Mechanical Properties Characterization of Uniaxially Aligned Cellulose Nano-Crystal Films Utilizing Buckling Stabilities	MML/NCNR MatSci
Radford University	Ashley, Joseph	Modeling Grain Boundaries in Thin Film Photovoltaics	CNST
Reed College	Ho, Ethan	3-Dimensional Structures for the NIST Chemistry WebBook: My Journey from Molecular Optimization to Self-Optimization	MML/NCNR ChemBio
Rochester Institute of Technnology	Krasniak, Carolyn	DNA-Controlled Purification of Carbon Nanotubes	MML/NCNR MatSci
Rowan University	Kosior, Jesse	Investigating Methods for Safe Vaccine Transportation	PML/Physics
Rowan University	Scott, Charles	Micro- and Meso-Porous Structure Analysis of CO_2 Capture Materials Using Gas Sorption	MML/NCNR MatSci
Rowan University	Torres, James	Cold Source Engineers: Maintenance and Operation of the PeeWee Cold Source	MML/NCNR MatSci
Saint John's University	Bujarski, Andrew	Comparing Different Approaches for Measuring Environmental Performance in the Manufacturing Industry	EL
Saint Mary's College of Maryland	Andre, Laura	Laser Interferometry for Radiation Dosimetry	PML/Physics
Saint Olaf College	Braafladt, Signe	The Comet Assay: Methods for Quantitative Image Analysis and Reproducibility	MML/NCNR ChemBio
Saint Olaf College	Stutzman, Mara	Stem Cell Enumeration: Using Simulations to Inform Experimental Design	ITL
Santa Clara College	Silva-Feaver, Maximiliano	AFM Applications of Optomechanical Transduction by a Microdisk Resonator	CNST
Smith College	Flores, Yadira	Measuring Sustainability in Commercial Buildings	EL
Smith College	Milosavljevic, Maja	Seasonal and Spatial Patterns in the Atmospheric Concentration of Greenhouse Gases	ITL
Smith College	Stoudt, Sara	Correcting Temperature Records for Biases Unrelated to the Climate	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Stanford University	Wu, Joseph	Smart and Synchronized!: Modeling the Effect of Time Offset in Power Flows Across the Smart Grid	ITL
State University of New York Albany	Brisbois, Chase	Probe-Assisted Deterministic Doping	PML/ElecEng
State University of New York Albany	Grisafe, Benjamin	Design and Characterization of Phase Shifting Photomasks for I-Line Projection Lithography	CNST
State University of New York Binghamton	Adhikari, Anil	Non-Destructive Analysis of Thermal Stress in Copper Through-Silicon Via Using Time Domain Reflectometry	PML/ElecEng
State University of New York Binghamton	Anderson, Scott	Micro-Viscometry of Reference mAB Protein Solution	MML/NCNR MatSci
State University of New York Binghamton	Levine, Casey	Parallel Programming to Quickly Generate Libraries of Images for 3D SEM-Based Dimensional Measurements	PML/ElecEng
State University of New York Binghamton	Michelson, Jonathan	Scanning Microwave Microscopy: A Promising Technique for 3D-IC Subsurface Metrology	PML/ElecEng
State University of New York Binghamton	O'Brien, Edward	High Resistance Characterization to 100 TΩ	PML/ElecEng
State University of New York Binghamton	Watrobski, Paul	Software Defined Radio Development for Spectrum Monitoring	ITL
State University of New York Geneseo	Bienstock, Mollie	Calibration of ^{22}Na Using the Sum-Peak Counting Method	PML/Physics
Swarthmore College	Collard, Jacob	Automatic Ontologies: Standardized Terminology Generation for Document Comparison and Search	ITL
Syracuse University	Cauffman, Stephen	Improving Situational Awareness in Incident Responders Using Unmanned Aerial Systems	EL
Tulane University	Byron, William	Residual Gas Effect on aCORN	PML/Physics
Tulane University	Kiffer, Lucianna	Adjustments and Additions to the OOF Software	ITL
University of Alabama	Wallace, Sergei	Modeling Laser Pulsed Heat Conduction in Solids for All-Optical Ferromagnetic Resonance Spectroscopy	CNST
University of California Berkeley	Hallock, Scott	Super Sheet Metal Stressing: The Stimulating Design Process of Two Straining Devices	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Florida	Carter, Jared	Synthesis, Crystal Structures, and Phase Transitions in (Na,Li)(Nb,Ta)O_3 Ceramics	MML/NCNR MatSci
University of Illinois	Willi, Joseph	Impact of Different Hose Stream Applications During Fire Suppression	EL
University of Maryland Baltimore County	Alexander, Brandon	*R*-separation of Laplace's Equation in Rotationally-Invariant Cyclidic Coordinates	ITL
University of Maryland Baltimore County	Dhanasekaran, Vignesh	Improvement of Systematic Uncertainties in Mass Calibration Using Robotic Comparators	PML/ElecEng
University of Maryland Baltimore County	Eurice, Gary	Analysis of Factors in Photovoltaic EVA Degradation	EL
University of Maryland Baltimore County	Jackson, Abigail	New Generation Dental Resin Composites	MML/NCNR ChemBio
University of Maryland Baltimore County	Jacques, Leonard	Interfacial Shear Strength Measurements for Hybrid Nanocomposites Using Fiber "Push" Methods	EL
University of Maryland Baltimore County	Maczka, Caitlyn	Evaluating Dual Platforms for Bone and Vascular Regeneration	MML/NCNR ChemBio
University of Maryland Baltimore County	Pan, Jane	Identifying Distinct Regions in Multi-Material Microstructure Images with Clustering Algorithms	ITL
University of Maryland Baltimore County	Sikder, Nasif	Semantic Refinement Tool Development	EL
University of Maryland Baltimore County	Vane, Chelsea	Application of Machine Learning Techniques for Manufacturing	EL
University of Maryland College	Kaplan, Maria	Uniaxial Orientation of Polymers: Fabrication of Anisotropic Organic Semiconductor Films	MML/NCNR ChemBio
University of Maryland College Park	Bajcsy, Andrea	Relating Quantitative Measurements to Human Assessments of Voting Ballot Mark Types	ITL
University of Maryland College Park	Catacora, Luis	D3 Spatial Decomposition Visualization Validation Tool for Cement Hydration	ITL
University of Maryland College Park	Du, Nick	Information Models for Sustainable Manufacture	EL
University of Maryland College Park	Eisenberg, Evan	Flammability Reduction in Upholstered Furniture	EL
University of Maryland College Park	Elahi, Syed	A New and Innovative Way to Conduct Uncertainty Analyses on HVAC&R Equipment!	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Golan, Rachel	Toxicity of TiO_2 Nanoparticles *in vitro* and *in vivo*	MML/NCNR ChemBio
University of Maryland College Park	Goldman, Joshua	Optical Calibration of Nanocalorimeter Chips Using Infrared Camera	MML/NCNR MatSci
University of Maryland College Park	Graybill, Joshua	Hydro-Mechanical Response of Thin-Film Polyelectrolyte Membrane Materials for Fuel Cells	MML/NCNR MatSci
University of Maryland College Park	Isser, Ariel	Towards Robust, Universal Polymer Grafting	MML/NCNR MatSci
University of Maryland College Park	Jamgochian, Arec	Development of a High Resolution Photonic Spectrometer	PML/Physics
University of Maryland College Park	Jin, Shelley	Mayday! Mayday!: Investigating the Performance of Radio Cables in High Temperature Environments	EL
University of Maryland College Park	Kim, Timothy	Large Image Visualization	ITL
University of Maryland College Park	Knizhnik, Gedaliah	Semantic Interpretation of Bayesian Inference in a Manufacturing Scenario	EL
University of Maryland College Park	Kordell, Alexander	Materials Informatics for the Materials Genome Initiative	MML/NCNR MatSci
University of Maryland College Park	Krummel, Gregory	Machine Learning for Adaptive Robot Coordination	EL
University of Maryland College Park	Land, Joshua	MakerBot Round Robin Study: Manufacturing Plan Precision	EL
University of Maryland College Park	Lawler, Christopher	Making the Robot Think Twice: Improvements to an Ontology-Based Agility Framework for Manufacturing Robotics	EL
University of Maryland College Park	Ledwell, James	Augmented Reality for Smart Manufacturing: A Google Glass Exploratory Project	EL
University of Maryland College Park	Marin, David	An Extraordinary Hall Effect Susceptometer for Fast Measurements of Magnetic Media	MML/NCNR MatSci
University of Maryland College Park	McCoy, Conor	Development of Low-Cost Data Acquisition Devices for Extreme Hazard Applications	EL
University of Maryland College Park	Mittal, Rohan	Unidirectional Ballistic Resistant Laminates	MML/NCNR MatSci
University of Maryland College Park	Oeste, Thomas	The Impact of Human-Robot Collaboration	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Rachuri, Swaksha	Molecular Cloning and Characterization of Adenylyl Cyclase Class II Secreted from *Pseudomonas Aeruginosa*	MML/NCNR ChemBio
University of Maryland College Park	Siegel, Jacob	Viewing Stem Cells in Three Dimensions on a Large Scale	ITL
University of Maryland College Park	Solomon, Tsega	Optimizing Online Proteolysis for Hydrogen Deuterium Exchange-Mass Spectrometry (HDX-MS)	MML/NCNR ChemBio
University of Maryland College Park	Wong, Christopher	Enzymatic Biodegradation of Traditional and Novel Restorative Dental Resins	MML/NCNR MatSci
University of Maryland College Park	Zhi, Bowen	Seeing is Believing: Visual Data Analytics for Smart Manufacturing	EL
University of Massachusetts Amherst	Dodd, Andrew	Towards Developing Composability in Modeling and Simulation of Additive Manufacturing Processes	EL
University of Michigan	Capraro, Gianluca	Advancing Manufacturing Process Diagnostics and Prognostics by Leveraging Supply Chain Strategies	EL
University of Michigan	Eyers, Bryan	The Effects of Shim Arm Depletion and Xenon Buildup on Estimated Critical Positions in NBSR for New- and Mid-Cycle Startups	MML/NCNR MatSci
University of New Haven	Wiercinski, Scott	Impact of Convective Heat on Firefighter Turnout Gear	EL
University of Oklahoma	Dachowicz, Adam	A Comparative Assessment of the LPV Algorithm for Materials Science Keyword Extraction	ITL
University of Oklahoma	Toms, Benjamin	Large-Eddy Simulation of Flow Over a Backward Facing Step	EL
University of Pittsburgh	Marksz, Eric	Applications of Laser-Cooled Lithium Ion Source Focused Ion Beam Technology for Materials Analysis and Processing	CNST
University of Puerto Rico	Barrios Fuentes, Nathaniel	Utilizing ANSI/ASHRAE Standard 37 for Volumetric Airflow Uncertainty	EL
University of Puerto Rico	Ortiz, Manuel	Real-Time Analysis of Route Origin Validation of Border Gateway Update Stream	ITL
University of Puerto Rico	Sandoval Casas, Jennifer	Testing an Electrical Power Frequency Disturbance Recorder (FDR) Device	PML/ElecEng
University of Puerto Rico	Serrano Garcia, William	Fabrication and Electrical Characterization of Rubrene Single - Crystal	PML/ElecEng

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Rochester	Sitaram, Ananya	Creating a Fast Piezo-Actuated Mirror for the Elimination of Fiber Noise	PML/Physics
University of South Carolina	Kuprenas, Rachel	An Analysis of the Effects of Simulation Parameters on CFD Aerodynamic Bluff Body Simulations Using Experimental Design Technique	EL
University of South Florida	Byrnes-Blanco, Laura	Examination of a 3D Printed Biocompatible Polymer for Stents	MML/NCNR MatSci
University of Texas Austin	Self, Jeffrey	Quasi-Elastic Neutron Scattering of Methanol Aggregates	MML/NCNR MatSci
University of Texas Austin	Tein, Ying-Heng	The Characterization of Relative Hydrogen-Bonding Strengths in AB Block Copolymer/C Homopolymer Blends	MML/NCNR MatSci
University of Texas Dallas	Miller, Ryan	Developing a Domain Specific Model Library and Supporting Tools for Manufacturing Modeling and Optimization	EL
University of Texas Dallas	Ploehn, Cathryn	The Authentication Equation: Visualizing the Convergence of Security and Usability of System-Generated Passwords	ITL
University of the District of Columbia	Baker, Collin	Advanced Plasma Etching for High-Aspect-Ratio Nanometer Silicon (Si) Trenches	CNST
University of the District of Columbia	Mayo, Kamala	Test and Measurement of Emerging Border Gateway Protocol Security Mechanism	ITL
University of Virginia	Chu, David	Understanding the Additive Manufacturing Digital Thread	EL
University of Virginia	Zeng, Kevin	Critical Geometries in Additive Manufacturing	EL
University of Washington	West, Aaron	Exploring the Structure of Surfactants with Rheo-SANS in Two Dimensions	MML/NCNR MatSci
Utah State University	Pound, Benjamin	Two-Dimensional Electron Gases at the Surface of Potassium Tantalate	CNST
Vanderbilt University	Madonna, Megan	Automating the Culture of Microbial Biofilms	MML/NCNR ChemBio
Virginia Polytechnic Institute and State University	Helsel, Michelle	Standard Testing Method for Density of Hydraulic Cement	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Virginia Polytechnic Institute and State University	Lichtman, David	Reproduction and Characterization of Commercial Cu-Ni-Zn Alloys	MML/NCNR MatSci
Virginia Polytechnic Institute and State University	Reynolds, Christopher	RM for Strain Measurements in SEM	MML/NCNR MatSci
Wake Forest University	Fogel, Derek	Residual Additive in Organic Photovoltaics	PML/ElecEng
West Virginia Wesleyan College	Cronise, Lauren	CT Imaging of the Lungs and Investigation of Dual Energy CT	PML/Physics
Yale University	Shi, Tanya	Measuring the Concentration of Specific Metallic Ions in Solution Through Induced Nanoparticle Aggregation	MML/NCNR ChemBio

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