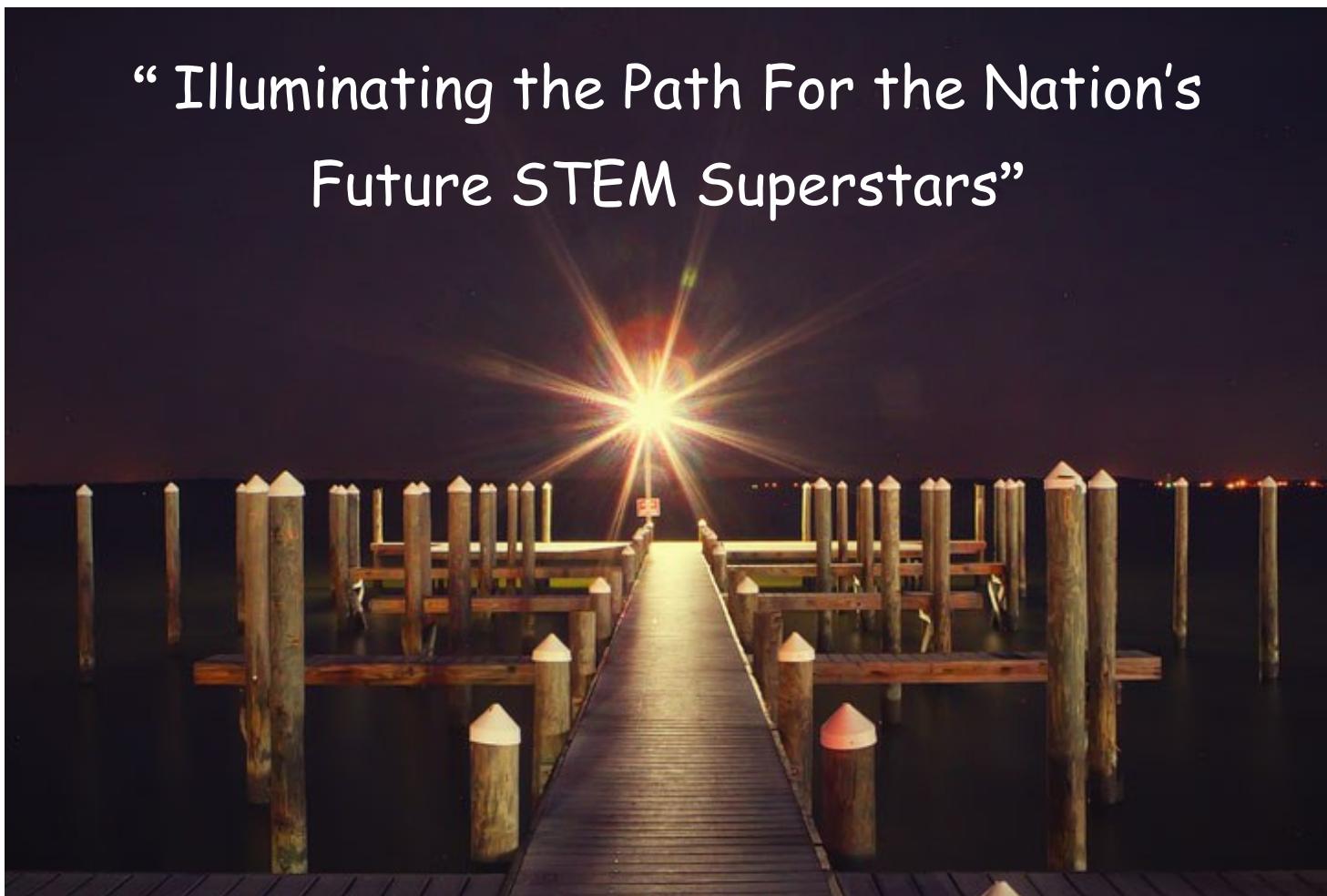


Summer Undergraduate Research Fellowship

# 20<sup>15</sup> SURF Colloquium

“ Illuminating the Path For the Nation’s Future STEM Superstars”



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

## SURF Students by Organizational Unit (OU)

- Center for Nanoscale Science and Technology (CNST)
- Center for Technology Laboratory (CTL)
- Engineering Laboratory (EL)
- Hollings Marine Laboratory, Charleston, SC (HML)
- Information Technology Laboratory (ITL)
- Material Measurement Laboratory (MML)
  - Chemical and Biochemical Sciences
  - Materials Science
- NIST Center for Neutron Research (NCNR)
- Physical Measurement Laboratory (PML)
  - Electrical Engineering
  - Physics

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**UNITED STATES DEPARTMENT OF COMMERCE**  
**National Institute of Standards and Technology**  
Gaithersburg, Maryland 20899-

Greetings!

On behalf of the Director's Office, it is a pleasure to welcome you to 2015 SURF Colloquium at the NIST Gaithersburg campus.

Founded by scientist in the Physics Laboratory (PL) with a passion for stem outreach, the SURF Program has grown immensely since its establishment in 1993. The first cohort of the SURF Program consisted of 20 participants from 8 universities primarily conducting hands-on research in the physics lab. Representing all STEM disciplines, this summer's cohort of the SURF Program includes 183 participants from 80 universities engaging in research projects in all 7 laboratories at the Gaithersburg campus. It's expected that the program will continue to grow in the future.

During your attendance at the SURF Colloquium, I encourage you to interact with the presenters. Aside from asking questions during the sessions, I recommend networking with presenters in between sessions and/or lunch. The colloquium is the perfect venue to exchange findings and new ideas from the most recent and rigorous research in all STEM fields.

Furthermore, I suggest chatting with NIST staff and scientist at the colloquium. Don't be afraid to ask questions about the on-going research in a NIST laboratory. Most staff and scientist love to talk about their role or research at NIST.

Moreover, I invite you to share your experience at the SURF Colloquium on the NIST Twitter Feed (@usnistgov) or the National Institute of Standards and Technology Facebook page using the hashtag, #2015SURFColloquium.

Lastly, I could not conclude this letter without mentioning the individuals which make the SURF Program at NIST possible. Thank you to the SURF Directors, the SURF mentors, the NIST Grant's Office, the National Science Foundation, and all the staff at NIST who play an integral role in making the SURF participants experience valuable. You are all greatly appreciated.

Again, welcome to the conference. I'm glad that you are here and I look forward to your participation in the SURF Colloquium.

Warm regards,

Brandi Toliver, PhD  
NIST SURF Program Manager

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# 2015 SURF STUDENT ABSTRACTS

## (Alphabetical by Last Name)

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

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<b>SURF Student Colloquium</b>		August 4-6, 2015	
NIST – Gaithersburg, MD			
			
Name:	Omar Y. Abou-Enein	Grant Number	70NANB15H189
Academic Institution:	Salisbury University	Major:	Computer Science and Mathematics
Academic Standing (Sept. '15):	Sophomore	Academic Standing (Sept. '15):	1st year graduate school
Future Plans (School/Career):	After attaining Bachelor's degrees in Mathematics and Computer Science, I plan to work towards Master's degree in Computer Science. In addition, I plan to continue to pursue work with Federal agencies. Through the various NIST intern programs, I have cultivated a great passion for robotics and sensor network research. My interest extends into the industries of which these research fields impact.	Future Plans (School/Career):	Graduate School Binghamton University
NIST Laboratory, Division, and Group:	Engineering Laboratory Intelligent Systems Division, Mobility and Manipulation Systems Group	NIST Research Advisor:	Dr. Yaw S. Obeng / Dr. Chukwudi Okoro
Title of Talk:	Inter-System Communication for Multi-Robot Control	Title of Talk:	Non-destructive analysis of the effects of thermal cycle and humidity in Copper Through-Silicon Vias using vector Network Analyzer
Abstract:	<p>Implementing new technologies within industry can pose many risks without proper tools for performance analysis. Investing in emerging technologies requires more than just insight into the reliability, precision, and efficiency of this equipment within an industry. The investment decision requires an ability to assess related metrics with relevancy, repeatability, and viability to ensure proper outcomes. With these principles in mind, the NIST Engineering Laboratory is working to provide new test methods for mobile manipulators.</p> <p>A mobile manipulator consists of an Automatic Guided Vehicle (AGV) and an onboard robot arm collaborating to accomplish tasks, such as assembly. Previous testing implementations for the NIST mobile manipulator included pre-determined AGV navigation paths and docking points measured by a ground truth measurement system. Once the AGV arrived and halted at its docking destination, the onboard robot arm would then begin to detect preprogrammed points on a test table known as the Reconfigurable Mobile Manipulator Artifact (RMMA).</p> <p>Performance measurement testing was restricted by the lack of communication between the AGV and collaborative robot arm. The robot arm previously could not know the actual AGV docking position which resulted in longer search times and a higher degree of failure in the robot arm's algorithm to find RMMA test points. The need to evaluate the AGV's ability to accurately navigate the robot arm to the RMMA in a wider range of test scenarios required the development of new performance testing methods. To achieve additional scenarios, collaboration between mobility and manipulator systems would need to be enhanced.</p> <p>The scope of this project included the integration of an off-the-shelf industrial PC onboard the AGV to facilitate collaboration between the AGV and robot arm. This PC functioned as the communication system between an additional onboard computer running ARToolkit freeware, which received input from a camera sensor, and an interface computer to the onboard robot arm. The integration allowed the manipulator robot base position to be modified based on the sensed RMMA pose and the AGV dock position. In addition, calibration tests were conducted on the ARToolkit camera sensor system to assess the effectiveness of this methodology for multiple mobile manipulator test scenarios. With this integration, low cost and easily implemented components now enable additional performance testing scenarios for future exploration and use within industry.</p>		

<b>SURF Student Colloquium</b>		August 4-6, 2015	
NIST – Gaithersburg, MD			
			
Name:	Anil Adhikari	Grant Number	70NANB15H166
Academic Institution:	State University of New York at Binghamton	Major:	Electrical Engineering
Academic Standing (Sept. '15):	1st year graduate school	Academic Standing (Sept. '15):	
Future Plans (School/Career):	Graduate School Binghamton University	NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, CMOS and Novel Devices Group
NIST Research Advisor:	Dr. Yaw S. Obeng / Dr. Chukwudi Okoro	Title of Talk:	Non-destructive analysis of the effects of thermal cycle and humidity in Copper Through-Silicon Vias using vector Network Analyzer
Abstract:	<p>Thermal stresses and the humidity are known to be major causes of failure in electronic devices, as they result in the formation of defects such as cracks, voids and delamination, leading to shorts/opens in the integrated circuits. Electronics devices undergo continuous temperature fluctuation when in use. This continuous thermal cycling generates thermal stresses due to the different coefficients of thermal expansion (CTE) of materials of construction. At the same time, reactive materials, such as copper, oxidize rapidly in presence of humidity at elevated temperatures that results in the deterioration of the electronic devices.</p> <p>With the emergence of three-dimensional stacked integrated circuits (3D-SIC), as the microchip of the future, the concern for stress and humidity related failures has increased. This is because the vertical electrical connections through the stacked chips are achieved with copper interconnects, that pass through the active silicon. Unfortunately, the large mismatch in the CTE of Copper (<math>17 \times 10^{-6}/^{\circ}\text{C}</math>) and Silicon (<math>2.3 \times 10^{-6}/^{\circ}\text{C}</math>) leads to the generation of significant stresses.</p> <p>In this work, radio-frequency (RF) based techniques were used for non-destructive fault-detection and to analyze the impact of thermal cycling at 85% humidity on the signal integrity of 3D-ICs enabled by Cu TSVs. Broadband RF signals (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 characteristics of the DUT were determined as a function thermal cycles and humidity conditions. From the frequency domain analysis, ABCD matrix, propagation constant, phase constant, attenuation constant and characteristics impedance were obtained. As the number of thermal cycle increases at constant humidity, the propagation loss and the impedance mismatch in the DUTs increased, suggesting drastic changes in the material properties.</p>		

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Ethan D. Allnutt	Grant Number 70NANB14H
Academic Institution: University of Maryland, Baltimore County	Major: Computer Science
Academic Standing Junior	
(Sept. '15):	
Future Plans (School/Career):	I plan on attending grad school but I have not decided on any schools at the moment.
NIST Laboratory, Division, and Group:	Innovation and Industry Services/Technology Partnerships Office
NIST Research Advisor:	Courtney Silverthorn
Title of Talk:	The need for information and API's in today's world
Abstract:	<p>In our ever growing world there is a constant need for information. What we have is never enough, so people seek means to gather up as much information as they can. It is important then, for groups that want to stay relevant in the public eye to make their information readily available in a way that does not inconvenience or hinder the average person. I seek to do this through the development of web API that facilitates the transfer of publicly available data from NISTTech's databases to Data.gov, a site meant to provide public access to machine readable datasets generated by the federal government. This API would pull non-restricted data from one of NIST's databases and then make only the data that it had pulled available for Data.gov, and then the public. This allows the public to know what technologies are available for licensing and can facilitate partnerships between laboratories and industries.</p>
Name: Luke Amatucci	Grant Number 70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Aerospace Engineering
Academic Standing Sophomore	
(Sept. '15):	
Future Plans (School/Career):	Career in the Aerospace Industry
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Structures Group
NIST Research Advisor:	DongHun Yeo, Marc Levitan
Title of Talk:	Experimental Methods of Pressure Transducer Data Correction
Abstract:	<p>When collecting pressure data of the surface of a model in a wind tunnel many pressure taps are made on the surface of the model. The taps are connected via plastic tubing to a pressure transducer module that is then attached to a data acquisition system (DAQ). When propagating through the plastic tubing pressure fluctuations get distorted and amplified, not unlike a musical instrument. Because of this amplification of data a transfer function must be written to be able to correct the signal from the DAQ. To create this transfer function there must be a ratio made between the pressure value collected and the pressure value at the surface of the model. A calculation of this ratio can be computed in theory, but before wind tunnel testing, a ratio needs to be determined from experimental data. The experimental results can be compared to the theoretical results to validate the experiment. After validating a transfer function it can be used to correct the signals collected by the DAQ and allow us to take pressure measurements of the surface of a model in the wind tunnel.</p>
To collect the data experimentally a device was designed to be able produce a pressure fluctuation at a continuous frequency. The pressure transducer module could be connected to this device through small tubes. Because the pressure transducer module cannot be directly connected to the device a tube of minimum length must be used to collect the 'real' values. The tube length and configuration used in the testing is then connected to the device as well. Using Fourier analysis techniques the amplitudes of the signals from both tubes can be computed. The two amplitudes can be used to compute an amplitude ratio across a range of frequencies that will be compared to theoretical values of amplitude ratio.	
This procedure is automated through LabView software that controls the DAQ and pressure fluctuation generator.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
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Academic Standing Junior	
(Sept. '15):	
Future Plans (School/Career):	I plan on attending grad school but I have not decided on any schools at the moment.
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This procedure is automated through LabView software that controls the DAQ and pressure fluctuation generator.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Khalil Anderson	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Computer Science
Academic Standing Sophomore	
(Sept. '15):	
Future Plans I plan of finished college and attempting to get an M.D./Ph.D. that will allow me to combine medicine with computer science	
(School/Career): NIST Laboratory, Engineering Laboratory, Smart Grid Program Office	
NIST Division, and Group:	
NIST Research Martin Burns	
Advisor:	
Title of Talk: Meters, Meters and More Meters: The Implementation of the Smart Grid Standard on the NIST Campus	
<b>Abstract:</b>	
Data is very important and contains useful pieces of information for people, so the federal government started two initiatives called Open Data and My Data. Open Data is data about the data created or maintained by the government; that the government wants people to have in order to allow more transparency into what the government does. My Data is giving consumers the ability to access their data such as their energy usage statistics. Energy usage is an important and fundamental measurement needed for many applications. The My Data initiative motivated the creation of the Green Button initiative which allows people to see their energy usage in discrete time intervals available from their utility providers such Electric and Gas services. NIST played a major role in creating a standard messaging format for data that passes through a Green Button service. This service would be provided by their Energy Service Provider or a Third Party collaborating with the Energy Service provider.	
<b>Abstract:</b>	
With the growth of consumer electronics in recent years, interest in organic electronics had grown considerably. Not only are organics made out of renewable materials making them useful in making truly green technology, they are also important in the wearable electronics industry due to their potential flexibility. One method of creating organic electronics is through inkjet printing. This method is has a number of advantages including being a relatively cheap and simple process and allowing for layer-to-layer alignment and large area processing. The major problem with inkjet printing however is that it is difficult to reliably create submicron patterns needed for high performance electronics. One method of creating submicron patterns is by printing solutions that will dewet on a previously printed line, creating a gap between the two. These self-aligning patterns could be very useful for various applications including the self-aligning of carbon nanotubes in the fine gap feature.	
I am researching the development of inks that can be printed to create submicron patterns. In creating these solutions, there are a number of constraints must be overcome. First the solvent/solute system for both solutions need to be selected so that the second solution can dewet without dissolving the first and both need to have high surface tensions due to the physical requirements of the printer. Additionally the molecular weight and concentration of the polymer solute needs to be fine-tuned to achieve a workable viscosity without making the solution too dilute to leave a pattern.	
Ink characteristics are evaluated by first studying drop formation with a real-time video camera. The printed features from well behaved inks are then characterized with both optical microscopy and atomic force microscopy. Finally, self-alignment is studied by printing overlapping features.	

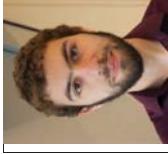
<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: David Anderegg	Grant Number 70NANB15H175
Academic Institution: Virginia Polytechnic Institute and State	Major: Materials Science and Engineering
Academic Standing Junior	
(Sept. '15):	
Future Plans Graduate School and Virginia Tech	
(School/Career):	
NIST Laboratory, Material Measurement Laboratory, Materials Science and Engineering Division, Functional	
Division, and Group: Polymers Group	
NIST Research Lee Richter	
Advisor:	
Title of Talk: Study of dewetting properties of inkjet-printed polymers	
<b>Abstract:</b>	
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<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<p><b>Name:</b> Joelle Baer</p> <p><b>Academic Institution:</b> Hamilton College</p> <p><b>Grant Number:</b> 70NANB15H190</p> <p><b>Major:</b> Physics</p>
<b>Academic Standing</b>	<p><b>Academic Institution:</b> Senior</p> <p><b>(Sept. '15):</b></p> <p><b>Future Plans</b> I plan to continue with physics in graduate school, possibly in the fields of experimental condensed matter or atomic physics.</p> <p><b>(School/Career):</b> NIST Center for Neutron Research, Neutron Condensed Matter Science Group</p>
<b>NIST Laboratory, Division, and Group:</b>	<p><b>NIST Laboratory,</b> NIST Research</p> <p><b>Division, and Group:</b> Wangchun Chen and Shannon Watson</p>
<b>Advisor:</b>	<p><b>Advisor:</b> Wangchun Chen and Shannon Watson</p>
<b>Title of Talk:</b>	<p><b>Title of Talk:</b> Here's the (In)Situ-ation: Optimizing and Testing a Prototype for Beamline Helium-3 Polarization</p>
<b>Abstract:</b>	<p>Polarized Helium-3 with a strong spin dependent neutron absorption cross section is used at the NIST Center for Neutron Research (NCNR) to study the magnetic structure of materials. <math>^3\text{He}</math> gas is placed inside of a glass cell along with small amounts of alkali metals and nitrogen. The <math>^3\text{He}</math> nuclei become polarized through Spin Exchange Optical Pumping (SEOP), where alkali-metal atoms are polarized by optical pumping and the resulting electronic polarization is transferred to <math>^3\text{He}</math> nuclei in spin-exchange collisions. SEOP requires high powered lasers, manipulated by optics, which illuminate the cell as it lies in a uniform magnetic field. These cells take 4–10 hours to reach the saturated <math>^3\text{He}</math> polarization depending on cell size and laser power. When the cells are placed on the beam line, the polarization decays exponentially with their characteristic relaxation times [1]. This decay correlates to a decreased intensity and polarization efficiency in its use as a polarizer or an analyzer for neutron scattering experiments.</p>
<b>Future Plans</b>	<p>I plan to pursue a Master's degree in an engineering related field</p>
<b>(School/Career):</b>	<p><b>NIST Laboratory:</b> Material Measurement Laboratory, Material Science Engineering Division, Functional Nanostructured Materials Group</p>
<b>NIST Research</b>	<p><b>NIST Research</b> Dr. Brian Boyce</p>
<b>Advisor:</b>	<p><b>Advisor:</b> Dr. Brian Boyce</p>
<b>Title of Talk:</b>	<p><b>Title of Talk:</b> Exfoliation and Study of Transition Metal Dichalcogenides</p>
<b>Abstract:</b>	<p>Following the exfoliation of a single-layer graphene in 2003, there has been wide spread interest in graphene and related 2-D materials. These 2-D materials are of interest for their unique chemical, mechanical and electronic properties that differ from their bulk counterparts. The unique properties of these materials offer new avenues to novel electronic and mechanical devices. In our current work we have studied transition metal dichalcogenides (TMDs) synthesized via chemical vapor transport (CVD). TMDs are of the form <math>\text{MX}_2</math> where 'M' is a transition metal and 'X' is chalcogen (S, Se, or Te). Like graphene they are weakly bonded between layers though van der Waals attraction. This allows the creation of samples using mechanical exfoliation to separate the layers. Using this technique we have exfoliated <math>\text{MoTe}_2</math> and <math>\text{NbSe}_2</math> onto samples of <math>\text{Si}/\text{SiO}_2</math> that were lithographically patterned. We have studied these exfoliated materials using a combination of Raman spectroscopy, optical microscopy, scanning electron microscopy, and atomic force microscopy. We have also begun studying the materials as suspended membranes over wells (<math>1\ \mu\text{m}</math> to <math>8\ \mu\text{m}</math>) with laser interferometry based on using the membrane as one etalon of a Fabry-Pérot interferometer. This work will form the technical basis to produce devices fully in house (synthesis to measurement) at NIST to study 2D materials both electrically and mechanically.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<p><b>Name:</b> Kode Arther</p> <p><b>Academic Institution:</b> Lewis &amp; Clark College</p> <p><b>Grant Number:</b> 70NANB15H139</p> <p><b>Major:</b> Physics and Mathematics</p>
<b>Academic Standing</b>	<p><b>Academic Standing</b> Senior</p> <p><b>(Sept. '15):</b></p> <p><b>Future Plans</b> I plan to pursue a Master's degree in an engineering related field</p>
<b>NIST Laboratory, Division, and Group:</b>	<p><b>NIST Laboratory:</b> Material Measurement Laboratory, Material Science Engineering Division, Functional Nanostructured Materials Group</p>
<b>NIST Research</b>	<p><b>NIST Research</b> Dr. Brian Boyce</p>
<b>Advisor:</b>	<p><b>Advisor:</b> Dr. Brian Boyce</p>
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<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Daniel Barcklow	Grant Number   70NANB15H114
Academic Institution: George Mason University	Major: Computer Engineering
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Career in Embedded Software Development	
NIST Laboratory, Division, and Group: Division, and Group: Communications Technology Laboratory, Wireless Networks Division, Spectrum Sharing Project	
NIST Research Advisor: Advisor: Dr. Michael Souriya	Title of Talk: Software-defined Radio Receiver Design with FPGA-based Hardware Acceleration
<b>Abstract:</b>	
<p>Software-defined radio (SDR) is a technology that focuses on the software approach to classical radio design. In many ways, SDR platforms are capable of outperforming their hardware-limited counterparts; SDRs are easily upgradeable, able to make decisions, flexible, reconfigurable, and relatively low cost, which makes them perfect tools for communications technology research. NIST CTRL is using SDRs to conduct research in radio frequency (RF) spectrum sharing metrology that would enable commercial wireless broadband use of Federal Government RF bands. Although there are many advantages to software-defined radio design, hardware implementations remain much faster and are more capable of providing real-time performance.</p>	
<p>The objective of my project was to find a way to better utilize the field programmable gate array (FPGA) portion of Xilinx's Zynq system-on-chip (SoC). The Zynq SoC is broken into two sections, the processing system (PS) and programmable logic (PL). The PS incorporates an ARM® dual-core Cortex-A9 application processing unit (APU), capable of running Linaro, an embedded distribution of Linux. The PL portion possesses FPGA fabric that is equivalent in both size and performance to Xilinx's Artix-7 FPGA Family.</p>	
<p>The advantage of the Zynq SoC lies in leveraging the FPGA fabric's ability to parallelize functions, pipeline operations, and stream information that would otherwise be too intensive or impossible for an embedded processor. The Zynq SoC provides SDR developers with a platform that has a small physical footprint, is portable, but still capable of performing rigorous and complex digital signal processing (DSP) operations. The goal of this project is to prototype a wideband RF spectrum sensor on the Zynq SoC that measures spectrum usage in real time, in support of dynamic spectrum sharing.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
Name: Rebecca Barolli	Grant Number   70NANB15H178
Academic Institution: Worcester Polytechnic Institute	Major: Chemical Engineering
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Pursuing a Master of Science degree in Fire Protection Engineering at Worcester Polytechnic Institute	
NIST Laboratory, Division, and Group: Division, and Group: Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Fire Group	
NIST Research Advisor: Advisor: Nelson P. Bryner	Title of Talk: Characterization of Exposure Conditions for Wildland/Wildland-Urban Interface Fire Fighters
<b>Abstract:</b>	
<p>In the United States, there are on average 75,000 wildfires annually. Only about 3% of these fires typically involve extreme fire behavior and are not quickly suppressed. Despite this small percentage, these fires have caused some of the largest amounts of loss in the history of the United States. The power of these fires can overwhelm suppression tactics and cause ignition of structures in nearby communities. There are 46 million structures in the wildland-urban interface (WUI) at risk in the U.S., and on average, 3000 structures lost annually. The WUI is considered the communities of structures intermixed with or neighboring wildland areas. There is little known information about the spread of these fires and the most effective suppression tactics.</p>	
<p>This project involved developing instrumentation to characterize the exposure conditions encountered by fire fighters as they extinguish fires. As part of this project, it was necessary to fabricate fuel packages that are representative of wildland vegetative fuels, a typical urban environment, and a wildland-urban interface community. Wildland fuels vary tremendously based on the location within the United States, and the fuels of southern California were selected due to the extensive damage caused by fires in this area. Residential fuel inventory studies were used to determine and incorporate realistic amounts of wood, inerts and hydrocarbons into the urban fuel package. The WUI fuel package includes the materials and porosities of each of the wildland and urban representations. The fuel packages were built small and large scale as a stacked array of sticks, also known as a crib.</p>	
<p>These cribs were burned in both laboratory-scale on the cone calorimeter and field-scale experimental burns. Smoke particulates and toxic gases produced were measured during these burns. Understanding the products of combustion for these fires will allow for improved design of more effective protective equipment for fire fighters. This knowledge will ultimately assist in protecting the 1.25 million fire fighters nationwide at the scene of a fire.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
	<b>Name:</b> Aaron Battier Pritzker <b>Academic Institution:</b> Harvey Mudd College <b>Grant Number:</b> 70NANB15H148
<b>Academic Standing:</b> (Sept. '15): Senior	<b>Academic Institution:</b> Harvey Mudd College <b>Major:</b> Physics
<b>Future Plans</b> <b>(School/Career):</b> Ph.D. program in physics	<b>Future Plans</b> <b>(School/Career):</b> Center for Nanoscale Science and Technology, Electron Physics Group
<b>NIST Laboratory,</b> <b>Division, and Group:</b> NIST Research	<b>NIST Laboratory,</b> <b>Division, and Group:</b> NIST Research
<b>Advisor:</b> Mark Stiles, Vivek Amin	<b>Advisor:</b> Title of Talk: Modeling Spin-Orbit Torques in Metal-Magnet Interfaces

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Lindsey Bass <b>Academic Institution:</b> Virginia Polytechnic Institute and State University <b>Grant Number:</b> 70NANB15H175 <b>Major:</b> Mechanical Engineering and Music
<b>Academic Standing:</b> (Sept. '15): Senior	
<b>Future Plans</b> <b>(School/Career):</b> After successfully obtaining both degrees, I will enter a graduate program related to Additive Manufacturing.	
<b>NIST Laboratory,</b> <b>Division, and Group:</b> NIST Research	<b>NIST Laboratory,</b> <b>Division, and Group:</b> Engineering Laboratory, Intelligent Systems Division, Production Systems Group
<b>Advisor:</b> Shawn Moylan	
<b>Title of Talk:</b> Residual Stress in Metal Additive Manufacturing Parts	

**Abstract:**  
One of the key barriers to widespread adoption of Additive Manufacturing (AM) for metal parts is the build-up of residual stresses. In the laser-based powder bed fusion process, a laser selectively fuses unheated metal powder layer by layer creating residual thermal stresses from the temperature gradients, which can lead to severe deformations and losses of part tolerances. In order to develop strategies to lesson these stresses, the stresses first need to be quantified. A thorough literature survey was completed utilizing multiple NIST library resources to determine the extent of prior research on measuring and modeling stresses at macro and micro levels. Among the various metal AM materials, AM technologies, and stress-measurement techniques, it was found that all test parts had mainly prismatic geometries. While dwell time  $\tau$  between layers was shown to influence residual stress with AM deposition processes, it is not well-studied in powder bed fusion processes. With this knowledge, and after interacting with researchers in MML and NCAR who have the capabilities to measure different levels of stresses, an experiment was designed with cylindrical parts to evaluate how diameter, hole size, and time between scanned layers affect residual stresses. A specimen tray was optimally arranged for both the powder bed fusion build process and the neutron diffraction stress-measurement technique. The measured residual stresses can be used to improve multi-physics models and simulations of AM processes to validate models and eventually lead to methods for reducing residual stress.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4-6, 2015



Name: Katherine Bellino	Grant Number	70NANB15H109
Academic Institution: Clemson University	Major:	Bioengineering, Electrical Concentration
Academic Standing (Sept. '15):	Junior	
Future Plans (School/Career):	Grad School followed by a career in Medical Devices	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, Nanoscale Metrology Group	
NIST Research Advisor:	Dr. Michael Gaitan	
Title of Talk:	Calculating the Uncertainty of High Frequency Accelerometer Calibrations using Laser Vibrometry	
<b>Abstract:</b>		
Accelerometers can be found anywhere from cell phones to cars to medical devices to nuclear power plants. The accuracy of these accelerometers is paramount in providing safety in many applications, hence the need for precise calibration. The calibration system itself consists of an air bearing shaker table capable of operating in a range of frequencies up to 50 kHz with displacements as small as nanometers. The primary source of uncertainty assessed in this project was the effect of transverse motion on the measured sensitivity. Even single axis accelerometers display a slight sensitivity to transverse motion, so any horizontal displacement of the shaker can impact calibration accuracy. In this project, transverse motion was measured using a laser vibrometer directed at the cylindrical surface of the shaker in two horizontal positions, 90 degrees apart. The vibrometer measures the velocity of the transverse motion and outputs a corresponding voltage. The calibration system uses this voltage to calculate a sensitivity value. Using this value, the ratio of transverse to primary acceleration is calculated. The uncertainty is then based on the peaks of the Root Sum Square of the two positions. This process was repeated for several different loads. Other sources of uncertainty evaluated in this project include magnetic effect, voltage electronics, and beam location.		

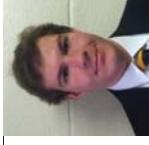


<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4-6, 2015
<b>Name:</b> Isabelle Berger	<b>Grant Number</b> 70NANB15H135
<b>Academic Institution:</b> George Washington University	<b>Major:</b> Mathematics
<b>Academic Standing (Sept. '15):</b> Junior	
<b>Future Plans (School/Career):</b> Planning on continuing my education in mathematics and finding a career that allows me to use it for the greater good	
<b>NIST Laboratory, Division, and Group:</b> Information Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Software Group	
<b>NIST Research Advisor:</b> Howard Cohl	
<b>Title of Talk:</b> Algorithms Behind the Symbolic Search and Verification for Generating Functions of Orthogonal Polynomials	
<b>Abstract:</b>	
Orthogonal polynomials have many useful applications in applied mathematics and physics. One of the most important properties of these polynomials is their generating functions. This talk will discuss my joint summer project in experimental mathematics with co-SURF student Catherine Traini. Our goal for this project was to develop and implement algorithms which would facilitate the search and verification of pre-existing and new generating functions for orthogonal polynomials in the Askey scheme. We were able to implement symbolic mathematics algorithms and corresponding code in Maple based on contributions by Bruno Salvy (National Institute for Research in Computer Science and Control (Inria), France). The algorithms utilize Zeilberger's algorithm to guess recurrence relations from a large but finite sequence of terms in the generating series and then derive ordinary differential equations with prescribed initial values. We use pre-existing symbolic methods which search for closed-form solutions to the derived initial value problems to search for new closed-form generating function representations. I will discuss these algorithms and how Catherine and I merged the initially developed sequential code into consolidated subroutine which we have applied to 15 orthogonal polynomials in the Askey scheme.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Matthew Bernstein	Grant Number   70NANB15H146
Academic Institution: Colorado School of Mines	Major: Engineering Physics
Academic Standing (Sept. 15): Senior	
Future Plans (School/Career): Possible Masters in Computer Engineering at the Colorado School of Mines. Early career in a Computer Engineering or Quantum Computation position	
NIST Laboratory, Division, and Group: NIST Research Advisor: Mudumalai Ranganathan	Communications Technology Laboratory, Wireless Network Division, Spectrum Sharing Project
Title of Talk:	Functionality for the Dynamic Spectrum Project Website
<b>Abstract:</b>	
The Spectrum Sharing Project includes a Measured Spectrum Occupancy Database (MSOD) with a web front end to display channel occupancy and power data from 3 <sup>rd</sup> Generation Partnership Project (3GPP) Long Term Evolution (LTE) cellular signals and Radio Frequency (RF) radar signals. The project, currently in a state of development, will be hosted by NIST and the National Telecommunications and Information Administration (NTIA), and will include data captured from sensors deployed at various strategic locations where spectrum sharing is planned. The web interface includes both client user) and administrative portals. Using the administrative portal, various system features and settings may be configured, such as graphical elements displayed to users, access privileges, sessions and sensor configurations. To be usable, the website needed additional administrative functionality. This talk will present an overview of the MSOD, and will cover the design and implementation of the following additional functionality: Graphical User Interface (GUI) Configuration interface, System Monitoring interface, and Service Control interface.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Andrew Blair	Grant Number   70NANB15H087
Academic Institution: Towson University	Major: Biology
Academic Standing (Sept. 15): Junior	
Future Plans (School/Career): Medical School	
NIST Laboratory, Division, and Group: NIST Research Advisor: Ashley Beasley Green, PhD	Material Measurements Laboratory, Biomolecular Measurement Division, Bioanalytical Science Group
Title of Talk:	MS Analysis of Protein BSA
<b>Abstract:</b>	
Proteins are polyptides formed from sequences of amino acids. These sequences are bonded in various ways to form primary, secondary, tertiary, and quaternary structures. The bond interactions of the tertiary structures will be addressed by evaluating the cysteine-cysteine disulfide bridges. These bridges are an important aspect of stabilization of the tertiary protein structure. In this current study, the disulfide linkages of SRM 927e: Bovine Serum Albumin (BSA) will be analyzed via mass spectrometry to characterize the tertiary structures of the protein. A proteomics-based mass spectrometric (MS) approach will be used to analyze the tertiary protein structure of SRM 927e. Prior to MS analysis, the peptide products are generated via enzymatic digest with trypsin or chymotrypsin. The intact protein is incubated at 95°C for 2 min to denature the protein, followed by reduction of the disulfide linkages with 5mM dithiothreitol at 60°C for 30 min. The samples are then alkylated with 15mM/L iodoacetamide at room temperature for 30 min in the dark to protect the cleaved peptide. A mass ratio of enzyme-to-total BSA protein (1:30 for trypsin and 1:20 for chymotrypsin) was used for digestion and the samples were incubated at 37°C (trypsin) and 25°C (chymotrypsin) overnight (~18 hours). Following digestion, the pH of the sample was reduced with 5 mL/TFA and the BSA tryptic fragments were concentrated in a SpeedVac and resuspended in 0.1% formic acid in water.	
The peptide fragments are compared in a reduced and non-reduced state for SRM 927e to analyze the difference in peptide profile. Analyses of the non-reduced BSA allow the identification of the inter- and intra-peptide disulfide bonds within the protein. The reduction of the disulfide bridges breaks the bonds between these residues which prevents analysis of the disulfide bonds. Therefore, the results from the analysis of the peptide profile from the reduced and non-reduced samples allow the characterization of the tertiary structure of SRM 927e.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Anna Michelle Blondermann <b>Academic Institution:</b> Montgomery College <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> Transferring to the University of Maryland, College Park, pursuing a career in software engineering and aerospace simulation <b>(School/Career):</b> Materials Measurement Laboratory, Biosystems and Biomaterials Division, Genome-Scale NIST Laboratory, Materials Measurement Laboratory, Biosystems and Biomaterials Division, Genome-Scale NIST Division, and Group: Measurement Group <b>NIST Research Advisor:</b> Arlin Stoltzfus <b>Title of Talk:</b> Fitness Measurements and Protein Evolution
<b>Abstract:</b>  Understanding the effects of mutations is a major challenge in genomics, evolution, and medicine. A new high-throughput technology called "Deep Mutational Scanning" has led to an unprecedented amount of data on the effects of mutations in proteins, with many potential uses.  Due to the newness of technology, DMS experiments still differ greatly in their power to discern effects on proteins, with unknown reasons. In this context, metrics designed to assess quality would be useful both for experimenters designing DMS protocols, and for downstream users of the resulting data.  Our main goals are to visualize DMS data through distribution graphs, develop and evaluate metrics to assess quality, and leverage this information in meta analyses and inference methods. Our quality metrics will discern the expected differences in the distribution of fitness effects between "missense" mutations that change one amino acid to another, causing a wide range of effects, "synonymous" mutations that change codons only, having very small effects, and "nonsense" mutations that truncate proteins expected to have strong, deleterious effects. Quantile normalization is used to compare studies that present fitness on different scales.  My research has focused on understanding DMS experiments, learning R for computational analysis, and writing scripts that read in DMS data, carry out calculations, and generate graphs automatically. We have confirmed that studies with more power, assessed by statistical cross-validation, tend to have a clearer separation between "missense" and "nonsense" mutations, with narrow distributions for each. We expect that metrics based on this distinction will be useful for comprehending the effects of protein mutations on fitness.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Matthew Bleakney <b>Academic Institution:</b> University of Maryland, Baltimore County <b>Academic Standing:</b> Sophomore <b>(Sept. '15):</b> I am interested in attending graduate school, but I am not sure what field I would enter in. My long term goal is to work in either industry or for the Department of Defense. After I retire I would like to be a part time professor or local high school teacher. <b>NIST Laboratory, Division, and Group:</b> Materials Measurements Laboratory <b>NIST Research Advisor:</b> Kirk Rice <b>Title of Talk:</b> Effect of gaps in backing support on ballistic performance of body armor
<b>Abstract:</b>  Recent changes in legislation that provides federal grant funding to qualifying law enforcement agencies for body armor have introduced an incentive to produce better-fitting body armor. The legislation "allows preferential consideration in Program grant awards to jurisdictions that provide armor vests to law enforcement officers that are uniquely fitted for such officers, including individual female officers." NIST has a long-standing role in the development of the performance standard specified by the Bureau of Justice Assistance in their administration of the Bulletproof Vest Partnership Grant Act, and our mission includes conducting research to support advancements in standards for public safety.  Common soft body armor constructions consist of many layers of high performance textile materials enclosed in a protective cover, which is referred to as an armor panel. Front and back armor panels are then inserted into a carrier having straps that are used to secure the body armor "vest" to the wearer's torso. Most body armor models consist of armor panels that lie flat, although such designs do not necessarily address the incentive in the legislation for improved fit. The fit of some body armor models is improved by shaping it into a non-planar form; however, standardized testing procedures provide considerable latitude in how the armor should be supported during a ballistic test. For example, the armor panel may be forced flat and placed on a flat clay surface for testing, or the armor panel may be placed on a contoured clay surface that matches the natural curvature of the armor panel. Also being contemplated is the possibility of introducing a standardized bust shape onto which the armor panel will be placed for testing. All of these options introduce questions about whether a potential gap between the armor panel and the clay surface might influence the ballistic performance of the armor panel.  This study investigates the role of an unsupported region behind an armor panel when tested in a flat configuration to generate recommendations for improved test protocols. Tests were performed with no gap (0 mm) between the clay backing support and the armor panel, as well as gaps of 20 mm, 40 mm, and 60 mm. To improve the sensitivity of the ballistic test, the armor panels are assessed at their estimated V50, the speed of a bullet expected to perforate armor 50 % of the time. Changes in failure statistics deviating substantially from the expected value indicate some influence due to the gap. These results will be further discussed in my presentation.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Jeffrey Brock	Grant Number   70NANB15H140 Major: Physics
Academic Institution: Miami University	
Academic Standing: Graduate Student in Physics, Miami University	
(Sept. '15):	
Future Plans (School/Career):	PhD in Physics, with the goal of entering academia
NIST Laboratory, Division, and Group:	Materials Measurement Lab, Materials Science and Engineering Division, Functional Polymers Group
NIST Research Advisor:	Adam Floyd Hannon
Title of Talk:	Nanostructure Characterization from X-Ray Scattering Techniques via Inverse Algorithms



## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4–6, 2015

Name: Jeffrey Brock

Grant Number | 70NANB15H140

Major: Physics

Academic Institution: Miami University

Graduate Student in Physics, Miami University

(Sept. '15):

Future Plans (School/Career):

PhD in Physics, with the goal of entering academia

NIST Laboratory, Division, and Group:

Materials Measurement Lab, Materials Science and Engineering Division, Functional

Polymers Group

NIST Research Advisor:

Adam Floyd Hannon

Title of Talk:

Nanostructure Characterization from X-Ray Scattering Techniques via Inverse Algorithms

### Abstract:

In recent years, the trends in the doubling of transistor density in integrated circuit devices predicted by Moore's law have approached a technological barrier due to traditional photolithography techniques reaching physical limits<sup>1</sup>. New fabrication techniques have been proposed to continue this trend, including the directed self-assembly (DSA) of block copolymers (BCPs)<sup>2</sup>, extreme ultraviolet lithography<sup>3</sup>, and multiple patterning approaches<sup>4</sup> all of which render structures with dimensions on the order of 10 nm. Characterizing the fabricated structures from these new methods non-invasively is important for quality control, but non-trivial characterization techniques are required to gauge internal structure<sup>5</sup> due to the small feature sizes involved. One potential method to accomplish this task is critical dimension small angle X-ray scattering (CDSAXS).

CDSAXS utilizes the principle that incident X-rays on a periodic structure array scatter at angles characteristic of the periodic pattern. The amplitude squared of the Fourier transform of the real space structure relates the scattered intensity profile with the sample structure. Since all phase information in the sample is lost in this process, inverse search methods are necessary to determine the real space structure. Using experimental data and a trapezoid stack model, a covariance matrix adaption evolutionary strategy method<sup>6</sup> was used to find the optimal geometric parameters that best reproduced measured scattering intensities of a variety of periodic nanostructures. By varying the number of trapezoids in the structure model, amount of data used in fitting, type of goodness of fit metric, and symmetry constraints, trends were observed for how different structures reproduced to experimental data. Analysis shows that the log-normal goodness of fit objective function offers the most consistent and best fitting solutions. Optimal refinement of solutions was attempted using Markov chain Monte Carlo fitting. The results demonstrate that using these different algorithms allows for accurate determination of the internal periodic structure of nanogratings, with feature sizes on the order of 10 nm.

[1] K. J. Kuhn, *13th International Workshop on Computational Electronics*, 37–40 (2009).

[2] D. F. Sunday et al., *Journal of Micro-Nanolithography MEMS and MOEMS* **12** (3) (2013).

[3] C. W. Gwyn et al., *Journal of Vacuum Science & Technology B* **16** (6), 3142–3149 (1998).

[4] C. Bercher et al., *Optical Microlithography XXI, Parts 1–3* **6924**, E9244–E9244 (2008).

[5] M. L. Schattenburg et al., *Nanostructure Science, Metrology and Technology*, 116–124 (2002).

[6] N. Hansen et al., *Evolutionary Computation* **11** (1), 1–18 (2003).

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Nathan Brockett	Grant Number   70NANB15H191
Academic Institution: The Pennsylvania State University	Major: Aerospace Engineering
Academic Standing	Senior
(Sept. '15):	
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group
NIST Research Advisor:	Yan Lu
Title of Talk:	A Proof-Of-Concept Additive Manufacturing Database

**Abstract:**  
An important next step for the Additive Manufacturing (AM) community is to develop design allowables for different AM materials and processes. Similar work has been done for metallic material using traditional manufacturing techniques in the Metallic Material Properties Development and Standardization (MMPDs) Handbook. These design allowables enable part designers to design parts with target properties, such as how the part will fatigue, or the yield load for a part of set dimensions. To develop reliable AM design allowables, a large number of well-documented builds, and the corresponding test data, are needed to derive relationships among part geometry, process parameters, and material properties. To store the data in a useful manner, the AM community requires a database and well-organized schema that allow for both collection of the necessary data, and advanced query of the collected data for analysis. This project is to design a proof-of-concept AM database and investigate its use for AM data analysis. Specifically, a prototype database was developed using NIST Materials Data Curation System (MDCS) that was designed for third party data curation under Material Genome Initiative and supports SPARQL query language and Representational State Transfer (REST) application programming interface (API).

The project has three steps, first develop a schema to hold and organize the data, second engineer an application to interchange data from a user and the database, and third perform proof-of-concept analysis of the data. The scope of this project's schema was limited to the process planning for Electro Optical Systems (EOS) machines and the corresponding mechanical test data. Observation of real AM part Building and the EOS User Manual were used to develop the process parameter part of the schema. The MMPSDs Handbook and American Society for Testing and Material (ASTM) mechanical testing standards were used to ensure the necessary test data was captured in the schema. The application to interchange data was developed in MATLAB using a REST API to connect to the NIST MDCS database. Both Python and R where explored as alternatives, but MATLAB was chosen due to its ability to analyze the data once imported from the database. The data used to populate the database came from an Edison Welding Institute (EWI) project and a Round Robin test project completed by NIST. These two projects provided two case studies to test the system. With the populated database, proof-of-concept data mining was performed to demonstrate the capability of the system. Future work includes improving the data model and extending the XML schema to cover various AM process and machine types.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
	<b>Name:</b> Lucas Brugulis
	<b>Academic Institution:</b> State University of New York Polytechnic Institute
	<b>Grant Number:</b> 70NANB15H152
	<b>Major:</b> Nanoscale Science
<b>Academic Standing</b> <b>(Sept. '15):</b>	<b>Academic Standing</b> : Senior
<b>Future Plans</b>	<b>Future Plans</b> : Graduate school
<b>(School/Career):</b>	<b>(School/Career):</b>
<b>NIST Laboratory, Division, and Group:</b>	<b>NIST Laboratory, Division, and Group:</b> Center for Nanoscale Science and Technology, Electron Physics Group
<b>NIST Research Advisor:</b>	<b>NIST Research Advisor:</b> Dr. Robert McMichael
<b>Title of Talk:</b>	<b>Title of Talk:</b> Measurement of magnetization dynamics on the nanoscale using nitrogen-vacancy centers in diamond
<b>Abstract:</b>	<p>The ability to detect homemade explosives (HMEs) in an efficient but reliable manner is of immediate interest for national security, forensic, and military applications. One of the primary techniques for detection of trace explosive residues is ion mobility spectrometry (IMS). Extensive literature exists on optimized explosives detection with IMS, and these instruments can detect many military-grade organic explosives at single particle levels. HMEs however are impure, and may contain precursors and by-products from their chemical synthesis. Recent years have seen a growing interest in the detection of HMEs, including the role that residual precursors and by-products play in detection. The detection of these compounds may also be useful to increase confidence of HME identification. The goal of this research is to optimize detection of precursors, by-products, and mixtures with their respective nitrate ester explosive. First, we determined what precursors and by-products gave reliable and strong signals, and determined their mobility values. Next the instrumental parameters were optimized to obtain maximum response, and limits of detection were determined. Finally, trace HME collections were simulated using controlled mixtures to examine the effect of these precursors and by-products on the explosive signal. This work found that precursors and by-products provide strong signals at roughly the same parameters of their corresponding explosive, and furthermore that their presence does not inhibit the explosive signal. Understanding the interaction of these mixtures can be used to increase confidence in HME detection, lower false positive rates, and provide a means of differentiating military-grade and homemade explosives.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Christopher Browne
	<b>Academic Institution:</b> Purdue University
	<b>Grant Number:</b> 70NANB15H143
	<b>Major:</b> Chemical Engineering
<b>Academic Standing</b> <b>(Sept. '15):</b>	<b>Academic Standing</b> : Junior
<b>Future Plans</b>	<b>Future Plans</b> : Graduate School
<b>(School/Career):</b>	<b>(School/Career):</b>
<b>NIST Laboratory, Division, and Group:</b>	<b>NIST Laboratory, Division, and Group:</b> Material Measurement Science Division, Surface and Trace Chemistry Analysis Group
<b>NIST Research Advisor:</b>	<b>NIST Research Advisor:</b> Edward Sisco and Thomas Forbes
<b>Title of Talk:</b>	<b>Title of Talk:</b> Optimized detection of Homemade Explosive Precursors and By-products using Ion Mobility Spectrometry
<b>Abstract:</b>	<p>The ability to detect homemade explosives (HMEs) in an efficient but reliable manner is of immediate interest for national security, forensic, and military applications. One of the primary techniques for detection of trace explosive residues is ion mobility spectrometry (IMS). Extensive literature exists on optimized explosives detection with IMS, and these instruments can detect many military-grade organic explosives at single particle levels. HMEs however are impure, and may contain precursors and by-products from their chemical synthesis. Recent years have seen a growing interest in the detection of HMEs, including the role that residual precursors and by-products play in detection. The detection of these compounds may also be useful to increase confidence of HME identification. The goal of this research is to optimize detection of precursors, by-products, and mixtures with their respective nitrate ester explosive. First, we determined what precursors and by-products gave reliable and strong signals, and determined their mobility values. Next the instrumental parameters were optimized to obtain maximum response, and limits of detection were determined. Finally, trace HME collections were simulated using controlled mixtures to examine the effect of these precursors and by-products on the explosive signal. This work found that precursors and by-products provide strong signals at roughly the same parameters of their corresponding explosive, and furthermore that their presence does not inhibit the explosive signal. Understanding the interaction of these mixtures can be used to increase confidence in HME detection, lower false positive rates, and provide a means of differentiating military-grade and homemade explosives.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Robert Buttles	<b>Grant Number</b> 70NANB15H168
<b>Academic Institution:</b> University of Maryland College Park	<b>Major:</b> Mechanical Engineering/Physics
<b>Academic Standing</b>	
Junior	
(Sept. '15):	
Future Plans	Working at a company or institution like Space Ex, where I get to help push the boundaries in fields related to space
(School/Career):	
NIST Laboratory, Division, and Group:	Physical Measurements Lab, Sensor Science Division, Thermodynamic Metrology Group
NIST Research Advisor:	Jacob Ricker, Dr. Jay Hendricks
Title of Talk:	Automation of an Optical Pressure Standard: A Noble Quest for Laser Modes
<b>Abstract:</b>	
<p>The Sensor Science division is working to redefine the Pascal in terms of the Boltzmann's constant in order to create a new primary method of pressure realization. This device is expected to outperform the current method (mercury manometers), will allow NIST to remove 500 kg of mercury from the lab, will drastically reduce the size of the current standards, and will be fully automated. Key to this novel technique is the ability to make best in the world measurements of the index of refraction. To do so, the group has built a device dubbed the "fLOC" or fixed-length optical cavity, which uses quantum mechanics theory to link the refractive index of helium gas to the temperature and pressure. How this works involves tuning a laser frequency to resonate in the fLOC. The problem is that when tuning the frequency, the cavity will resonate at several transverse electromagnetic (TEM) modes. However, to make accurate pressure measurements, the same mode must be used every time. The solution to finding the correct laser mode is to use the visual intensity patterns and a Serial Camera controlled by a Netduino in order to determine the laser mode. After decoding the JPEG and analyzing the transformed color space, the Netduino can determine whether the laser is on the correct mode, or whether it needs to look for a new mode. With the automatic mode locking, data collection will be made easier and can be made without human interaction.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Carson J Bryant	<b>Grant Number</b> 70NANB15H082
<b>Academic Institution:</b> Vanderbilt University	<b>Major:</b> Chemistry and Applied Mathematics
<b>Academic Standing</b>	
Junior	
(Sept. '15):	
Future Plans	Graduate School (Chemistry)
(School/Career):	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Biosystems and Biomaterials Division, Cell Systems Science Group
NIST Research Advisor:	Donald Atha, Witas Reipa
Title of Talk:	Development of a Reproducible Electrochemical Method for Quantifying Oxidative Stress
<b>Abstract:</b>	
<p>Induction of oxidative stress in human cells can result in the accumulation of reactive oxygen species (ROS) and can lead to the development of a wide range of diseases, including AIDS, Huntington's, Parkinson's, and Alzheimer's. One metric of the relative strengths of oxidizers implicated in causing pathogenic oxidative damage via ROS production is the effective redox potential experienced by the cells. Therefore, establishing the relationship between the strength of the oxidative action, characterized by redox potential, and biomolecular consequences is critical to elucidating the thermodynamic framework of oxidative damage.</p> <p>Conventional techniques used to induce ROS production and oxidative damage in mammalian cells include addition of chemical oxidizers and/or exposure to ionizing radiation. However, the oxidizing strength of these methods and reagents can be difficult to precisely quantify and to subsequently describe in thermodynamic terms. Our approach for achieving controlled, reproducible oxidative stress in mammalian cells is treatment under potentiostatic conditions.</p>	
<p>First, we investigated the cytotoxic effect of applying an electrochemical potential gradient to growing cultures of Chinese hamster ovary (CHO) cells using a bipolar electrode method. A constant current was applied along a confluent cell layer on the flask bottom, creating a potential gradient across the length of the surface. Potential gradients ranging from -100 mV to +250 mV (vs. Ag/AgCl) were generated over short (1 h to 2 h) and long (72 h) treatment periods. Calcein AM and ethidium homodimer-1 dyes were introduced after treatment as biomarkers for live and dead cells, respectively, and were imaged with a fluorescence microscope. Images were analyzed for integrated pixel density with a custom ImageJ software macro.</p> <p>Cell viability gradients were produced within a range of treatment levels. Cells subjected to high oxidative potentials underwent apoptosis, while cells subjected to neutral or reductive potentials remained alive. These results will be compared with DNA strand break damage as analyzed by single cell gel electrophoresis (Comet assay). This demonstrates the advantage of potentiostatic treatment as a reproducible platform for quantifying oxidative stress and for testing antioxidant efficacy.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> William Byron <b>Grant Number</b>   70NANB15H165 <b>Academic Institution:</b> Tulane University <b>Major:</b> Physics and Math <b>Academic Standing</b> Graduate <b>(Sept. '15):</b>
<b>Future Plans</b> <b>(School/Career):</b>	In Fall of '15 I will be hiking in Oregon and Washington for 6 weeks and then returning to New Orleans to tutor Physics and Math.
<b>NIST Laboratory, Division, and Group:</b>	Physical Measurement Laboratory, Radiation Physics Division, Neutron Physics Group
<b>NIST Research Advisor:</b>	Scott Dewey
<b>Title of Talk:</b>	Residual Gas Effect on aCORN
<b>Abstract:</b>	
<p>The degree of angular correlation between the beta electron and antineutrino in neutron decay is denoted by the dimensionless parameter “<math>\alpha</math>”. 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 “<math>\alpha</math>” had systematic uncertainties on the order of 5%. The aCORN (a CORrelation in Neutron decay) experiment is designed to obtain a systematic uncertainty of less than 1%. The experiment 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 antineutrino. In the experiment the proton travels several meters through a <math>10^{-7}</math> torr vacuum pressure before being detected. A potentially important systematic error associated with the velocity dependent removal of protons by the residual gas is being analyzed. Initially it is assumed that the residual gas consists of pure molecular hydrogen. The effect is being assessed with a Monte Carlo treatment that follows individual protons as they travel through the residual gas and via a measurement of the experimental parameter at both the nominal operating pressure and a significantly elevated controlled pressure.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Megan Cain <b>Grant Number</b>   70NANB15H181 <b>Academic Institution:</b> West Virginia University <b>Major:</b> Chemical Engineering <b>Academic Standing</b> Senior <b>(Sept. '15):</b>
<b>Future Plans</b> <b>(School/Career):</b>	A career in the Materials Science field
<b>NIST Laboratory, Division, and Group:</b>	Materials Measurement Lab (MMI); Materials Measurement and Science Division (MMSD); Nanomechanical Properties Group (09)
<b>NIST Research Advisor:</b>	Brian Bush
<b>Title of Talk:</b>	Length Scale Effects on the Mechanical Properties of Soft Materials
<b>Abstract:</b>	
<p>Hydrogels constructed from poly (ethylene glycol) (PEG) are three-dimensional crosslinked polymer networks that are capable of absorbing large quantities of water and exhibit mechanical properties that mimic those of natural tissues. This makes them suitable for a variety of bio engineering uses including tissue scaffolds, drug delivery, and contact lenses. However, the scale at which the hydrogels are tested has been shown to alter the mechanical properties recorded and can range over several orders of magnitude for qualitatively similar materials<sup>[1,2]</sup>. Thus, it is of interest to determine the effects of indenter size on the extracted mechanical properties of PEG hydrogels.</p> <p>In this experiment, the mechanical properties of PEG hydrogels were measured with a range of applied forces and indenter sizes to determine their effect on the resultant mechanical properties. Hydrogels were fabricated at weight concentrations of 5 wt% and 10 wt%. Bulk polymer methods were used to calculate the gel fraction and swelling ratio of the hydrogels in order to determine the extent of crosslinking and average pore size, respectively. AFM testing with probes of varying radii (e.g. 10 nm, 150 nm, 1.3 <math>\mu</math>m, and 4.4 <math>\mu</math>m) was conducted by indenting to a maximum applied load of 2 nN to 100 nN, holding at constant displacement for 15 s, and then retracting the probe from the surface. The force relaxation response during the hold period was modeled to extract indentation modulus and viscoelastic and poroelastic time constants which were then used to approximate pore size. Preliminary results indicate the gels are heterogeneous with indentation moduli on the order of several kilopascals and pore sizes in the range of 1 nm to 2 nm. However, a final mechanical analysis to determine whether these properties are affected by indenter size has not been completed at this time; these calculations are currently underway.</p>	
<p>[1] Z. Drira and V. Yadavalli, <i>Journal of the Mechanical Behavior of Biomedical Materials</i>, 2013, <b>18</b>, 20-28.  [2] S. P. Zuttyak and J. B. Leach, <i>Biomacromolecules</i>, 2010, <b>11</b>, 1348-1357.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD August 4-6, 2015	
Name: Matthew Calamari	Grant Number   70NANB15H166 Major: Mechanical Engineering
Academic Institution: Binghamton University	
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Look for a career in Engineering	
NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Production Systems Group	
Advisor: Greg Vogl	
Title of Talk: Data Analysis and Validation for Sensor-Based Diagnostics of CNC Linear Axes	
<b>Abstract:</b>	
Computer numerical control (CNC) linear axes are common tools used in manufacturing processes. Along these axes there are small errors due to degradation of the axis which can cause imperfections in the parts being made by the machines. Currently measuring these errors is done using a laser method to detect movement or angular change. Although this is highly effective, it can be a long and complicated process, and manufacturers prefer not to shut down production to test their machines. Clearly, a faster method that is just as accurate is needed. The Prognostics and Health Management for Smart Manufacturing Systems (PHM4SMS) project at the National Institute of Standards and Technology (NIST) is developing a sensor box method for detecting linear axis errors due to degradation. This method uses accelerometers, inclinometers and a rate gyroscope and measures acceleration, angular position and angular velocity data collected for three different axis speeds. The data is collected along the entire axis travel, and the method ‘fuses’ the data to calculate the straightness and angular errors along an axis of a machine tool.	
This SURF project works on developing the data analysis code within MATLAB for the sensor box method. The data analysis code must be able to read in all saved data from the sensor box and manipulate it to produce straightness and angular error curves plotted against the axial position. The code uses the data along with various filters, interpolation, and integration, to yield the estimated straightness and angular errors for every desired axis position. The MATLAB results for the sensor box method are compared to the reference “laser method” results to determine the accuracy of the sensor box method. In addition, more research into different sensors and data acquisition modules is necessary for improvements to the method. Simulations were produced within MATLAB for various accelerometers and data acquisition modules to increase the accuracy of the sensor box method. According to the simulations, the estimated straightness error has an RMS uncertainty of $0.52 \mu\text{m}$ using a certain accelerometer that can measure down to 0 Hz.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD August 4-6, 2015	
	
Name: Juana Alejandra Cerna Sanchez	Grant Number   70NANB15H084 Major: Public Health
Academic Institution: American University	
Academic Standing (Sept. '15): Graduated	
Future Plans (School/Career): MD/PhD programs	
NIST Laboratory, Division, and Group: Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis and Modeling Group	
NIST Research Advisor: John Lu	
Title of Talk: 3D to 1D: Variances of Tumor Measurements from CT Patient Data Sets with Linear Scale Analysis of Volume Measurements	
<b>Abstract:</b>	
The purpose of this project was to assess variability, including reader variability, in tumor measurements when there are “no change” conditions using a linear scale model for computed tomography (CT) data sets. This paper reports the statistical data analysis of the Quantitative Imaging Biomarker Alliance (QIBA) 1B data sets containing CTs of 32 non-small lung cancer patients interpreted by 10 readers. Reader variability of spherical (normal) and non-spherical nodules was quantified in this analysis using mean, standard deviation (SD), and mean absolute deviation (MAD) measurements. The readers and measurements in the data were divided into two phases: one in which the reader had independent readings of each CT and the other where the readers had locked, sequential readings. Unidimensional (1D), bidimensional (2D) and volumetric (3D) measurements were the three sizing measurements used to analyze inter-reader variability. The 2D and 3D measurements were transformed to linear diameter measurements with equivalent area or volume of spherical objects. The variability (SD) values for mean percent difference are very comparable across the three measures using the linear scale model. For Phase 1 the 2D and 3D mean percent difference ( $\pm SD$ ) was $(10.0 \pm 25.1\%)$ , $(11.5 \pm 20.2\%)$ respectively and for phase 2 $(0.54 \pm 9.9\%)$ , $(1.3 \pm 10.3\%)$ , respectively. Results indicate that phase two, locked sequential reads, eliminate bias and reduce variance. We also observe the significant variability among readers. The observed large biases (outliers) in phase 1 were attributed to four of the five readers; for phase 2 the outliers were attributed to only two readers. The results validate our proposed linear scale approach of volume measurements are preferable to the previous non-linearized models due to the comparability of the results across the three sizes.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Maria A. Chaudhry
	<b>Academic Institution:</b> Montgomery College
	<b>Academic Standing:</b> Graduate Student, Junior at UMBC/U MUC
	<b>(Sept. '15):</b> Transferring to University of Maryland Baltimore Campus(UMB), Master in Computer Future Plans
	<b>(School/Career):</b> Science /Joining Accenture Federal Services as a career at the end of august
	<b>NIST Laboratory,</b> Material Measurement Laboratory, Biosystems and Biomaterials division, Cell Systems
	<b>Division, and Group:</b> Science Group (644.04)
	<b>NIST Research Advisor:</b> Talapady N. Bhattacharya
	<b>Title of Talk:</b> Developing Websites using Visual Studio and SQL Server
	<b>Abstract:</b> A user friendly website is an important tool for people to navigate through. Research data of scientists should be accessible for users through website. Consistent navigation throughout the website allows users to feel comfortable about where they are and what they are looking for. A good usability website makes it easy and fast to find the information users need.
	The main reason for developing our web projects was to make them user friendly, efficient, search data faster, and able to download the data. Visual Studio and SQL Server software were used to approach this model. Visual Studio contains C#, ASP.NET and HTML programming languages. ASP and HTML controls are used for different design purposes; C# coding for programming and SQL queries to get the data from database. Web Service is used to load the data faster. Furthermore, we created functionality for users to download and read the data in Excel worksheet. Each website's data has its own scope, and we tried to meet user needs by providing them the data in the most efficient manner.
	We also created clear labels, home page and few selections of pages to give users a sense of where they are and how to get back. These websites adapt to match user needs in almost every possible way. Search functions are accessible to visitors with an auto fill component which suggests to the user what kind of data is in the database. This function is a way to quickly find the information users might be looking for. To conclude, these websites efficiently provide specific data according to user needs.
	<a href="https://wschwchemd01.nist.gov/cellimage/default.aspx">https://wschwchemd01.nist.gov/cellimage/default.aspx</a>
	<a href="https://wschwchemd01.nist.gov/indexing/default.aspx">https://wschwchemd01.nist.gov/indexing/default.aspx</a>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
	<b>Name:</b> Eddie Chang
	<b>Academic Institution:</b> University of Maryland College Park
	<b>Grant Number:</b> 70NANB15H163
	<b>Major:</b> Mechanical Engineering & Physics
	<b>Academic Standing:</b> Junior
	<b>(Sept. '15):</b> Graduate school, research career in energy
	<b>Future Plans (School/Career):</b> Center for Nanoscale Science and Technology, Electron Physics Group
	<b>NIST Laboratory, Division, and Group:</b> Center for Nanoscale Science and Technology, Electron Physics Group
	<b>NIST Research Advisor:</b> Ihabz McCelland, Kevin Twedt
	<b>Title of Talk:</b> Modeling Electrochemical Lithiation of Tin with Li MOTS
	<b>Abstract:</b> Lithium ion batteries, commonly used in portable consumer electronics, show promise for heavy-duty applications such as hybrid and fully electric vehicles. While graphite is the current choice anodic material, efforts are directed towards studying materials which may surpass graphite as anodes for energy storage devices with high power and energy densities. Silicon and tin are two popular candidates for the next generation of commercial battery anodes owing to their excellent specific capacities of 4200 mAh/g Si and 992 mAh/g Sn, while other options such as tin nanoparticles encapsulated by carbon have also been explored. <sup>1</sup> Great focus exists on constructing, cycling and evaluating the performance of batteries constructed with these materials, but studying interactions of lithium ions on the nanoscale with electrolytic and anodic materials may allow more precise methodologies for selecting, studying, and evaluating battery materials. This can be done with recent technology which uses photoionization of laser-cooled atoms to create a high brightness beam of Li ions that can be focused to the nanometer scale onto the surface of a sample.
	It is first necessary to establish this new technology as a viable tool to study electrochemical lithiation of battery materials. To investigate this, samples of tin were lithiated using both a 3-electrode cell set-up and a focused beam of ions to study the behavior of lithium in each case. Tin was selected due to the easily visible changes it undergoes upon lithiation. <sup>2</sup> Different doses of lithium were delivered to observe various stages of the formation of lithium-tin alloys. Thus far, certain aspects of lithiation via electrochemistry and focused ion beam appear similar. However, more detailed analysis is required to study the effects on crystallography and sample composition as a function of dose and to determine whether the new technology is a good model for behavior of lithium in anodic materials.
	<sup>1</sup> J. Mater. Chem. A, 2013, 1, 8710 <sup>2</sup> Chem. Mater., 2014, 26, 4102-4108

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Seong Ik Cheon
Academic Institution:	College of William and Mary
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Grad school for Chemistry
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction group
NIST Research Advisor:	Shonali Nazare, Szabolcs Matko
Title of Talk:	Hot seat: Fire Protective Performance of Barrier Fabrics
Abstract:	<p>In residential upholstered furniture (RUF), the polyurethane foam (PUF) is the most flammable component. Barrier fabrics (BFs) are often used to protect PUF from heat and flames. For this purpose, the barrier fabrics are placed between the outer layer (cover fabric) and the polyurethane foam. Textile industry has successfully developed barrier fabrics using variety of fiber blends and flame retarding technologies. Range of commercially available BFs includes a variety of textile structures including highloft (thick fiber mesh), nonwoven battings (thin, pressed/needle punched fiber), knitted, and woven structures. However, the test methods for evaluating barrier fabrics have been limited only as quality control (pass/fail) tool. None of these tests provides an effective tool for quantitatively screening BFs. Efforts for developing a test method to quantify barrier effectiveness are ongoing.</p> <p>Thermal protective performance of BFs is a function of a number of variables including its ignitability, gas permeability, heat transfer properties, and char structure. Three different open-flame ignition test methods have been employed to assess protective performance of barrier fabrics. The test methods vary in sample orientation, sample configuration, type and severity of ignition sources. The component test (BF only) provides quantitative data while the composite tests (combination of BF, CF, PUF) provide qualitative (pass/fail) information. Data for various BFs subjected to different tests will be discussed. Careful interpretation of burning behavior of BF composite specimens in addition to the quantitative data will be used to evaluate thermal protective performance and ranking of BFs.</p>
Name:	Nathan Christie
Academic Institution:	Carnegie Mellon University
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Master's or PhD in Materials Science & Engineering followed by either industry or research
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymer and Complex Fluids Group
NIST Research Advisor:	Debra Audus
Title of Talk:	Modeling Competition between Polymerization and Phase Separation with a Webtool
Abstract:	<p>In an effort to accelerate the design and development of new materials, specifically polymeric materials, I have aided in the development of a webtool that takes relevant input parameters and utilizes them to generate phase boundaries and critical properties of polymer blends and solutions. The development of the webtool, which previously included models for polymer blends (Flory-Huggins and Lattice Cluster Theory) and polyelectrolyte solutions (Vorn-Overbeek), is supported by the Materials Genome Initiative (MGI), a white house sponsored initiative whose goal is to bring new materials to market two times faster and two times cheaper, and the Center for Hierarchical Materials Design (CHM4D), a NIST sponsored center for advanced materials research. This webtool allows researchers to model their systems and make predictions upon changes in conditions such as temperature or concentration. Thus far, the webtool has focused on systems composed of polymers with a fixed length or, equivalently, a fixed number of monomers. My work extends these capabilities to include a model of polymerization, the Free Association Model. Within this relatively straightforward model, the solution is initially composed of monomers in a solvent. The monomers then react to form polymers of various lengths, which are in equilibrium with one another. Additionally, the system can undergo phase separation yielding two distinct phases composed of different distributions of polymer lengths; thus, the Free Association Model can be used to model competition between polymer chain formation and separation in fluids. Models of polymerization, like the Free Association Model, can also describe phenomena that are less commonly thought of as polymerization such as the formation of fibrils by a globular protein, Actin, or the formation of chains of nanoparticles that interact through both van der Waals interactions and dipolar interactions. In addition to describing the details of the Free Association model, I will also present some of the technical details associated with the development of the webtool and the calculation of phase coexistence curves.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Seong Ik Cheon
Academic Institution:	College of William and Mary
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Grad school for Chemistry
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction group
NIST Research Advisor:	Shonali Nazare, Szabolcs Matko
Title of Talk:	Hot seat: Fire Protective Performance of Barrier Fabrics
Abstract:	<p>In residential upholstered furniture (RUF), the polyurethane foam (PUF) is the most flammable component. Barrier fabrics (BFs) are often used to protect PUF from heat and flames. For this purpose, the barrier fabrics are placed between the outer layer (cover fabric) and the polyurethane foam. Textile industry has successfully developed barrier fabrics using variety of fiber blends and flame retarding technologies. Range of commercially available BFs includes a variety of textile structures including highloft (thick fiber mesh), nonwoven battings (thin, pressed/needle punched fiber), knitted, and woven structures. However, the test methods for evaluating barrier fabrics have been limited only as quality control (pass/fail) tool. None of these tests provides an effective tool for quantitatively screening BFs. Efforts for developing a test method to quantify barrier effectiveness are ongoing.</p> <p>Thermal protective performance of BFs is a function of a number of variables including its ignitability, gas permeability, heat transfer properties, and char structure. Three different open-flame ignition test methods have been employed to assess protective performance of barrier fabrics. The test methods vary in sample orientation, sample configuration, type and severity of ignition sources. The component test (BF only) provides quantitative data while the composite tests (combination of BF, CF, PUF) provide qualitative (pass/fail) information. Data for various BFs subjected to different tests will be discussed. Careful interpretation of burning behavior of BF composite specimens in addition to the quantitative data will be used to evaluate thermal protective performance and ranking of BFs.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Ramon Collazo-Martis	Grant Number   70NANB15H171
Academic Institution: University of Puerto Rico, Rio Piedras Campus	Major: Computer Science
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	After getting my bachelor degree I want to go to Grad School.
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group
NIST Research Advisor:	Rene Peralta
Title of Talk:	Combinational Circuit Optimization: New Results
<b>Abstract:</b>	
In this work we present efficient circuits using only AND and XOR gates, that is, addition and multiplication modulo 2. One goal is to find the smallest number of gates that produces the desired output. It is also important to have circuits with low-depth and few AND gates. These properties are of interest in cryptography and can be used in fully homomorphic encryption, zero-knowledge proofs, and secure multiparty computation.	
<b>Abstract:</b>	
Heavy fermions materials are a class of inter-metallic compounds which exhibit an extremely high effective electron mass, upwards of $1000m_e$ , due to competition between the Kondo and the RKKY interactions. These interactions cause these materials to lie on the edge of magnetic instability, giving them the ability to reach many different exotic phases, such as antiferromagnetic order and unconventional superconductivity, also found in high temperature superconductors. In a previous study, it was found that CeRhIn <sub>5</sub> , a well-known heavy-fermion compound, antiferromagnetically orders at $T_n=3.8$ K with an incommensurate structure under ambient pressure but also goes superconducting at $T_c=2.1$ K under applied pressure. In our current study we explore the magnetic ordering of Ce <sub>1-x</sub> Yb <sub>x</sub> RhIn <sub>5</sub> as a function of Yb concentration through x-ray diffraction, magnetometry, and neutron diffraction. We have found that adding Yb to the Ce <sub>1-x</sub> Yb <sub>x</sub> RhIn <sub>5</sub> parent compound changes the magnetic structure from an incommensurate ( $\mathbf{k}=[\frac{1}{2}, \frac{1}{2}, 0.297]$ ) to commensurate ( $\mathbf{k}=[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ ) at ambient pressure, information gained from this study furthers our understanding of the link between antiferromagnetic ordering and unconventional superconductivity.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Ramon Collazo-Martis	Grant Number   70NANB15H171
Academic Institution: University of Puerto Rico, Rio Piedras Campus	Major: Computer Science
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	After getting my bachelor degree I want to go to Grad School.
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group
NIST Research Advisor:	Rene Peralta
Title of Talk:	Combinational Circuit Optimization: New Results
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In this work we present efficient circuits using only AND and XOR gates, that is, addition and multiplication modulo 2. One goal is to find the smallest number of gates that produces the desired output. It is also important to have circuits with low-depth and few AND gates. These properties are of interest in cryptography and can be used in fully homomorphic encryption, zero-knowledge proofs, and secure multiparty computation.	
<b>Abstract:</b>	
Heavy fermions materials are a class of inter-metallic compounds which exhibit an extremely high effective electron mass, upwards of $1000m_e$ , due to competition between the Kondo and the RKKY interactions. These interactions cause these materials to lie on the edge of magnetic instability, giving them the ability to reach many different exotic phases, such as antiferromagnetic order and unconventional superconductivity, also found in high temperature superconductors. In a previous study, it was found that CeRhIn <sub>5</sub> , a well-known heavy-fermion compound, antiferromagnetically orders at $T_n=3.8$ K with an incommensurate structure under ambient pressure but also goes superconducting at $T_c=2.1$ K under applied pressure. In our current study we explore the magnetic ordering of Ce <sub>1-x</sub> Yb <sub>x</sub> RhIn <sub>5</sub> as a function of Yb concentration through x-ray diffraction, magnetometry, and neutron diffraction. We have found that adding Yb to the Ce <sub>1-x</sub> Yb <sub>x</sub> RhIn <sub>5</sub> parent compound changes the magnetic structure from an incommensurate ( $\mathbf{k}=[\frac{1}{2}, \frac{1}{2}, 0.297]$ ) to commensurate ( $\mathbf{k}=[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ ) at ambient pressure, information gained from this study furthers our understanding of the link between antiferromagnetic ordering and unconventional superconductivity.	

SURF Student Colloquium	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Andres Correa Hernandez	Grant Number   70NANB15H092
Academic Institution: Boise State University	Major: Materials Science & Engineering
Academic Standing   Sophomore	
Future Plans   Obtain a Ph.D. in Materials Science & Engineering	
(School/Career):	
NIST Laboratory: Material Measurement Laboratory, Materials Measurement Science Division, Materials	
Division, and Group: Structure and Data Group	
NIST Research Advisor: Eric J. Cockayne	
Title of Talk: Density Functional Theory Studies of Carbon Dioxide Interaction with Oxide Surfaces	
<b>Abstract:</b> With the increasing levels of atmospheric carbon dioxide posing imminent threats related to global warming and ocean acidification, carbon-capture technologies, which have the ability to significantly reduce the amount of CO <sub>2</sub> entering the atmosphere, have drawn great interest. In an effort to further expand these technologies we simulated the interaction of CO <sub>2</sub> with nanoparticulates of two different oxides: α-MnO <sub>2</sub> and olivine. α-MnO <sub>2</sub> is a solid oxide that is nanoporous, with a large active surface area, offering great potential for capturing carbon dioxide. Olivine, specifically the forsterite (Mg <sub>2</sub> SiO <sub>4</sub> ) end member, is one of the most abundant minerals commonly found in the Earth, and captures carbon through natural weathering processes. Accurate density functional theory (DFT) electronic structure calculations can help to quantify the interaction of carbon dioxide with the solids, and to assist in the design of new materials with desired properties (new technologies). While numerous studies have investigated the interaction of CO <sub>2</sub> with bulk solids, studies of interactions with nanoparticle surfaces are more limited. Scripts were devised and carried out to run parallel DFT computations on a computer cluster. DFT energy minimization calculations were performed to find the binding positions, and energies, of CO <sub>2</sub> at various positions on the nanoparticiles. Afterwards, more advanced DFT techniques were used in order to better understand these systems. Our results show that CO <sub>2</sub> captured by olivine transforms into a CO <sub>3</sub> <sup>2-</sup> ion, in agreement with the natural reaction. In α-MnO <sub>2</sub> , we compare the binding energy of CO <sub>2</sub> inside the pore with the binding energy of CO <sub>2</sub> on the external surface.	

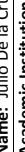
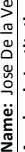
SURF Student Colloquium	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Shannion Craig	Grant Number   70NANB15H146
Academic Institution: Colorado School of Mines	Major: Engineering Physics
Academic Standing   Senior	
(Sept. '15):	
Future Plans   MS in Applied Mathematics and Statistics with a computational emphasis	
(School/Career):	at Colorado School of Mines
NIST Laboratory: Engineering Laboratory, Applied Economics Office	
Division, and Group: NIST Research	
Advisor: Joshua Kneifel	
Title of Talk: Calculating Sustainability Performance of Residential Buildings	
<b>Abstract:</b> Lawmakers desire better environmental sustainability and energy efficiency in new buildings. However, we currently lack a good measurement tool for sustainability and energy efficiency. Using whole building energy simulations, Life Cycle Costing (LCC), and Life Cycle Assessment (LCA), the Applied Economics Office (AEO) is developing metrics and tools to aid sustainable building design. These new metrics assess twelve (12) environmental performance categories and integrate economic performance metrics, yielding science-based measures of the business case for investment choices in high-performance sustainable buildings. The Building Industry Reporting and Design for Sustainability (BIRDS) tool allows users to easily and rapidly compare energy use, life cycle costs, and environmental impacts of a building designed to meet different levels of energy efficiency. As of May 2015, BIRDS (v2.0) included a residential building database of ten (10) building types designed to meet four editions of the International Energy Conservation Code (IECC) in 228 cities across the U.S. (9,120 unique building designs).	
My research expanded BIRDS in size, scope, and functionality to be incorporated into BIRDS (v3.0). This required the creation of generalized code for the calculations involved in residential sustainability analysis. Using this code, I re-generated this residential buildings database and generated another database for 240,000 building designs based on NIST's Net Zero Energy Residential Test Facility (NZERTFF). I expanded the user's choices to include incremental energy efficiency measures, comfort and indoor air quality metrics, mortgages, and various discount rates. I also automated the analysis of these databases at the state and national level.	
Moving forward, this project developed the framework to generate sustainability calculations for custom building designs based on inputs from whole building energy simulation software. This allows BIRDS to continue expanding by incorporating more building types, design choices, and complexity of economic incentives in the future.	

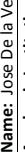
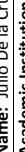
<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Kiersta S. Davis
Academic Institution:	Montgomery College
Academic Standing	Junior
(Sept. '15):	Grad School, PhD in Biochemistry and Genetics from The George Washington University,
Future Plans	Future Plans
(School/Career):	Geneticist
NIST Laboratory,	NIST Laboratory, Material Measurement Laboratory, Biomolecular Measurement, 645
Division, and Group:	Division, and Group:
NIST Research	Mark Lowenthal
Advisor:	Using evolution to predict novel N-glycosylation on non-canonical protein motifs
<b>Abstract:</b>	
Glycosylation is an important co-translational modification that significantly influences the function and stability of proteins. N-linked glycosylation is known to occur at a (canonical) consensus motif in the pattern N-X-S/T where "X" is any amino acid other than proline, but has also been observed on rare occasions on other primary sequence motifs. The literature describes fewer than ten proteins reported to be N-glycosylated at "non-canonical" motifs in the conformation N-X-C, where a cysteine replaces the serine or threonine as seen in the canonical consensus motifs. It is important to note that although a protein may contain a consensus motif, it does not dictate that a glycan <i>will</i> be attached (site occupied), but rather indicates that there is the <i>potential</i> at that site for glycan attachment. Because of the functional importance of N-glycosylation, developing a tool to predict glycosylation site occupancy <i>in silico</i> would greatly benefit researchers. The tools that currently exist to predict N-glycosylation are based on prior knowledge of secondary and tertiary protein structures and are often non-specific.	
<b>Abstract:</b>	
We compute closed-form expressions for oscillatory and damped spherically symmetric fundamental solutions of the Helmholtz equation in hyperspherical and hyperbolic geometry. We are using the R-radius hypersphere and R-radius hyperboloid model of hyperbolic geometry. These models represent Riemannian manifolds with positive constant and negative constant curvature respectively. We also derive Gegenbauer expansions for these fundamental solutions in geodesic polar coordinates.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Thinh Dang
Academic Institution:	American University
Academic Standing	Major: Mathematics
(Sept. '15):	Junior
Future Plans	Undecided
(School/Career):	Information Technology Laboratory, Applied and Computational Mathematics Division,
NIST Laboratory,	NIST Mathematical Software Group
Division, and Group:	Howard Cohl
NIST Research	Howard Cohl
Advisor:	Fundamental solution of the Helmholtz Equation in hyperbolic and hyperspherical geometry
<b>Abstract:</b>	
We compute closed-form expressions for oscillatory and damped spherically symmetric fundamental solutions of the Helmholtz equation in hyperspherical and hyperbolic geometry. We are using the R-radius hypersphere and R-radius hyperboloid model of hyperbolic geometry. These models represent Riemannian manifolds with positive constant and negative constant curvature respectively. We also derive Gegenbauer expansions for these fundamental solutions in geodesic polar coordinates.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Kyle Davis	<b>Grant Number</b> 70NANB15H155
<b>Academic Institution:</b> The College of New Jersey	<b>Major:</b> Computer Science
<b>Academic Standing</b>	<b>Senior</b>
<b>(Sept. '15):</b>	
<b>Future Plans (School/Career):</b>	Planning either to pursue a career that combines my interests in computer science and financial analysis, or continue my degree with a focus in Human Computer Interaction.
<b>NIST Laboratory,</b>	Information Technology Laboratory, Applied & Computational
<b>Division, and Group:</b>	Mathematics Division, High Performance Computing & Visualization Group
<b>NIST Research Advisor:</b>	Sandy Ressler
<b>Title of Talk:</b>	Integration of Web-Based 3D Modelling with Leap Motion Tracking and Oculus Rift
<b>Abstract:</b>	
<p>The purpose of my summer research was to explore the capabilities of web-based 3D graphics and virtual reality. This was done through a number of methods, all utilizing Extensible 3D Graphics Document Object Model (X3DOM), a JavaScript library that allows the creation and manipulation of 3D objects within a web browser. Graphics are placed directly into the HTML Document Object Model (DOM). Using the HyperText Markup Language (HTML), the DOM lets us use the web development infrastructure to create graphics, even though it was never intended to do so. This also means that real-time changes can be made to the graphics while the page is running, without the use of plugins or extensions, which is an extremely powerful way of sharing information. In conjunction with X3DOM, both the Leap Motion and Oculus Rift were utilized. The Leap Motion is an inexpensive tool that is used to track the user's hands and gestures and translate those movements into the computer. The Oculus Rift is a virtual reality headset that allows the user to view a 3D environment. The culmination of this project is a tool to convert 3D models into something that can be read and interpreted by the Oculus and interacted with by the Leap Motion.</p>	
<b>Name:</b> Mark Dear	<b>Grant Number</b> 70NANB15H191
<b>Academic Institution:</b> Pennsylvania State University	<b>Major:</b> Computational Mathematics
<b>Academic Standing</b>	<b>Junior</b>
<b>(Sept. '15):</b>	
<b>Future Plans (School/Career):</b>	Attend graduate school in computer science
<b>NIST Laboratory,</b>	Information Technology Laboratory, Software and Systems Division, Information Systems
<b>Division, and Group:</b>	Group
<b>NIST Research Advisor:</b>	Walid Keyrouz
<b>Title of Talk:</b>	Experiments in Numerical Reproducibility
<b>Abstract:</b>	
<p>Numerical reproducibility is one of the core assumptions that underlie the use of modeling and simulations to derive computational measurements. Unfortunately, it is precisely this reproducibility that has become quite difficult to achieve with modern architectures in High Performance Computing (HPC). Reproducing numerical results obtained with finite-precision numbers (e.g., float and double) require the operations to execute in a particular order because arithmetic operations on such numbers are not generally associative and commutative. So when they are not executed in that order problems occur. Modern HPC systems use multicore processors as well as cluster and accelerator computing. HPC takes advantage of the many processing elements in a cluster by distributing computations among the various cores available in a system. Unfortunately, these systems do not allow the programmers let alone the users to specify the order of execution of operations when coding operations in a straightforward manner. Hence reproducibility cannot be guaranteed in these systems. We are currently running numerical reproducibility experiments that implement a variety of algorithms for reducing large vectors of finite-precision numbers to their sums. These algorithms have differing reproducibility properties. We will document the experiments and present results from a reproducibility perspective.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Kyle Davis	
<b>Academic Institution:</b> The College of New Jersey	<b>Grant Number</b> 70NANB15H155
<b>Academic Standing</b>	<b>Senior</b>
<b>(Sept. '15):</b>	
<b>Future Plans (School/Career):</b>	Planning either to pursue a career that combines my interests in computer science and financial analysis, or continue my degree with a focus in Human Computer Interaction.
<b>NIST Laboratory,</b>	Information Technology Laboratory, Applied & Computational
<b>Division, and Group:</b>	Mathematics Division, High Performance Computing & Visualization Group
<b>NIST Research Advisor:</b>	Sandy Ressler
<b>Title of Talk:</b>	Integration of Web-Based 3D Modelling with Leap Motion Tracking and Oculus Rift
<b>Abstract:</b>	
<p>The purpose of my summer research was to explore the capabilities of web-based 3D graphics and virtual reality. This was done through a number of methods, all utilizing Extensible 3D Graphics Document Object Model (X3DOM), a JavaScript library that allows the creation and manipulation of 3D objects within a web browser. Graphics are placed directly into the HTML Document Object Model (DOM). Using the HyperText Markup Language (HTML), the DOM lets us use the web development infrastructure to create graphics, even though it was never intended to do so. This also means that real-time changes can be made to the graphics while the page is running, without the use of plugins or extensions, which is an extremely powerful way of sharing information. In conjunction with X3DOM, both the Leap Motion and Oculus Rift were utilized. The Leap Motion is an inexpensive tool that is used to track the user's hands and gestures and translate those movements into the computer. The Oculus Rift is a virtual reality headset that allows the user to view a 3D environment. The culmination of this project is a tool to convert 3D models into something that can be read and interpreted by the Oculus and interacted with by the Leap Motion.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Jose De la Vega <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> I am planning to pursue a PhD in cyber security here in the United States. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Laboratory, Computer Security Division, Secure Systems & Applications Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Michael Jorga <b>Title of Talk:</b> Coloring the Facets of the Cloud Rubik's Cube
	<b>Name:</b> Julio De la Cruz Natera <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> I am planning to pursue a PhD in cyber security here in the United States. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Laboratory, Computer Security Division, Secure Systems & Applications Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Michael Jorga <b>Title of Talk:</b> Coloring the Facets of the Cloud Rubik's Cube
	<b>Name:</b> Michael Jorga <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> I am planning to pursue a PhD in cyber security here in the United States. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Laboratory, Computer Security Division, Secure Systems & Applications Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Michael Jorga <b>Title of Talk:</b> Coloring the Facets of the Cloud Rubik's Cube
	<b>Name:</b> Aurelien Delaitre <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> Right now my future plans are to get a Master degree in Computer Science and build a big Cybersecurity company in Puerto Rico. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Lab, Software and Systems Division, Software Quality Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Vadim Okun <b>Title of Talk:</b> Fuzzing bugs out of Wireshark to test static analyzers

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Julio De la Cruz Natera <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> I am planning to pursue a PhD in cyber security here in the United States. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Laboratory, Computer Security Division, Secure Systems & Applications Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Michael Jorga <b>Title of Talk:</b> Coloring the Facets of the Cloud Rubik's Cube
	<b>Name:</b> Jose De la Vega <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> Right now my future plans are to get a Master degree in Computer Science and build a big Cybersecurity company in Puerto Rico. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Lab, Software and Systems Division, Software Quality Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Vadim Okun <b>Title of Talk:</b> Fuzzing bugs out of Wireshark to test static analyzers
	<b>Name:</b> Aurelien Delaitre <b>Academic Institution:</b> University of Puerto Rico, Rio Piedras Campus <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans:</b> Right now my future plans are to get a Master degree in Computer Science and build a big Cybersecurity company in Puerto Rico. <b>(School/Career):</b> <b>NIST Laboratory:</b> Information Technology Lab, Software and Systems Division, Software Quality Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Vadim Okun <b>Title of Talk:</b> Fuzzing bugs out of Wireshark to test static analyzers

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
<b>Name:</b> Moira Dewey	<b>Grant Number</b> 70NANB15H168
<b>Academic Institution:</b> University of Maryland College Park	<b>Major:</b> Computer Science
<b>Academic Standing</b>	<b>Grade:</b> Junior
<b>(Sept. '15):</b>	<b>Academic Standing</b> Junior
<b>Future Plans</b>	<b>Programmer;</b> I am leaning towards going to graduate school, but am still uncertain.
<b>(School/Career):</b>	I think I would like to go into graphics programming.
<b>NIST Laboratory,</b>	<b>NIST Laboratory,</b> Engineering Laboratory, Fire Research Division, Flammability Reduction Group
<b>Division, and Group:</b>	<b>Division, and Group:</b>
<b>NIST Research</b>	<b>Research Advisor:</b> William Pitts
<b>Advisor:</b>	
<b>Title of Talk:</b>	<b>Title of Talk:</b> Realization Through Visualization: Understanding How Barrier Fabrics Affect Flame Spread on Upholstered Furniture
<b>Abstract:</b>	<p>Historically, a large fraction of fire fatalities in the United States have been attributed to ignited mattresses and residential upholstered furniture. While mattresses have become safer through the establishment of regulations that have led to reductions in their flammability, upholstered furniture has been less successfully regulated to reduce flammability. As such, research is being done to develop methods to improve the fire safety of upholstered furniture. Our experiment investigated how several different factors in combination affect the burning behavior of upholstered furniture. These factors include fabric material (either 100% cotton or a blend of polyurethane and polypropylene), the type of inner polyurethane foam, the use of polyester padding and wrapping, and the use of different kinds of barrier materials, which are placed between the highly flammable foam inside the cushion and the outer cover fabric in order to reduce or slow down a fire. In the experiment, real-scale mockups were assembled and ignited, and various aspects of fire behavior were characterized. In particular, one aspect was the flame spread rates over the surfaces of the cushions forming the mock-up. To do this in a standardized fashion, grids with one square-inch blocks were mapped over the surfaces of the back and seat cushions, and a time series of snapshots of the seat and back cushion surfaces of each chair were collected from videos taken of the burning mock-ups. For each snapshot, an image of the outline of the flame spread was created with Adobe Photoshop. Once all the outlines were available for each snapshot in the time series, they were mapped onto the grid; each outline representing the extent of the flame spread at a given time. Through this visualization, each variable's effect on the flame spread rates can be characterized.</p>

<b>SURF Student Colloquium</b>	
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August 4-6, 2015	
	
<b>Name:</b> Melissa Deschamps	<b>Grant Number</b> 70NANB15H162
<b>Academic Institution:</b> University of Massachusetts-Amherst	<b>Major:</b> Chemical Engineering
<b>Academic Standing</b>	<b>Grade:</b> Junior
<b>(Sept. '15):</b>	<b>Academic Standing</b> Junior
<b>Future Plans</b>	<b>Graduate School</b>
<b>(School/Career):</b>	<b>Materials and Measurement Laboratory, Materials Science and Engineering Division,</b>
<b>NIST Laboratory,</b>	<b>Division, and Group:</b> Polymer and Complex Fluids Group
<b>NIST Research</b>	<b>Research Advisor:</b> Paul Salipante
<b>Advisor:</b>	
<b>Title of Talk:</b>	<b>Title of Talk:</b> The Effect of Electrolyte Concentration on Irreversible Colloid Adsorption
<b>Abstract:</b>	<p>Particle adsorption at a liquid-solid interface can be a complex process involving many different timescales and interaction forces. Many technical and biological applications depend on controlled adsorption, for instance biomaterials, biological systems, filtration, coatings, and separation processes. The adsorption process for these applications is highly dependent on many unknown solvent, particle, and interface properties. This impairs the collection of experimental data which can be validated by current theories and models. To better understand the effect of electrostatic repulsion on the adsorption process, we developed a simplified experiment to track individual colloidal particles as they adsorb to the interface using light microscopy. Our colloid system is comprised of varying electrolyte solutions and micron sized silica particles. After the colloids are introduced to the system, gravity forces the particles towards the interface. The particles are trapped near the surface and the degree of hydrodynamic coupling is modified by adjusting salt concentration. Observations were made using bright field microscopy and the surface coverage was calculated in MATLAB through data imaging. We saw that increased interface mobility leads to faster adsorption kinetics and higher total surface coverage while slow diffusion leads to clustering. Data gathered on the effect of electrolyte concentration on adsorption in this basic system will add to the understanding of diffusive dynamics that can be applied to more complex systems.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<p><b>Name:</b> Lamouguin Yenkodikoi Douti</p> <p><b>Academic Institution:</b> University of Maryland, College Park</p> <p><b>Academic Standing</b> 1<sup>st</sup> year Graduate school</p> <p><b>(Sept. '15):</b> Future Plans Graduate school at the University of Maryland, College Park, PhD</p> <p><b>(School/Career):</b> NIST Laboratory, Material Measurement Laboratory, Material Measurement Science Division, Division, and Group: Nanomaterials Research Group</p> <p><b>NIST Research</b> Jingyu Liu, Hino El Hadri</p> <p><b>Advisor:</b> Jingyu Liu, Hino El Hadri</p>
	<p><b>Title of Talk:</b> Loss of functionalized gold nanoparticles in commonly used containers</p> <p><b>Abstract:</b> The manufacturing and application of engineered materials (ENMs) exhibited a rapid development in recent years. Significant control over the particle's chemical properties, geometry and surface charge were achieved. Nevertheless, assessing whether these ENMs may lead to adverse environmental, health and safety risks is of great importance. This assessment mainly relies on controlled laboratory experiments that simulate environmental and biological behaviors. One common source of error in interpreting the experimental data resides in the difference between the effective dosage and the loading dosage. To improve the reliability of testing assays, a detailed study quantifying particles loss in commonly used containers is needed. In this study, gold nanoparticles (AuNPs) with different functionalities (bPEI, PVP and citrate) at concentration between 5 ppb and 5000 ppb were incubated in glass (untreated or coated with silane) and polymer (polypropylene, polycarbonate, polyethylene and polypropylene protein low binding) containers on a vortex shaker. Recovery was determined by measuring AuNP concentration using ultraviolet-visible spectroscopy (UV-vis) and inductively coupled plasma mass spectrometry (ICP-MS) after acid digestion of incubated solution.</p> <p>Loss of AuNPs was found to depend highly on the material of the container and the AuNP surface coating. An extensive loss (&gt;50%) was observed after incubating negatively charged AuNPs (citrate stabilized) in polymer containers compared to an untreated-glass container. This result was reversed for positively charged AuNPs. Particle loss was directly related to the exposure surface area with evident particle absorption on the container surface. A seven day kinetic study demonstrated that particle loss was relatively rapid during the first 24 hours. Overall, the results suggest that a major driving force for particle surface adsorption (loss) is electrostatic in nature. Hence, this study provides important insights regarding the selection of containers when performing assays with functionalized AuNPs.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<p><b>Name:</b> Elizabeth Donoghue</p> <p><b>Academic Institution:</b> Denison University</p> <p><b>Academic Standing</b> College graduate, planning to enroll in grad school for Fall of 2016</p> <p><b>(Sept. '15):</b> Future Plans Gap year doing STEM outreach and research, followed by graduate school to pursue a PhD in physics.</p> <p><b>(School/Career):</b> NIST Laboratory, Physical Measurement Laboratory, Quantum Measurement Division, Quantum Optics</p> <p><b>NIST Research</b> Alan Migdall</p> <p><b>Advisor:</b> Alan Migdall</p> <p><b>Title of Talk:</b> Repurposing a Light Field Camera for Optical Characterization</p> <p><b>Abstract:</b> Across multiple disciplines, the need for high precision measurements is rising. In systems involving optical beams, this high level of precision in turn requires that the beams be well characterized for the best possible measurements. Repurposing an existing commercial light field camera has the potential to do this better than current commercial waveform sensors.</p> <p>A Shack-Hartmann waveform detector consists of an array of microlenses in front of a many-pixel sensor. When light passes through this lens array, where the light hits the pixels behind each lens provides information about the direction of the light's waveform at that lens position. Using the distribution of the light behind each microlens makes it possible to reconstruct the waveform, yielding both phase and intensity information.</p> <p>This project was to repurpose the Lytro camera into a Shack-Hartmann waveform sensor. Our work involved finding an alternative way to read the files created by the camera, as the built-in software was not designed for our needs. Once we had access to this information, it was then necessary to write a program for spot-detection in the area associated with each of the lenslets. A preliminary calibration of the camera was necessary in order to make the conversion possible. The performance of the camera as a waveform sensor was then tested.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Nicholas Dow	Grant Number   70NANB15H144 Major: Mechanical Engineering
Academic Institution: Rowan University	
Academic Standing   Senior	
(Sept. '15):	
Future Plans   I plan on graduating and exploring graduate school.	
(School/Career):	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Fire Fighting Technology Group
NIST Research Advisor:	Craig Weinschenk
Title of Talk:	Impact of Convective Heat Transfer on Fire Fighter Personal Protective Equipment
<b>Abstract:</b>	
Firefighting is an incredibly dangerous occupation. Nearly 30,000 fire fighters were injured on the fireground in 2013, and 97 died. One of the most important ways fire fighters protect themselves is through the use of personal protective equipment (PPE). By studying the limits and capabilities of this equipment, firefighter safety can be improved.	
For this project, fire fighter PPE was tested in full-scale live-fire experiments at the Delaware County Emergency Services Training Center. These experiments provided data on the thermal conditions that a fire fighter may be exposed to in a typical residential fire. Laboratory-scale experiments were also conducted. These experiments used a purpose-built flow loop, where PPE was subjected to high temperature flows to demonstrate the impact of convective heat transfer under strictly controlled and repeatable conditions. The full-scale tests can also provide feedback to best design laboratory scale experiments to replicate real exposures.	
Utilizing data acquired at both scales helps to quantify the conditions that PPE should be expected to perform to as set by current or future National Fire Protection Association (NFPA) standards. Ultimately, the goal of this research is to give fire fighters a better understanding of the limits of their equipment.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Kristina Dungan	Grant Number   70NANB15H097 Major: Physics
Academic Institution: Denison University	
Academic Standing   1 <sup>st</sup> year graduate student	
(Sept. '15):	
Future Plans   I will be continuing on to get my PhD in Physics at the University of Illinois at Urbana-Champaign	
(School/Career):	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Quantum Optics Group
NIST Research Advisor:	Dr. Joshua Bienfang
Title of Talk:	Time-tagging for High-Precision Single-Photon Detection
<b>Abstract:</b>	
Devices capable of measuring the arrival times of single photons and other particles at high frequencies are crucial to scientific experiments and engineering. These time-tagging apparatus are commonly implemented using Field Programmable Gate Arrays (FPGAs) due to their high speeds and their programmability, and are mainly time-to-digital converters (TDCs), which only measure time intervals. However, for our purposes in high-precision single-photon detection, absolute time-tags are required and therefore we have created a Time Domain Quantizer (Bord) with 100 picosecond timing resolution and the ability to count photons, or other events, at $500 \times 10^6 \text{ s}^{-1}$ . This summer, we have done significant work testing a unique time-tag encoding system that we developed last summer. This system is based on a high-speed (10 GHz) 4-bit latched counter and a high-speed FPGA. Our main focus has been to determine which performance metrics are relevant to characterize our device based on the wider field, and then to make those measurements. Towards this goal, extensive research was done on other published reports of time-tagging systems and we have measured the quantization error of our system, which is the uncertainty in identifying the actual time of uniformly distributed temporal events that occur mainly at the time-bin boundaries. Through our experiments we have measured a quantization error for the device of less than 2%, or 4 picoseconds. Measurement of such small time intervals is difficult; however, we are currently developing a method to achieve more accurate results. Other areas that we will characterize include the differential non-linearity (DNL), the maximum count rate, and the temperature dependence of the system. These efforts are aimed towards publishing an article describing the design and performance of our time-tag encoding system.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Joshua Chaim Eisendorfer	Grant Number   70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Aerospace Engineering
Academic Standing   Junior	
(Sept. '15):	
Future Plans: Post-undergraduate studies plans:	
(School/Career): Graduate School for Aerospace Engineering and work in the field of National Security	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, Nanoelectronics Group	
NIST Research Advisor: Dr. Angela Hight Walker	
Title of Talk: Hyperspectral Imaging Analysis (HIA) For Raman Mapping	
<b>Abstract:</b> Raman spectroscopy is a technique in which in-elastically scattered photons are collected on a charge-coupled device (CCD). These photons correlate to the vibrations between each atom in a sample, and provide a ‘fingerprint’ by which different molecules or structures can be identified.	
The goal of hyperspectral imaging is to obtain the spectrum with multiple peaks for each pixel area in a sample, and techniques such as Raman spectroscopy gather complex spectra at each spatially resolved position on a sample, resulting in terabits of data. A myriad of tools are available to analyze the information-rich files, which, in the Hight Walker lab, consist of information taken from samples of graphene, a 2-dimensional (2-D) hexagonal lattice of carbon atoms. Graphene has received much attention in the scientific community because of its extraordinary properties, which include a high electrical and thermal conductivity, as well as an enormously large strength-to-weight ratio. Raman Spectroscopy is particularly well suited to the study of graphene, and, by observing spectral changes in Raman features such as the D (defect), G (graphite), and G' (second-order graphite) peaks, we can identify several properties of the sample, including the thickness and disorder. This analysis can be done at a single diffraction limited point, or across an entire mm <sup>2</sup> sample, resulting in a hyperspectral cube, which is a 3-dimensional representation of data taken over a sample.	
Since this imaging results in thousands of data-rich files, dedicated hyperspectral imaging analysis tools must be used to extract information from this data. To that end, both commercial as well as open-source programs exist that perform this analysis. These programs are written in multiple languages (Python, MATLAB, etc.) and can interact with multiple data formats, from JPEG/PNG images to formatted text files. Inspectra is written in MATLAB and aims to provide Raman analysis, and was originally designed by a former SURF student. Features of the Inspectra program include the ability to create smoothed/unsmeared heat maps, the removal of cosmic rays, as well as subtracting background interference. My goals are to dramatically improve this code with additional features and user interface capabilities. Examples of this are: a re-haul of the GUI, automatic directory updating, the ability to title any saved file. Additionally, current spectra will be saved in text files, and the cosmic ray remover algorithm will be updated to remove cosmic rays from sample data without impinging on the rest of the data.	
My future plans include a re-haul of the fitting capabilities of this program, allowing mixtures of Lorentzian and Gaussian fits which are critical to Raman analysis, as well as the automation of an xyz-nano positioning stage to interact with Raman collection software.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Leila Ettehadieh	Grant Number   70NANB15H168
Academic Institution: University of Maryland College Park	Major: Bioengineering
Academic Standing   Junior	
(Sept. '15):	
Future Plans (School/Career): I would like to work at a biomedical engineering organization that develops and tests prosthetics or a pharmaceutical company. I also hope to continue on with my studies in graduate school.	
NIST Laboratory, Division, and Group: Engineering laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group	
NIST Research Advisor: Joseph Falco	
Title of Talk: Test Methods for Evaluating the Ability of a Robotic Hand to Detect Slip	
<b>Abstract:</b> Slip detection of grasped objects is an important part of human interactions with their surrounding environment and is a functionality developers are trying to replicate in robotic-hand designs using tactile sensors. Tactile sensors are typically mounted on the outer surface of the finger phalanges or palm and are used to detect finger-object touch and slip, discriminate textures, and provide feedback for manipulation control. This project supports the development of a test method to measure the slip detection capabilities of robotic hands equipped with tactile sensing.	
In this project, a bio-inspired tactile sensor system (BioTac) and a NIST developed neural network based slip detection algorithm were used. First, a test device with modular slip artifacts was designed and 3D printed. Slip artifacts consisted of different materials including a Polyvinyl chloride (PVC) pipe, paper, duct tape, and a 3D printed textured cylinder. Experiments were conducted where the BioTac sensor was placed against each covering and data was collected at various speeds. Half the data for each artifact type collected was used to populate and train the neural network for the slip detection algorithm while the other half was used to determine how well the algorithm performed. Algorithm performance was benchmarked using a fully trained network and performance comparisons were presented using simplified training scenarios using subsets of the artifacts to determine tradeoffs between training efficiency and slip detection performance. The neural network was able to learn and detect slip faster and more accurately for rough surfaces in comparison to smoother surfaces. In addition, the neural network algorithm was tested for its ability to discriminate texture. Test device texture artifacts were identified most accurately when they were spinning against the BioTac sensor at fast speeds. In the future, this data will help create grasp performance metrics and test methods to help the developers and end-users of robotic hands to evaluate slip detection and texture discrimination characteristics.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: John Fischer	Grant Number 70NANB15H146
Academic Institution: Colorado School of Mines	Major: Mechanical Engineering
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Graduate school and continuing research in energy technologies including hydrogen fuel cells and batteries.	
(School/Career): NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Laboratory, Division, and Group:	
NIST Research Advisor: Joseph Dura	
Title of Talk: Understanding Interfacial Structures of Ultrathin Self-Assembled Nafion®	
<b>Abstract:</b>	
Polymer electrolyte membrane (PEM) fuel cells show promise for a wide range of applications due to their high power output and low operating temperatures. While the structure and transport properties of bulk PEMs for fuel cell applications have been studied extensively, much less is known about these materials at interfaces, which is relevant for the catalyst layers (CLs) of PEM fuel cells - where device performance is largely determined.	
Self-assembly (SA) has been proposed as a method to reproduce Nafion® films similar to those in CLs. Reported differences in structure and properties between SA and spin coated (SC) films indicate that characteristics of thin films can vary with coating technique [1]. These dissimilarities could be caused by differences at the substrate interface and/or in the bulk-like structure. While the mechanism for the differences is not yet fully understood, candidates include effects of shear and the kinetics of interfacial bonding.	
Since SA preparation techniques differ throughout literature, a standardized protocol for creating smooth and uniform SA Nafion® thin films must first be established in order to systematically investigate both the bulk-like and interfacial properties and their differences from SC films. Using x-ray reflectivity (XRR) in both dry (<10% RH) and humidified (>90% RH) environments, quartz crystal microbalance (QCM), and ellipsometry, we have studied the structure and swelling vs. thickness for ultrathin Nafion® films (<10 nm) to separate interfacial from bulk-like characteristics.	
Future investigations will explore SA Nafion® in-situ during binding to substrates using a QCM. This will help to identify bonded or entangled layers, as well as quantify deposition rates. Ultimately neutron reflectometry will resolve differences from SC samples that may exist in interfacial structure and water uptake in the bulk-like portion of the film.	
[1] Kusoglu, et al., <i>Adv. Funct. Mater.</i> <b>2014</b> , <i>24</i> (30) pp 4763-4774	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Tony Feric	Grant Number 70NANB15H163
Academic Institution: University of Maryland College Park	Major: Chemical Engineering
Academic Standing Junior	
(Sept. '15):	
Future Plans Plan to attend graduate school to study biomedical engineering.	
(School/Career): NIST Laboratory, Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group	
Division, and Group: NIST Research Division	
Advisor: Dr. Kevin McGrattan	
Title of Talk: Modeling Smoke Venting of a Compartment Fire	
<b>Abstract:</b>	
Consolidated Fire and Smoke Transport (CFAST) is a numerical model that predicts the thermal environment caused by a fire within a compartment. Every compartment contains an upper and lower gas layer, with the fire driving combustion products from the lower to the upper layer via the plume. The temperature within each layer is uniform, and its change with respect to time is calculated by a set of ordinary differential equations derived from the fundamental laws of mass and energy conservation. The transport of smoke and heat within a compartment is governed by empirical correlations that are situation specific.	
As a fire burns in a compartment, smoke rises and forms a layer along the ceiling. If there is a shaft or a vent located on the ceiling, the smoke can escape. However, under specific conditions, the ambient air beneath the layer of smoke can also be expelled, which significantly reduces the amount of smoke that is exhausted from the compartment. This phenomenon is referred to as plug-holing, and CFAST requires an empirical correlation to accurately model this behavior. The goal of this project was to develop an expression for the relative amounts of smoke and ambient air in the exhaust flow after the onset of plug-holing. To determine this expression, a compartment containing a smoke layer and a ceiling vent was constructed in a more complex model known as the Fire Dynamics Simulator (FDS), which is a computational fluid dynamics model of fire. The temperature and the depth of the smoke layer, the height of the ceiling, and the dimensions of the ceiling vent were all varied to observe how the amount of smoke exhausted through the vent was affected by these conditions. After analyzing the results of the experiment, it was deduced that the fraction of smoke exhausted was correlated with the volume flow rate of air leaving the ceiling vent, the temperatures of the smoke layer and ambient air in the room, and the depth of the smoke layer.	

## SURF Student Colloquium

NIST – Gaithersburg, MD  
August 4–6, 2015



Name:	Ryan Franklin	Grant Number	70NANB15H182
Academic Institution:	Hood College	Major:	Chemistry
Academic Standing (Sept. '15):	Senior		
Future Plans (School/Career):	I plan to go to grad school for a Ph.D in Material Science, then focus on ballistic armor design or related field. The school has yet to be determined.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Joseph Curtis		
Title of Talk:	Construction and Molecular Dynamics of a Nanodisc for Membrane Protein Simulation		

### Abstract:

Phospholipid nanodiscs are used to stabilize membrane proteins when the protein is removed from its native biological environment by providing interaction with a lipid bilayer, allowing the protein to be isolated without denaturing. An amphiphatic polymer (Polystyrene-co-maleic acid) (SMA) has been used to encircle a discoidal lipid bilayer, keeping it from dispersing. Using small-angle neutron scattering (SANS), a structural mapping ( $\pm 2 \text{ \AA}$ ) of the protein may be obtained from this stabilized structure.

To confirm experimental results, computer modeling is commonly used to predict the SANS profile of proteins. If the experimentally determined neutron scattering profile matches the theoretical computer generated profile, experimental researchers are reassured their results are valid. Predictive modeling of SANS profiles for membrane proteins was not possible since no suitable nanodisc model had been created, leading to uncertainty in the structure of the membrane proteins being studied. Also, the interaction and orientation between the bilayer and the SMA polymer had not yet been precisely determined through experimental studies. In our research, we used computer modeling and molecular dynamics to construct and simulate a nanodisc. In the process of creating this nanodisc for membrane protein modeling, we simulated the behavior of the SMA polymer belt, providing insight into this interaction. The lipid used was 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) since this lipid was also used in research studies. Parameters for the SMA polymer were developed through CGENFF by analogy to known structures. A miniaturized DMPC patch was also equilibrated with SMA polymer for preliminary design validation and polymer behavior simulations. By analyzing the polymer dihedrals for this initial simulation, we predicted the rotational volume each polymer strand would require, allowing for accurate polymer orientation in the full nanodisc.

## SURF Student Colloquium

NIST – Gaithersburg, MD  
August 4–6, 2015

Name:	Jennifer Freedberg	Grant Number	70NANB15H184
Academic Institution:	Rensselaer Polytechnic Institute (RPI)	Major:	Physics
Academic Standing (Sept. '15):	Sophomore		
Future Plans (School/Career):	After I get my BS in physics, I plan on earning my PhD in physics. In the future, I would like to be a professor of physics at a large research institution.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Laboratory, Quantum Optics Group		
NIST Research Advisor:	Alan Migdall and Sergey Polyakov		
Title of Talk:	Improving Optical Detectors to Better Measure Bioluminescent Effects in Genetically Engineered Mice		

### Abstract:

Improving signal-to-noise ratio is the cornerstone of all measurement sciences. This can be done by increasing the sensitivity and/or decreasing the noise of the instrument, in this case, a detector. Early generation detectors from our group were less sensitive to light and were very temperature dependent, so any variance in the environment's temperature increased noise. Using a transimpedance amplifier (TIA), a device which converts current to voltage and amplifies the signal, I designed, built and tested a more sensitive detector and reduced temperature dependence. I will discuss my experimental results using the improved detector and compare them to the earlier generation. Finally, I will evaluate my modified detector and suggest improvement for future detectors. This work is motivated by collaborative effort between NIST and Swiss scientists from EPFL (Ecole polytechnique fédérale de Lausanne) to miniaturize a detector while maintaining a high degree of signal-to-noise to measure weak bioluminescent effects in genetically engineered mice. Our collaborators in Switzerland infuse mice with luciferin, a substrate which emits visible light when enzymatically oxidized by luciferase. The light emitted in this catalytic reaction is then monitored by our optical detector. Because the amount of light detected is proportional to the cell's metabolic rate, we can determine the metabolic rate of the mouse's cells.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Connor Galvin	Grant Number 70NANB15H110 Major: Biology
Academic Institution: Miami Dade College	Academic Standing Sophomore
Academic Standing (Sept. '15):	Academic Standing (Sept. '15): Junior
Future Plans (School/Career): Biochemical research	Future Plans (School/Career): Graduate school – unknown location; followed by work in a research lab
NIST Laboratory: Materials Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Division, and Group: Structure and Function Group	NIST Laboratory, Materials Measurement Lab, Materials Measurement Science Division, Materials Division, and Group: Measurement Science Division Office
NIST Research Advisor: Travis Gallagher	NIST Research Advisor: Robert Cook
Title of Talk: Protein Crystallography	Title of Talk: Mapping Mechanical Properties of Polymer and Polymer Composites Using Nanoindentation
Abstract:	Abstract: The chemical behavior of a protein is determined by its three dimensional conformation, thus knowing a protein's structure is important to understanding how it functions biologically. X-ray diffraction is the most successful method of protein structure determination. This project was directed towards the production of diffraction quality crystals of the NIST RM 8670 antibody. Attempts were made at crystallizing the full, intact antibody as well as the isolated Fab (antigen-binding) and Fc (constant region) fragments. Although the intact antibody has yet to crystallize, crystals of both the Fab and Fc fragments have been extensively cultivated in order to optimize quality and obtain the best structural data. Bar-shaped Fc crystals grew from solutions containing polyethylene glycol and calcium acetate, while pyramidal Fab crystals grew from high concentration ammonium sulfate. Preliminary diffraction data to about 3 angstrom resolution has been collected from both types of crystal and improvement is expected in the near future.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Andrew Gayle	Grant Number 70NANB15H089 Major: Mechanical Engineering and Materials Science
Academic Institution: Duke University	Academic Standing Junior
Academic Standing (Sept. '15):	Future Plans (School/Career): Graduate school – unknown location; followed by work in a research lab
NIST Laboratory, Division, and Group: Materials Measurement Lab, Materials Measurement Science Division, Materials Division, and Group: Measurement Science Division Office	NIST Research Advisor: Robert Cook
Advisor:	Title of Talk: Mapping Mechanical Properties of Polymer and Polymer Composites Using Nanoindentation
Abstract:	Abstract: Carbon nanotubes (CNTs) are cylindrical carbon molecules, with walls formed by thin sheets of carbon – often one or several atoms thick. Due to their immense strength at small size, high thermal conductivity, controllable electrical conductivity, and other properties, CNTs are frequently used in polymer matrices as composites. However, current dispersal techniques often result in non-uniformity of CNTs in the matrix. The first step in improving the distribution is developing a reliable method to measure the distribution. This project aims to measure the CNT distribution by determining mechanical properties at the nano-scale and then mapping the surface of a CNT-polymer composite. Nanoindentation is ideal for mapping a relatively small area, with X and Y dimensions ranging from hundreds to thousands of micrometers. Nanoindenters use very small indentations to obtain mechanical properties by measuring continuous load, displacement, and time data during the indentation, allowing for efficient mapping of a small area without being destructive to the sample. By fitting the nanoindentation output data to viscoelastic-plastic deformation equations, the properties of a sample at a single indent can be determined. Measurements and modeling of an array of indentations can be used to generate a map of material properties. Previous viscoelastic-plastic models are incomplete; thus a new model was developed not only for CNT-polymer composite mapping, but also for determining materials properties of polymers, ceramics, and metals.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Justin Goh	Grant Number   70NANB15H141 Major: Mechanical Engineering
Academic Institution: Montgomery College	
Academic Standing   Junior	
{Sept. '15}; Future Plans   I plan on attending graduate school after I earn a Bachelor's Degree in Mechanical Engineering. After finishing graduate school, I hope to work at a leading tech company that deals with robotics and exo-skeletons.	
(School/Career): NIST Laboratory, Intelligent Systems Division,	
Division, and Group: Manipulation and Mobility Systems Group	
NIST Research Advisor: Karl Van Wyk	
Title of Talk: Test Method for Evaluating Robotic Hands' Center of Pressure and Normal Force Sensing Modalities	
Abstract:	Hans Moravec, known for his work in robotics and artificial intelligence, wrote over 25 years ago, "It is comparatively easy to make computers exhibit adult level performance on intelligence tests or playing checkers, and difficult to give them the skills of a one-year old when it comes to perception and dexterity." Although significant advancements have been made to improve the dexterity of robots, this statement still remains true today. Fortunately, one avenue for improving dexterity is through tactile sensing. Tactile sensors provide touch-related information by measuring kinetic events during interaction with its environment. This information can then be used to develop more intelligent grasping and manipulation control schemes.
	Our goal for this project is to develop a test method for measuring how well a robotic hands' tactile sensors can resolve contact center of pressure (COP) and normal force directionality. These sensory signals can be used for grasp planning (placing of fingers on an object), touch-based object tracking, and grasping and manipulation control. In particular, the Biotac, a biomimetic tactile sensor by SynTouch, was investigated. The Biotac was designed to replicate the sensing capabilities of the human fingertip by having a similar physical layout (an elastomeric skin encapsulating a rigid, bone-like core). In addition, it possesses a spatial distribution of touch-sensitive electrodes, high-frequency pressure transducer, and a temperature sensor. In order to fully realize time-varying COP and force normal profiles on surfaces in three-dimensional Cartesian space, a sophisticated test bed is necessary. First, the Biotac sensors were seated in a 3D printed reflective structure to enable 6 degree-of-freedom (DOF) Cartesian tracking via a motion capture system. Then, an algorithm was programmed to convert the 6-axis load cell data to a three-dimensional normal force vector and centers of pressure. Next, a weighted centroid scheme was used to resolve raw Biotac data into COP and normal force directions. After data collection, Biotac data was transformed to the load cell coordinate system where results can be compared. At this point, an average error and confidence intervals are calculated between the two measurements of COP and normal force directions which indicate the Biotac prediction accuracies for these two sensing modalities.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Ryan Goldband	Grant Number   70NANB15H166
Academic Institution: Binghamton University, State University of New York	Major: Computer Engineering
Academic Standing   Senior	
{Sept. '15}; Future Plans   Obtain a M.S. undecided where (School/Career):	
NIST Laboratory, Physical Measurements Laboratory, Semiconductor and Dimensional Metrology Division, Division, and Group: Surface and Nanostructure Metrology Group	
NIST Research Advisor: Ronald Dixon	
Title of Talk: Implementing Interferometry for Stage Drift Correction	
Abstract:	This talk discusses using an interferometric encoder to monitor, and ultimately correct, the stage drift in a critical dimension atomic force microscope (CD-AFM). Over the course of a scan, the coarse-positioning stage slowly drifts relative to the AFM head. This can cause the apparent shape and/or orientation of the resulting image to be distorted. An example of this would be that a circular feature scanned using a CD-AFM could appear to be elliptical in shape. For many applications the apparent shape of features in the x-y plane is of secondary importance. The most important measurements, such as the width and cross-sectional profile of a feature, are typically performed using the fast-scan axis. Since these measurements only rely upon data taken from a single fast-scan line, the results are relatively insensitive to drift. However, even for fast-axis measurements, knowledge of the relative location of the tip and sample is important. Furthermore, monitoring and correction of the stage drift could enable more accurate measurement of feature shape in the x-y plane. This is the field of contour metrology, and at present, the stage drift presents serious challenges in using CD-AFM for contour measurements.
	This presentation covers both major components of the project: (1) the use of the Renishaw fiber optic laser encoder and interpretation of its quadrature output to create a graph that updates in real time to display the stage drift, and (2) the design and fabrication of parts in order to mount the laser heads and mirrors inside of the CD-AFM. Finally, the next steps and potential extensions of this effort will be discussed.

## SURF Student Colloquium

NIST – Gaithersburg, MD  
August 4-6, 2015



Name: Joshua Goldman

Academic Institution: University of Maryland College Park

Academic Standing: Junior

(Sept. '15): Future Plans

Graduate school

(School/Career): NIST Laboratory, Materials Measurement Science Division, Materials

Division, and Group: for Energy and Sustainable Development Group

NIST Research David Lavan

Advisor:

Title of Talk: Optical calibration of nanocalorimeter chips using an infrared camera

**Abstract:**

Nanocalorimetry is the high-sensitivity measurement of thermal and thermodynamic properties of samples with mass on the order of nanograms. With our system, a fast heating rate and higher resolution measurement (up to 200Khz sampling rate) are possible. The measurement is based on a microfabricated sensor chip used in a four-probe system, where the sample is heated using applied current and its resistance is simultaneously measured. Temperature data is derived from resistance using a sensor chip-unique *a priori* calibration fit. In this talk I describe a calibration method whereby an infrared thermal camera with a microscopic lens measures the heater of the sensor chip and calculates temperature (using its proprietary calibration factors) over a range of applied voltage. Simultaneously, resistance of the chip is calculated using four-wire measurement. However, raw data from the camera is not accurate unless the subject is a blackbody. We must determine 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 the calibration process, the temperature of the platinum heater is compared to a reference platinum surface which remains at room temperature (or another controlled temperature).

This process is automated with a LabVIEW virtual instrument (VI) controlling a digital data acquisition system. The VI can generate an emissivity fit, correct temperature data from the camera, and generate a temperature-resistance fit with configurable voltage steps. Overall, the calibration process is much faster. We can calibrate up to 500° C and then extrapolate further. We validated this method of calibration by using a fit to measure the melting point of an aluminum sample.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4-6, 2015



Name: Madeleine Gordon

Academic Institution: College of Charleston

Academic Standing: Graduated

(Sept. '15): Future Plans

Fall internship at Berkeley National Laboratory then graduate school in fall of 2016.

(School/Career): NIST Laboratory, Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division,

Division, and Group: CMOS and Novel Devices Group

NIST Research Joseph Robertson

Advisor:

Title of Talk: Biomimetic Membranes for Structure-Function Determination of Membrane Proteins

**Abstract:**

Characterizing the interfaces of biomimetic membranes is essential for better understanding the structural biology of functional membrane proteins and to develop better biosensors. Here, we are investigating a model membrane based on a self-assembled thiolipid as a platform for the characterization of protective antigen (PA63), the pore forming component of anthrax toxin. To investigate the ion-conductance properties of the PA63-membrane system, we used electrochemical impedance spectroscopy (EIS). From EIS we studied the kinetics and behavior of membranes tethered to gold surfaces in different environments such as varying detergents, polyethylene glycols and proteins. The data collected enables us to calculate essential information such as protein surface coverage, pore size and protein channel size along with providing valuable insights into the driving kinetic forces behind membrane formation and destruction.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
Name: Daniel Graham	Grant Number: 70NANB15H137
Academic Institution: Centre College	Major: Chemistry and Computer Science
Academic Standing (Sept. '15): Senior	
Future Plans [School/Career]: Thinking about going to graduate school in computational chemistry.	
NIST Laboratory, Division, and Group: Materials Measurement Lab, Chemical Sciences Division, Chemical Informatics Research Group	
NIST Research Advisor: Thomas Allison, Kari Irikura, Peter Linstrom	
Title of Talk: Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	
<b>Abstract:</b>	The NIST Chemistry WebBook is a popular reference database for researchers, engineers, and students. It contains theoretical and experimental information such as molecular structure, thermodynamics and spectral data on approximately 130,000 molecules. Our primary focus this summer was to optimize 3-dimensional (3D) molecular structures for compounds in the Webbook. Our secondary focus was to utilize the vibrational frequencies and intensities that were computed by developing a web application to display the infrared (IR) spectrum in a user-friendly manner.
	The 3D structures were optimized using an efficient multi-step process. Starting with a classical molecular mechanics (MM2) approach, we refined initial structures created from 2D structural drawings. Quantum chemistry methods implemented in the Gaussian09 software package were used to produce accurate structures using the PM6 semi-empirical and B3LYP density functional theory (DFT) methods. DFT is more computationally expensive, but has a reputation for yielding molecular structures that are in good agreement with experimental results. Before uploading to the WebBook, we checked the structures for accuracy and consistency with existing WebBook information.
	The web application is constructed in JavaScript using the plotting package Flot to interactively display the IR spectrum of the molecule. The spectrum plot is linked to a 3D representation of the molecule that can be visualized through the JSMol package. Users can select individual frequencies to see the corresponding normal mode molecular vibrations. We hope this functionality will be included in the next release of the WebBook.
	3D structures and IR spectra are important in areas such as drug discovery, experimental simulation, and communication to non-chemists. We were able to optimize more than 20,000 molecules this summer, ensuring that the WebBook remains a valuable resource for scientists and educators.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Joshua Reeves Graybill	Grant Number: 70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Mechanical Engineering
Academic Standing (Sept. '15): Senior	
Future Plans: Graduate degree in mechanical engineering with a focus on materials science. Career at a national research laboratory or in industry.	
(School/Career): NIST Laboratory, Materials and Measurement Laboratory (MML), Materials Science and Engineering Division, and Group: Division (MSE), Functional Polymers Group	
NIST Research Advisor: Bradley Frieberg, Gery Stafford	
Title of Talk: In-situ hydro-mechanical stress response of aged perfluorinated ionomer (PFSI) membranes for fuel cell applications.	
<b>Abstract:</b>	Perfluorinated ionomers (PFSI) are a critical component in hydrogen fuel cells, as both the proton exchange membrane (PEM) and the binder within the catalyst layer. Of particular interest to the PEM fuel cell community, is a better understanding of the failure mechanisms of the polymer membranes that result from hydration cycling and long term aging effects. Both of these processes result in mechanical fatigue and ultimately failure of the fuel cell with time and directly affect the lifetime and durability of the fuel cell. Within the catalyst layer the PFSI binder, in particular the benchmark material Nafion, experiences confinement on the order of tens of nanometers. Understanding and measuring the mechanical behavior of thin films on this length scale is difficult and hard to obtain experimentally. In-situ stress measurements of polymer thin films and the resulting mechanical properties are not only of interest to the polymer membranes community but of great interest to polymer science as well as in industry. Therefore to understand the mechanical properties of thin films is critical, given the properties of films thinner than 100 nm can be significantly different from the bulk. Recently, we have developed a cantilever bending technique to investigate the swelling induced stresses in Nafion thin films. By measuring the deflection of a Nafion thin film coated on a silicon substrate and exposing the film to various humidity environments, the swelling-induced stress-thickness of the thin film could be measured directly. To determine long-term aging effects we subjected thick and thin Nafion films to humidity cycling at different aging intervals for both dry and wet storage conditions. As the films aged it was found that the shear, and consequently, the Young's modulus values increased with the age of the film. In particular it was observed that the aging of Nafion films in both humid and arid environments over extended periods of time produced similar effects to that of thermal annealing. This effect is in part related to a possible cross-linking between polymer chains effectively increasing the modulus properties and stiffening the material.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> William Brady Gunnarsson <b>Academic Institution:</b> University of Maryland, College Park <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> Future Plans <b>(School/Career):</b> NIST Laboratory, Division, and Group: <b>NIST Research Advisor:</b> Dr. Nhan Nguyen <b>Title of Talk:</b> Sample Alignment Automation for Internal Photoemission Spectroscopy
	<b>Name:</b> William Brady Gunnarsson <b>Academic Institution:</b> University of Maryland, College Park <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> Planning to pursue a Ph.D. in Electrical Engineering after graduation, followed by a career in engineering research. <b>(School/Career):</b> Physical Measurement Laboratory, Semiconductor & Dimensional Metrology Division, NIST Laboratory, Physical Measurement Laboratory, Semiconductor & Dimensional Metrology Division, NIST Division, and Group: Nanoelectronics Group <b>NIST Research Advisor:</b> Dr. Nhan Nguyen <b>Title of Talk:</b> Sample Alignment Automation for Internal Photoemission Spectroscopy
	<b>Abstract:</b>  At the core of most modern electronic technologies are heterogeneous material systems with extremely refined electron transport properties. These properties are largely determined by the energy barriers at interfaces between different materials, so naturally precise method is needed to characterize energy barriers. Internal photoemission spectroscopy (IPES) is a novel technique to directly measure barrier heights and other properties of heterogeneous interfaces. IPES uses light to eject charge carriers from one solid (emitter) to another (collector) across the interface. The light is varied across a range of photon energies, and the resulting photocurrent is measured for multiple voltage biases. At NIST, the material systems (devices) whose properties will be measured are fabricated on wafers, each device with a diameter on the order of 100 microns. In order to perform IPES with high efficiency, the wafer must be carefully positioned to center the focused light on the correct device, thereby maximizing the intensity of light incident on the device. The current IPES setup at NIST requires this action to be performed manually by adjusting linear positioning stages until the photocurrent through the device is maximized. For my project, this process will be automated using precision positioning stages driven by stepper motors, interfaced with the electrometer and incorporated into the IPES control interface using Visual C++. The stages will automatically scan the XY plane to identify the position at which the photocurrent is maximized, and (time permitting) an additional stage will position the focusing lens along the Z axis to correct for aberrations in focal length as the wavelength of light is varied, also optimizing position based on photocurrent measurement. The automation software will create a simpler, faster, and more user-friendly procedure for IPES sample alignment.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Elise Green <b>Academic Institution:</b> University of Maryland, College Park <b>Academic Standing:</b> Sophomore <b>(Sept. '15):</b> After I graduate from University of Maryland, I hope to go to graduate school to study robotics or a related field. <b>NIST Laboratory:</b> Engineering Lab, Intelligent Systems Division, Cognition and Collaboration Group <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Craig Schlenoff <b>Title of Talk:</b> Representing Robot Capabilities for Automated Planning of Manufacturing Assembly Robots
	<b>Abstract:</b>  Robot systems are complex and involve a wide range of features and performance characteristics. With the growth of robotic technology, it has become increasingly important to be able to represent this information in a useful way. For manufacturing assembly robots, a useful way to represent robot capabilities is to encode the information into a computable-interpretable knowledge representation which can be fed into a planning system to facilitate automated robot planning. We used OWL (Web Ontology Language) to create an ontology which represents the different components of a robot capability. This includes the characteristics of the robot, the action(s) to be performed, and the object (with their associated characteristics) which the action affects. This ontology provides the basic structure for representing a robot capability, and users would enter the specific characteristics of their own robots, actions, and objects within this structure. In addition, an existing converter from OWL to PDDL (Planning Domain Definition Language) was then modified in order to be able to utilize the robot capability information to create assembly plans.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Grace Hahn	Grant Number   70NANB15H141
Academic Institution: Montgomery College	Major: Biochemistry
Academic Standing (Sept. '15): Junior	Academic Institution: Colorado School of Mines
Future Plans (School/Career): Graduate School, University of Maryland, College Park	Academic Standing (Sept. '15): Senior
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical Measurement Science Group	Future Plans (School/Career): Grad School
NIST Research Advisor: Dr. Melissa M. Phillips	NIST Laboratory:
Advisor:	Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Mass and Force Group
Title of Talk: Quantification of Anthocyanins in Cranberry Standard Reference Materials by LC-Absorbance-MS.	NIST Research Advisor: Gordon Shaw Title of Talk: Calibrating a Mass Sensor
<b>Abstract:</b> <p>Antioxidants inhibit cell damaging oxidation reactions by neutralizing free radicals. The consumption of antioxidant-rich foods is linked with many health benefits such as the prevention of urinary tract infections, the risk reduction of cardiovascular diseases, and the regression of cancerous tumor growth. Anthocyanins are antioxidants and the natural pigments in many plants. In fruits such as cranberries and blueberries, the anthocyanin structure is comprised of one of the five anthocyanidin bases (cyanidin, delphinidin, peonidin, petunidin, and malvidin) bonded to one of three glycoside functional groups (glucoside, galactoside, and arabinoside). The National Institute of Standards and Technology (NIST) provides a variety of <i>Vaccinium</i> berry Standard Reference Materials (SRMs) that food manufacturers and testing laboratories use for quality assurance.</p> <p>Due to the high anthocyanin content present in cranberries, an instrumental method for anthocyanin screening is needed for Standard Reference Materials 3281 Cranberry Extract, and 3284 Cranberry-Containing Solid Oral Dosage Form. LC-Absorbance-MS was used to detect the absorbance of the analytes at 520 nm and confirm analyte identity based on the mass-to-charge ratio. An instrumental method was developed based on the successful separation and the identification of all combinations of anthocyanin compounds present in the Standard Reference Materials. Quantification was performed using Allura Red AC (FD&amp;C Red 40) as an internal standard, as it provides a similar absorbance signal to the analytes. Extraction studies were conducted to determine optimum conditions prior to quantification by LC-Absorbance-MS.</p>	
<p><b>Abstract:</b>  <p>Microelectromechanical systems (MEMS) are microscale sized objects that couple a mechanical motion to an electric signal. Many of these systems include a resonator, such as a cantilever, whose oscillations are the motion transduced into a signal. These resonator systems are particularly useful for accurate physical measurement. For instance, we can build mass sensors with MEMS oscillators, since their resonant frequencies change if mass is added. My project was to calibrate such a mass sensor, using a fused silica parallelogram flexure as the resonator. The base of the parallelogram flexure was mechanically fixed to a ceramic support with a proof mass at the distal end. The proof mass ensured that the flexure's transverse displacement was approximately rectilinear and that higher order vibrational modes were suppressed. The velocity of this flexure was transduced to a voltage signal via a laser Doppler vibrometer. This core component of a vibrometer is a two-beam interferometer, and the path length of its test beam directly depends on the motion of the flexure. For this reason, the velocity of the flexure's motion determines the frequency of the heterodyne FM signal generated by the vibrometer. A shift in this frequency results from the Doppler effect generated by the motion of the sensor.</p> <p>We repeatedly lifted a small aluminum wire (~30 <math>\mu</math>m) onto and off of the flexure using a robotic arm controlled by a Newport Universal Motion Controller Driver. The motion controller was given a string of ASCII commands to automate these repetitions. The string of ASCII commands were programmed in LabVIEW, and sent to the motion controller via a general purpose interface bus (GPIB). With each repetition, the resonance frequency of the sensor shifted in response to the added mass. This general approach can be used to examine the resonator's linearity and sensitivity as a mass sensor.</p> </p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Grace Hahn	Grant Number   70NANB15H141
Academic Institution: Montgomery College	Major: Biochemistry
Academic Standing (Sept. '15): Junior	Academic Institution: Colorado School of Mines
Future Plans (School/Career): Graduate School, University of Maryland, College Park	Academic Standing (Sept. '15): Senior
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical Measurement Science Group	Future Plans (School/Career): Grad School
NIST Research Advisor: Dr. Melissa M. Phillips	NIST Laboratory:
Advisor:	Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Mass and Force Group
Title of Talk: Quantification of Anthocyanins in Cranberry Standard Reference Materials by LC-Absorbance-MS.	NIST Research Advisor: Gordon Shaw Title of Talk: Calibrating a Mass Sensor
<b>Abstract:</b> <p>Antioxidants inhibit cell damaging oxidation reactions by neutralizing free radicals. The consumption of antioxidant-rich foods is linked with many health benefits such as the prevention of urinary tract infections, the risk reduction of cardiovascular diseases, and the regression of cancerous tumor growth. Anthocyanins are antioxidants and the natural pigments in many plants. In fruits such as cranberries and blueberries, the anthocyanin structure is comprised of one of the five anthocyanidin bases (cyanidin, delphinidin, peonidin, petunidin, and malvidin) bonded to one of three glycoside functional groups (glucoside, galactoside, and arabinoside). The National Institute of Standards and Technology (NIST) provides a variety of <i>Vaccinium</i> berry Standard Reference Materials (SRMs) that food manufacturers and testing laboratories use for quality assurance.</p> <p>Due to the high anthocyanin content present in cranberries, an instrumental method for anthocyanin screening is needed for Standard Reference Materials 3281 Cranberry Extract, and 3284 Cranberry-Containing Solid Oral Dosage Form. LC-Absorbance-MS was used to detect the absorbance of the analytes at 520 nm and confirm analyte identity based on the mass-to-charge ratio. An instrumental method was developed based on the successful separation and the identification of all combinations of anthocyanin compounds present in the Standard Reference Materials. Quantification was performed using Allura Red AC (FD&amp;C Red 40) as an internal standard, as it provides a similar absorbance signal to the analytes. Extraction studies were conducted to determine optimum conditions prior to quantification by LC-Absorbance-MS.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Tyler Heisel	<b>Grant Number</b> 70NANB15H113
<b>Academic Institution:</b> Millersville University of Pennsylvania	<b>Major:</b> Computer Science
<b>Academic Standing:</b> Senior	
<b>(Sept. '15):</b>	
<b>Future Plans:</b> Aviation or Explosive Ordnance Disposal (EOD) Officer in the US Navy	
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b> Information Technology Laboratory, Software and Systems Division, Software Quality Group	
<b>NIST Research Advisor:</b> Mary Laamanan	
<b>Title of Talk:</b> Digital Forensics using Extensible Markup Language (XML)	
<b>Abstract:</b> In an age where nearly all forms of communication are digital and most people's business occurs in some form of electronic way, the field of digital forensics is becoming increasingly meaningful. Collecting data and maintaining reliable information within the field of digital forensics is essential to criminology. Many languages can be used to represent this data; however, Extensible Markup Language (XML) tends to be the language of choice. It is a versatile language that can be used for a multitude of projects. In my project's case, XML is being used to represent the state of information on a hard drive. Currently, the Digital Forensics XML (DFXML) schema is being used to represent this information. The goal of my project was to write a script that would take the current DFXML files and convert them into the Cyber Observable expression (CyBOX) schema.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Hannah Hastings	<b>Grant Number</b>
<b>Academic Institution:</b> Bryn Mawr College	<b>Major:</b> Physics
<b>Academic Standing:</b> Senior	
<b>(Sept. '15):</b>	
<b>Future Plans:</b> Graduate School	
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b> Physical Measurements Laboratory, Sensor Science Division, Optical Radiation Group	
<b>NIST Research Advisor:</b> Cameron Miller	
<b>Title of Talk:</b> The World-Wide State of Solid State Lighting Measurements	
<b>Abstract:</b> Solid state lighting (SSL) products have become popular because of benefits they provide such as durability, energy efficiency, and longer lifetimes. As SSL products are now widely used for general lighting purposes, NIST began a Measurement Assurance Program (MAP) in 2010 with support of the Department of Energy to provide proficiency testing for laboratories around the world to make sure that as SSL product use increased, laboratories existed that were capable of measuring these products. MAP 1, the first version of the MAP (another version, MAP 2, began in 2015), consisted of six different lamps and 118 laboratories participated. Measurements of each lamp's total luminous flux, RMS voltage and current, electrical power, luminous efficacy, chromaticity coordinates x and y, correlated color temperature, and color rendering index were taken by NIST, then by the laboratory, and then by NIST again. The differences between NIST's measurements and the laboratories' measurements for each property were calculated and analyzed for whether or not they potentially came from a random process and for the deviation of the laboratories' measurements from NIST's. This analysis was done by fitting each distribution of measurement differences to a normal distribution and calculating the correlation coefficient and standard deviation of the differences.	
<b>Overall results of the analysis show that measurements of each property were closely correlated with a normal distribution. Measurements of current in certain lamps however had lower correlation coefficients and the standard deviation of the distribution of current measurement differences was much greater than expected. The hypothesis is that these issues seen in measuring the current of some solid state lighting products are caused by lamps inducing high frequency electricity when operated by power supplies that use a digital waveform generator. The transmission of the high frequency electricity effected by the capacitance and inductance in the wires of the measurement system makes an accurate measurement difficult to obtain. An experiment was designed to test this hypothesis in which lamps were measured multiple times using three different power supplies and varying the resistance, capacitance, and length of the wires in the system.</b>	

SURF Student Colloquium	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Janelle Henrich	Grant Number   70NANB15H084
Academic Institution: American University	Major: Mathematics, Economics
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Graduate School	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group
NIST Research Advisor:	Antonio Farina and Paul Kienzle
Title of Talk:	Inversion of Quasielastic Neutron Scattering Data from Differing Instruments
<b>Abstract:</b>	
At the NIST Center for Neutron Research, user scientists employ a variety of neutron scattering instruments to study material dynamics. Quasielastic neutron spectrometers are used to determine the dynamic structure factor of the sample. Data collected in the energy domain are often Fourier transformed to obtain the Intermediate Scattering Function (ISF), the function which describes the dynamics of the system in the time domain. The different instruments differ mainly for their energy resolution and energy windows. However, despite overlap in these two quantities, the data on a single sample from two different instruments do not always overlap and form a continuous ISF curve. This is problematic, because utilizing multiple instruments provide more and different information on a sample which can be essential for the characterization of a material's dynamics. However, there is currently not a single, standardized, statistically sound method of reconciliation, and scientists utilize a number of different methods to combine data sets from different instruments.	
This talk discusses the investigation into the reason for this mismatched data, and the subsequent attempts to create a single statistically sound algorithm to resolve the discrepancies. To complete this investigation, code was used to create artificial data in which the true ISF function was known, and the artificial data was manipulated to create the discrepancies found in previous experiments. In addition, measurements from the high-flux backscattering spectrometer and disk-chopper time-of-flight spectrometer on propylene carbonate were combined to then test the algorithm.	

SURF Student Colloquium	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Emily Hermann	Grant Number   70NANB15H140
Academic Institution: Miami University	Major: Physics and Mathematics
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Graduate school for high energy/particle physics	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Operations and Engineering Group
NIST Research Advisor:	Dagistan Sahin
Title of Talk:	Dynamic Reliability Assessment of the NIST NBSR Thermal Shield Cooling System
<b>Abstract:</b>	
Safe and efficient operation of any nuclear reactor and each of its subsystems is of great importance. The thermal shield and the thermal shield cooling system (TSCS) of the NIST NBSR reactor are in place to remove heat dissipated in the reactor shielding during reactor operation. If the TSCS is not operational, the NBSR reactor can not operate. The lead shielding surrounding the reactor core may melt due to high temperatures. Therefore, the reliability and operation of the TSCS is crucial. To maximize the reliability of the system, it is first necessary to quantify risks and failure mechanisms. Traditionally, this quantification is provided by a probabilistic risk assessment (PRA) using a series of event and fault trees to generate cut sequences and overall failure probabilities. A complex system such as the TSCS, which contains both mechanical and digital components, allows for numerous dynamic interactions between its components, introducing time dependence into the system. This time dependence makes it difficult to accurately model the TSCS using previous practices. To more accurately model the system, the Markov/cell-to-cell mapping (CCMT) technique is employed. Using the Markov technique, diagrams outlining the transitions of the components between configurations are made. The CCMT is used to advance the system state through discrete transitions over discrete time steps. The controlled variable space is defined only by the significant variables in the system and discretized by dividing the continuous range of possible values into a finite number of intervals. Using the Markov/CCMT methods, a matrix of transition probabilities between states is created. Using this matrix, the likelihood of a failure event, in this case, reactor shutdown, occurring can be quantified by finding each event's PDF (probability density function) and CDF (cumulative density function). Once the reliability model of the system has been constructed, it can be integrated with an existing PRA and used to determine what further upgrades or replacements can be made to decrease the frequency with which reactor rundown occurs, hence improving system reliability.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Kaitlyn Hillgartner	Grant Number 70NANB15H146
Academic Institution: Colorado School of Mines	Major: Chemical Engineering
Academic Standing (Sept. '15):	Colorado School of Mines, Senior
Future Plans (School/Career):	I plan on attending graduate school, hopefully at Colorado School of Mines, to earn my MS in either chemistry or chemical engineering.
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group
NIST Research Advisor:	Jonathan Seppala
Title of Talk:	3D Printing Temperature and Speed Effects
Abstract:	3D printing processes such as stereo lithography, selective laser sintering (SLS), and fused filament fabrication (FFF), can be used to create objects inaccessible to traditional manufacturing processes, either due to unusual shape or lack of volume (prosthetics, medical implants). Since 3D printing is a useful but complicated process which typically results in a fragile final product, it is important to understand how operating conditions, such as extrusion temperatures and print speeds will affect the quality and strength of the print. This project focuses on how extrusion temperature and print speed combinations effect the mechanical properties of welds prepared by FFF while simultaneously monitoring the temperature profile of each layer during the printing process.
Acrylonitrile butadiene styrene (ABS) layers were printed at print speeds of 10mm/s, 31.6mm/s, and 100mm/s, and extrusion temperatures from 200°C to 260°C. The path of the printing process was fixed such that each layer was printed in one direction. During the printing process, each sample was filmed using an infrared (IR) camera to obtain thermal intensity profiles for each layer. The intensity profiles were converted into temperature profiles from an offline calibration of intensity and temperature using the IR camera and a thin ABS ‘washer’ sample on a hot stage. Next, mode 3 shear tests were performed on a tensile stage and normal force data was used to determine the strength of individual welds of the printed objects.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Brian Hillsley	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County (UMBC)	Major: Computer Engineering
Academic Standing (Sept. '15):	4 <sup>th</sup> year
Future Plans (School/Career):	I am interested in pursuing a PhD in manufacturing or computer technology. I want to work in an interdisciplinary environment where can apply my expertise in software and hardware design, but also learn more about mechanical systems, physics, and chemistry. Life is the best school I know, and it is infi-disciplinary.
NIST Laboratory, Division, and Group:	NIST Research, Engineering Laboratory, Intelligent Systems, Production Systems Group
NIST Research Advisor:	Brandon Lane
Title of Talk:	One Layer Deep: Investigating Scan Path Strategies for Individual Print Layers
Abstract:	In the commercial market, AM (additive manufacturing), more well known as <i>3D printing</i> , has grown tremendously in popularity and complexity. With a price and a “frustration-curve” holding the technology from being a part of every home, it is an area where great progress will be made in the coming years. Commercial systems have become simple enough for end-users with little technical background to operate. However, these simplifications have hidden the complexity of developing machine-controller instructions. Of the different AM technologies, L-PBF (laser-based powder bed fusion) is the primary focus of this project, which involves heating spots of metal powder with a laser to form solid shapes.
This project explores the steps taken to create toolpaths from individual layers of 3D models which can then be exported as G-code (RS-274), a compatible language for AM machines. G-code includes instructions for moving a tool, extruder, or laser spot along the machines X, Y, and Z axes and includes other control commands specific to the type of machine such as setting the extrusion volume or laser power. To create G-code, the 3D model must be processed with certain parameters to form a toolpath. A toolpath is a sequence of points a machine tool should follow. For L-PBF, these points must include information about whether the laser is on or off.	
The process of generating machine code, such as G-code, for L-PBF machines, is ultimately concealed by proprietary software developed by companies that work closely with the manufacturers of the machines. With a focus on its application to L-PBF, this project built an API (Application Programmable interface) from the bottom-up for generating toolpaths to be exported as G-code for individual print layers. The software provides a flexible and extendable API for describing complicated toolpath strategies that allow the designer of a print to control the composition of individual regions of a single layer.	
The work put into this software has helped identify the overall complexity of G-code generation for metal PBF machines and will help in the production of NIST's first custom additive manufacturing machine, which is currently in its design phase.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Donald Hong	Grant Number   70NANB15H172
Academic Institution: University of Maryland, Baltimore County (UMBC)	Major: Biochemistry and Molecular Biology
Academic Standing   Senior	
(Sept. '15); Future Plans   Graduate school or biochemist career	
(School/Career); NIST Laboratory, Material Measurement Laboratory (MML), Biomolecular Measurement Division (BMD), Division, and Group; Bioprocess Measurements Group 645.07	
NIST Research Advisor: Dr. Jeffrey Hudgens	
Title of Talk: Analysis of New HDX-ETD Software for Higher Resolution in Epitope Mapping	
<b>Abstract:</b>	
Today, the biopharmaceutical industry is a multi-billion dollar business stretching from investments into research on new biochemical molecules to the development and manufacture of synthetic drugs for clinical trials. With such a huge industry, careful steps must be taken to analyze the quality of synthesized drugs/molecules and their function. These drugs/molecules could be involved in protein-protein/antigen-antibody interactions and must be analyzed with high resolution to ensure that they work. Hydrogen-deuterium exchange mass spectrometry (HDX-MS) can view the interactions in solution with a high enough resolution. HDX involves the exchange of the hydrogens on the amide backbone of the protein with deuterium in a deuterium oxide solution. This allows a heat map to be produced to show the different sites of the molecule during the interactions that are exposed to the solution over a set time period. As the year pass, there is a need for higher resolution of molecule interactions such as epitope mapping during an IgG binding to an antigen or viewing the active site of protein-protein interactions. Electron transfer dissociation (ETD) can allow for higher resolution through of fragmenting ions in a mass spectrometer that allows the viewer to take protein down to the smallest functional unit. This coupled with HDX could improve the resolution of analysis but there are two competing methods of ETD that are used in the field: top-down ETD and bottom-up ETD. Top-down ETD is the analysis of intact proteins while bottom-up ETD enzymatically/chemically digests proteins into smaller peptides before mass spec analysis. To confirm which method provides the higher resolution, my tenure at NIST/IBR focused on new computer software that will be used to compile and analyze ETD data from both methods. Software already exists to analyze HDX-MS data for proteomic studies, but there has not been any recent software that allows for the analysis of HDX-MS/ETD data. The new software I am evaluating contains both regular HDX-MS capabilities in addition to the new HDX-MS/ETD. I have been testing the regular HDX-MS capabilities on already well analyzed proteins such as ubiquitin and human AGP. With regards to the HDX-MS/ETD capabilities, more proteins must be analyzed; in addition to ubiquitin and AGP, to determine which ETD method provides the higher resolution need for epitope mapping.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Jard Horn	Grant Number   70NANB15H172
Academic Institution: University of Maryland, Baltimore County (UMBC)	Major: Mechanical Engineering
Academic Standing   Senior	
(Sept. '15); Future Plans   I am planning to enter a career in sustainable energy production and storage, while pursuing a graduate degree in mechanical engineering.	
NIST Laboratory, Division, and Group; Energy and Sustainable Development Group, Facility for Adsorbent Characterization and Testing	
NIST Research Advisor: Dr. Laura Espinal	
Title of Talk: Challenges in the reliable measurement of high pressure CO <sub>2</sub> adsorption isotherms	
<b>Abstract:</b>	
Sustainable technologies to capture and store CO <sub>2</sub> are being developed to mitigate the effect of CO <sub>2</sub> emissions on the environment. One such technology is the use of adsorbent materials to selectively adsorb CO <sub>2</sub> from large scale stationary sources of carbon emission. While advances are being made, the pace of innovation is significantly slowed by a lack of reproducibility in measurements, particularly conducted at high pressure, due to a lack of standardized protocols and sample preparation methods. NIST recently launched the Facility for Adsorbent Characterization and Testing (FACT Lab), a state-of-the-art laboratory commissioned to establish testing procedures and provide reliable material property data. We designed an internal round robin test (RRT) using three different gas sorption instruments in the FACT Lab. The RRT involved measuring high pressure CO <sub>2</sub> adsorption isotherms at 20 °C on the NIST reference material RMV-8852 (zeolite ZSM-5). Results reveal the various experimental parameters that play a role in reproducibility of data.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name:	Jonathan Huff
Academic Institution:	Boise State University
Academic Standing:	Senior
(Sept. '15):	Grad school at Boise State
Future Plans:	Graduate school for artificial intelligence; researcher
(School/Career):	NIST Laboratory, Materials Measurement Science Division, Materials Measurement Laboratory, Materials Measurement Science Division,
NIST Research Division, and Group:	Nanomechanical Properties Group
Advisor:	Douglas Smith
Title of Talk:	Displacement Metrology for Nanomechanical Testing
<b>Abstract:</b> A Fabry-Pérot interferometer consists of two partially transparent parallel mirrors separated by some distance. When laser light passes into the cavity, a fraction is transmitted through each mirror while the rest reflects and interferes within the cavity. The intensity of the light transmitted through, and reflected from, the cavity varies periodically with changes in either the wavelength of the laser or the length of the cavity, resulting in interference fringes. If the cavity length is varied while the laser wavelength remains constant, the change in transmitted or reflected light intensity can be related to the change in cavity length, allowing for high accuracy displacement measurement. Difficulty arises when attempting to track length changes greater than one quarter of a wavelength because the slope of the interference fringes goes to zero at minima and maxima, resulting in regions of low sensitivity.	
My work was focused on characterizing an experimental interferometer based on the Fabry-Pérot design that will be able to sense displacement changes on the subnanometer scale over several micrometers. By modulating either the cavity length (with a piezo actuator) or the laser wavelength (using a rapidly tunable laser) and employing lock-in amplifiers to read the intensity of the modulation signal and its second harmonic, a polar plot can be constructed that allows for tracking of displacements across multiple fringes without loss of sensitivity. Such a system holds promise for the field of nanomechanical testing where subnanometer displacement measurements can be used to measure sample elongation or contraction as well as sensing the deflection of a load cell for the purpose of measuring applied force.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Steven Hudak
Academic Institution:	University of Maryland, Baltimore County
Academic Standing:	Senior
(Sept. '15):	Graduate school for artificial intelligence; researcher
Future Plans:	Engineering Laboratory, Systems Integration Division, Systems Engineering Group
(School/Career):	NIST Research Division, and Group:
NIST Research Advisor:	Yung-Tsun Tina Lee
Title of Talk:	A Comparison of Standard Representations of Predictive Models
<b>Abstract:</b> The manufacturing industry makes use of predictive models for many reasons, e.g., to achieve gains in productivity. Predictive models can be produced in numerous ways: from standalone data mining platforms, from a plethora of data mining libraries in various programming languages, and even from custom code. To obtain results from these predictive models (i.e., scores), consumer programs must either be designed to work with the specific program that produced the model or both producer and consumer programs must agree on a standard representation. A standard representation allows predictive models generated by any producer program to be scored by any consumer program that understands the standard representation. This increases the manufacturer's flexibility in choosing producer and consumer programs, and reduces the costs of translating between different representations. Predictive Model Markup Language (PMMI), an XML-based format, is the de facto standard for communicating commonly used predictive models. Portable Format for Analytics (PFA) is a recently developed a JavaScript Object Notation (JSON)-based format capable of communicating any predictive model. To assist manufacturers in deciding which use cases are ideal for each format, PMMI and PFA are thoroughly evaluated using detailed and relevant evaluation criteria.	

	<b>SURF Student Colloquium</b> NIST – Hollings Marine Lab, Charleston, SC to be presented at <b>The Medical University of South Carolina Research Day 2015</b>	<b>Name:</b> Samuel Huntington <b>Grant Number</b>   70NANB15H081 <b>Academic Institution:</b> The Citadel <b>Academic Standing</b>   1 <sup>st</sup> Year Graduate Student <b>(Sept. '15):</b> Graduate school at the Purdue University studying analytical chemistry <b>Future Plans:</b> Graduate school at the Purdue University studying analytical chemistry <b>(School/Career):</b> Material Measurement Laboratory, Chemical Sciences Division, Environmental Chemical Division, and Group: Sciences Group <b>NIST Research</b> Michael B. Ellisor <b>Advisor:</b>	<b>Title of Talk:</b> A Novel Method for Tin Speciation in Complex Biological Matrices  <b>Abstract:</b> Butyl tin compounds have been widely used as pesticides, antifouling agents, and PVC stabilizers. Although organotin-based antifouling paints have been banned globally since 2008 due to their toxic nature, the persistent nature of these compounds in the aquatic environment continues to be a major source of concern for the marine environment. With an increased effort to monitor the health of marine environments, the analysis of butyl tins in a variety of biological samples has become necessary. Current methods used for Sn speciation in biological matrices at NIST generally involve tedious and somewhat hazardous sample preparation methods utilizing microwave-assisted extraction with tetramethylammonium hydroxide (TMAH), followed by a series of steps where the analytes of interest are derivatized, back extracted in organic solvents, and undergo solid phase extraction (SPE) clean-up prior to gas chromatography (GC) inductively coupled plasma (ICP) mass spectrometry (MS). In a novel method, an anionic acid labile surfactant was used to extract mono-, di-, and tri-butyl tin from marine tissue and subsequently facilitate the derivatization process required for GC-ICP-MS analysis. The use of TMAH was eliminated, however back extraction and SPE-clean-up was still required. The tin species were analyzed by GC-ICP-MS with the hope of adapting the method to liquid chromatograph ICP-MS eliminating the need for potentially harmful organic solvents. Isotope dilution was employed to determine the concentration of n-butylin compounds.
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	<b>SURF Student Colloquium</b> NIST – Gaithersburg, MD August 4-6, 2015	<b>Name:</b> David Indictor <b>Academic Institution:</b> Binghamton University, State University of New York <b>Academic Standing</b> Senior <b>(Sept. '15):</b> Unspecified graduate school/Unspecified career in computer communications or computer technology <b>NIST Laboratory,</b> Communications Technology Laboratory, Wireless Networks Division, Spectrum Sharing <b>Division, and Group:</b> Project <b>NIST Research</b> Timothy A. Hall <b>Advisor:</b>	<b>Title of Talk:</b> Spectrum Sharing for Wireless Communications with Occupancy Prediction  <b>Abstract:</b> The rise of smartphones has created a great demand for wireless data usage. Spectrum available for wireless data usage is a limited resource in the sense that signals must be separated either in space, time, frequency, or code. As part of President Obama's initiative to create an additional 500 MHz of spectrum available for non-government use, our project is to enable technology that permits commercial use of government-held spectrum through spectrum sharing. For example, efforts are underway to make the 150 MHz of broadband space centered at the 3.5 GHz band currently used by Navy air marshalling radar systems available for wireless broadband use in a way that will not interfere with the Navy's operations. The Spectrum Access System will govern the spatial and temporal distribution of spectrum space for priority-based spectrum sharing. This system will respond to sensors monitoring spectrum activity and employ prediction algorithms to make sharing decisions.  In addition to giving an overview of the project as a whole, an investigation of different algorithms that can predict LTE activity is presented. A prediction algorithm studying partial periodic pattern mining was implemented and analyzed. This prediction algorithm counts the number of instances of commonly occurring patterns in the previous activity of a channel, which it then uses to predict future availability within the channel. It allows for partial patterns by utilizing wildcards, which allow sequences that differ minimally to be consolidated into one pattern. The effectiveness and accuracy of this algorithm in predicting open time slots available for use was measured on previously captured data. We compare our results to the results obtained by the original authors of the algorithm as well as the results obtained from other prediction algorithms. The implications of our results in the larger context of the Spectrum Sharing Project will be discussed.
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<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Samantha Isaac	Grant Number 70NANB15H181
Academic Institution: West Virginia University	Major: Physics & Mathematics
Academic Standing Sophomore	
(Sept. '15):	
Future Plans [School/Career]:	I plan on earning a Ph.D. in physics however I am currently unsure of which field in physics that I will focus on.
NIST Laboratory,	NIST Center for Neutron Research, Neutron Condensed Matter Science Group
Division, and Group:	
NIST Research Advisor:	Leland Harriger
Title of Talk:	Monte-Carlo Modeling of Multiplexed Neutron Spectroscopy
Abstract:	Multiplexing of a crystal analyzer-detector system produces about an order of magnitude increase in the collection rate of triple axis neutron spectrometers. Using the recently developed mode of operation, Rowland defocusing, a sample image reproduced by the multiplexed analyzer is projected onto the Rowland circle and then viewed by a position sensitive detector (PSD) through a radial collimator. This ability to use a radial collimator just before the PSD greatly increases the signal-to-noise ratio. This geometry can be implemented on multiplexed triple axis with no design modification. However, a much more powerful spectrometer can be designed by expanding the multiplexing of crystals to a 150° coverage of the detector angle (A4) – an Inverse Rowland Inelastic Spectrometer (IRIS). In a second design, a Low Energy Anti-Focusing spectrometer (LEAF) superimposes multiple Rowland circles with each encompassing its own reduced IRIS design, permitting a wide range of energies and A4 to be sampled at once.
	In order to quantitatively measure viability and throughput, I have built virtual models employing the Rowland defocusing geometry. Using Monte Carlo simulations, I was able to show that when the position of the sample image and collimator focal point matched, the collection rate was optimized. Simulations are currently running to accurately reproduce measured calibration results of a multiplexed triple axis spectrometer in the Rowland defocusing geometry. A virtual model of IRIS and LEAF will then be constructed and simulations will be run in order to confirm an increase in collection rate.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Ariel Isser	Grant Number 70NANB15H168
Academic Institution: University of Maryland College Park	Major: Bioengineering
Academic Standing Senior	
(Sept. '15):	
Future Plans Graduate School	
(School/Career):	
NIST Laboratory,	Material Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials
Division, and Group:	Group
NIST Research Advisor:	Swarnavo Sarkar
Title of Talk:	Predicting Bulk Properties of Photocurable Monomers from Molecular Dynamics Simulations
Abstract:	Photopolymerization is a synthetic technique that uses photons to initiate a radical reaction that grows a polymer network from monomers. It is used for a wide range of applications, including nano- and microfabrication, coatings and surface modification, additive manufacturing, and in-situ polymerizations of dental restorative materials. Current gaps in our understanding of how starting materials and curing processes affect the physical and chemical properties of photocured polymers make new material discovery for these applications a time-consuming and expensive process. While there is ongoing work to accelerate this process through computational tools that can predict macroscopic properties of photopolymerized materials by simulating polymer network growth, the tools require accurate inputs for the bulk properties of the initial system of unreacted monomers. In this project, software based on molecular dynamics simulations was developed to predict several bulk properties, such as viscosity and heat capacity, for a given molecule. These calculations can be useful for the acceleration of material discovery, both by providing inputs for network growth simulations and by allowing experimentalists to pre-screen monomers before deciding to synthesize them in the laboratory. The consistency and accuracy of the software was first tested and validated on simple, well-characterized systems, including water and methyl methacrylate. Then, the bulk properties of two larger, photocurable monomers commonly used in the dental industry, bisphenol A glycidyl methacrylate (bis-gma) and triethylene glycol dimethacrylate (tegDMA) were calculated and compared to existing experimental data.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4–6, 2015



Alaina Jackson

Name: Alaina Jackson

Academic Institution: Bowie State University

Grant Number: 70NANB15H188

Major: Computer Technology

Academic Standing: Senior

(Sept. '15):

Future Plans: Graduate School at Bowie State University

(School/Career):

NIST Laboratory, Division, and Group:

NIST Research

Advisor: Judith E. Terrill

Title of Talk: Automating the Testing of Immersive Visualizations in a CAVE

**Abstract:**

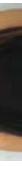
We describe a new test designed to automatically report on the status of the High Performance Computing and Visualization Group software system running the CAVE immersive visualization environment. At its lowest level our software system uses Open Graphics Library (OpenGL). OpenGL is the computer industry's standard application program interface for programming Graphics Processing Units (GPUs). This standard does not guarantee that the pixels displayed in a demo will be exactly the same when displayed with different GPUs and different drivers. So an image generated with identical inputs at two different times may both be correct, but not have identical outputs. My hypothesis is that an image generated with identical inputs from one GPU will not be the same output when displayed on a different GPU.

I have developed a technique to verify that the system is working properly even though our environment is constantly changing. With my designed test, I am able to generate new images on the current software system and record them from different positions based on what their normal state should be. For the best results, I have repeated this test with different hardware and software configurations such as the Nvidia Quadro Fx 4800, and 2000, and compared each of the test results with what their normal state should be. My final result concludes that with different GPU's, the generated images show little to no difference from the original image.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4–6, 2015



Malik Montay-Jackson

Name: Malik Montay-Jackson

Academic Institution: University of Maryland Baltimore County

Grant Number: 70NANB15H172

Major: Computer Science

Academic Standing: Sophomore

(Sept. '15):

Future Plans: Grad School: Master's Degree in some area of Computer Science.

(School/Career):

NIST Laboratory, Division, and Group:

NIST Research

Advisor: Alden Dima

Title of Talk: Improving the Unigram Classification Model

**Abstract:**

Scientific journals are a crucial foundation for scientists to further their research and accelerate innovation in the academic community. Producing such a journal, however, has become an extremely tedious task as researchers must manually evaluate thousands of articles to decide if they are relevant for the journal. Fortunately, advancements in Natural Language Processing and Machine Learning allow us to create models that train computers to automatically classify scientific articles, up to a certain range of accuracy. The current classifier model created to confront this issue uses unigrams in a vector called a bag of words representation (BOW). Unfortunately, this model has certain limitations in extracting semantic information from documents. For example, words such as specific and near have unique contextual meanings when phrased together than when analyzed individually. The current unigram model is unable to make use of such unique phrases. Could the classifier's accuracy, precision, and recall scores be improved by including bigram, trigram, and quadgram word phrases into the BOW? The author of this project hypothesizes that adding a high amount of un-concentrated N-Gram phrases to the BOW will create information noise and actually decrease performance while a highly selective N-Gram filtering algorithm will increase performance. The experiment to confirm this hypothesis concludes with varied results based on combinations of factors however; holistically, the N-Gram based classifier model outperforms the unigram based model.

<b>SURF Student Colloquium</b>		NIST – Gaithersburg, MD	
		August 4-6, 2015	
Name: Karina Jones	Grant Number	70NANB15H156	
Academic Institution: Savannah State University	Major:	Electrical Engineering	
Academic Standing			
(Sept. '15): Senior			
Future Plans: Plan to attend graduate school right after obtaining undergraduate degree.			
(School/Career):			
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Semiconductor and Dimensional Metrology, Nanoelectronics Group			
NIST Research Advisor:			
Dr. Emily Bittle			
Title of Talk: Electrical Contact to Organic Single Crystal Semiconductors in Field Effect Transistor Structures			
Abstract:	<p>Organic semiconductors have unique transport properties and have been used in light emitting diodes found in TVs and smart phone screens. They also have high potential for future applications in flexible electronics such as organic photovoltaics and wearable electronics. Organic semiconductors are interesting because they are relatively inexpensive to produce compared to inorganic semiconductors and are a lot more flexible. In order to tap the full potential of organic semiconductors, there must be a better understanding of the charge transport through these materials and through their interfaces with different metal contacts. The organic/metal interfaces we studied compare organic single crystal semiconductor Rubrene with platinum and Pentacene with gold. We find that the platinum and Rubrene interface is less resistive than gold and Rubrene. This project aims to clarify what occurs in the electronic interfaces of single crystal organic transistors with the use of DC characterization and AC impedance spectroscopy. These techniques will help distinguish electronic interface behavior from pure transistor behavior, which will help form a better understanding of the physics happening within these devices.</p>		
Name: Tim Kamaldinoff	Grant Number	70NANB15H152	
Academic Institution: SUNY Polytechnic Institute - Albany	Major:	Nanoscale Engineering	
Academic Standing			
(Sept. '15): Senior			
Future Plans: PhD in Biomedical Engineering and a career in government laboratory or industry with a focus on biomaterials and tissue engineering.			
(School/Career):			
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biosystems and Biomaterials Division, Group			
NIST Research Advisor:			
Dongbo Wang and Sumona Sarkar			
Title of Talk: Determination of Mineralizing Phenotype in <i>in vitro</i> Tissue Cultures Using Confocal Laser Scanning Microscopy			
Abstract:	<p>Regenerative medicine is at the forefront of medical innovation. Cells used in these therapies must be well characterized and validated for their intended biological function. Mineralization is often used in <i>in vitro</i> cultures as an indicator of stem cell potency or to monitor bone tissue formation. Matrix mineralization occurs through different pathways, which are not yet well understood for <i>in vitro</i> cultures. Some mechanisms are cell-mediated processes resulting in physiological or pathological mineralization, while others may arise from physicochemical processes from cell culture components.</p>		
We hypothesized that each type of calcification can result in different patterns of mineral deposition over the time course as cells grow into mature osteoblast. A mouse pre-osteoblastic cell line MC3T3-E1 (SC4), was chosen as a robust <i>in vitro</i> cell culture model to monitor and characterize mineralization over time. Cells were cultured on polymeric 2D films and 3D nanofiber microenvironments, then characterized at weekly time points over 4 weeks using immunofluorescent staining and confocal and fluorescent microscopy.	<p>Since mineralization is controlled by organic and inorganic components of the matrix, the cultures were stained for calcium deposits, using calcein fluorophore, and osteocalcin, a late stage protein marker of osteoblast differentiation, where expression is linked to the extracellular mineralization. Additionally, the cell actin cytoskeleton and nuclei were stained in order to observe spatial distribution of cells in relation to mineral formation. Different spatial and morphological patterns of mineral, osteocalcin, and cells were observed after 28 days of culture. We categorized mineral morphologies as fibrillary, granular, or sheet like, and observed different mineral morphologies through the thickness of the cell layers.</p>		
In conjunction with fluorescent microscopy observations, parallel samples were prepared for analysis using broadband coherent anti-Stokes Raman scattering microscopy to characterize the chemical composition of the different mineral morphologies. Correlations between mineral morphology, spatial localization and chemical characteristics may lead to better understanding of mineralization in <i>in vitro</i> cultures, and help to identify physiologically relevant mineral patterns.			

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Anton Kienzle
Academic Institution:	Haverford College
Academic Standing	Sophomore
(Sept. '15):	
Future Plans:	Natural science researcher
(School/Career):	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Systems Engineering group
NIST Research	
Advisor:	Tom Hedberg, Allison Barnard Feeney
Title of Talk:	Review of Machine Learning in Manufacturing from 2010 to 2015
<b>Abstract:</b>	
Machine learning, wherein a computer algorithm's output improves when given more data, has been used across domains for decades but has not been applied widely in manufacturing. Widespread use of machine learning in manufacturing enterprises would improve everything from decision making to task efficiency and accuracy. This paper seeks to identify processes in the production life cycle for which machine-learning techniques have been applied and to determine the extent of this research so as to focus further research. A survey of the Engineering Village™-database for articles on the application of machine-learning to the production life cycle, with emphasis on manufacturing itself, yielded 190 articles. These articles were classified by various machine-learning tags applied by Engineering Village, and then further categorized by machine-learning application. Frequent categories of similar applications — scheduling, the production process, and optimization — were grouped to emphasize rarer types of application. Little further research is needed in these categories of application. Articles related to development of machine-learning architectures and algorithms for manufacturing and the application of those architectures and algorithms to specific factories were all prevalent. This survey found limited research related to production-line creation or selection decisions, production-line health monitoring, and supplementary quality-control information, and these areas would benefit from further research. Even though some research has identified strong connections both between design and manufacturing, and between supply chain management and manufacturing, very few papers develop properly informed machine learning algorithms through broad information sharing across the product life cycle. A significant impact may be achieved through application of machine learning in the context of more comprehensive information use and sharing in the product life cycle.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Jillian Kasner
Academic Institution:	Hood College
Academic Standing	Senior
(Sept. '15):	
Future Plans:	After graduation, I plan to work in Cryptology or Cyber Security.
(School/Career):	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis, & Modeling Group
NIST Research	William Guthrie
Advisor:	
Title of Talk:	Redeveloping the GUM.validate Function in the Metrology Package for R
<b>Abstract:</b>	
Uncertainty can occur due to random error and user error. Uncertainty analysis uses these errors to verify if, in this case, the variation in measurement is due to the uncertainty. One of the available resources for measurement uncertainty analysis is the metrology package in R. The function GUM.validate performs this verification process.	
For ten days, I conducted an experiment with one of the NIST 3D Printers. Then applied the gathered data to the GUM.validate function to determine if the measurement variation of the 3D printed boxes was within the specifications provided by MakerBot.	
Over the course of the summer, we have made multiple changes to the GUM.validate function. This function checks the validity of the uncertainty analysis by comparing the simulated values to the input values provided by the user. The function now uses copulas which allows correlation among different distribution types; uniform, normal, triangular, and beta. The function performs an optimization to make the correlation of the copulas more precise. I will discuss these changes, as well as others, during my presentation.	

## SURF Student Colloquium

NIST – Gaithersburg, MD  
August 4–6, 2015



Name: Tatjana Kiryutina

Academic Institution: Montgomery College, Rockville

Academic Standing (Sept. '15): University of Maryland, College Park, transfer student

Major: Chemical and Biomolecular Engineering

Future Plans (School/Career): Graduate School

(School/Career):

NIST Laboratory:

Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical

Division, and Group: Measurement Science Group

NIST Research Advisor: Dr. Jeanita Pritchett

Title of Talk: Method Development and Validation of Targeted Metabolomics Approach for

Nanotoxicity Assessment

**Abstract:**

Metabolomics is the study of chemical processes involving metabolites, the intermediates and products of metabolism. It involves collecting quantitative data to gain an overall understanding of metabolism. Metabolites under study reveal how chemical functions are being carried out in an organism, its developmental status, and disease information of a biological system inside the organism.

The overall goal of this project is to quantitatively measure nanotoxicity via metabolism. My contributions are developing a method for the targeted liquid chromatography tandem mass spectrometry (LC-MS/MS) approach and evaluating the robustness of this approach. The metabolites chosen for this project are amino acids, which contribute to 10% to 15% of metabolic energy generated by animals and are precursors of many different rather than untargeted metabolites, such as hormones and neurotransmitter substances. This approach is deemed targeted instead of observing global differences in the entire metabolome.

The liquid chromatography method development involved running known concentrations of standard L-amino acids through the normal phase column, then adjusting the organic to inorganic gradient of the mobile stationary phase was chosen because amino acids are polar molecules and better adhere to the column, resulting in a suitable separation method. The fragmentor voltage and collision energy in the mass spectrometer were optimized with flow injection analysis mode for each of the target analytes.

For method development and validation, standard L-amino acid solutions of varying concentrations in 90 % (v/v) Acetonitrile were prepared. Multiple runs were carried out for each solution to confirm the reproducibility and robustness of the method. The instrument response was plotted against the concentration for each amino acid in a standard curve. Each standard curve exhibited a linear relationship which was supported by R-squared values close to one. In future nanotoxicity assessments, instrument response and the standard curve equations can be used to determine the concentrations of amino acids in biological samples.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4–6, 2015



Name: Emmie Knoblock

Academic Institution: Smith College

Academic Standing (Sept. '15): Junior

Future Plans (School/Career): Graduate school, seeking a PhD in biochemistry or biomedical science

NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials Group

NIST Research Advisor: Diane Bienek

Title of Talk: Assessing Healing Properties of an Airbrushed Chitosan Wound Dressing

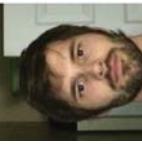
**Abstract:**

The purpose of this project was to assess the in vitro growth and activity of keratinocytes grown on airbrushed nanofiber scaffolds containing chitosan and to quantify their antimicrobial properties. Chitosan is a polysaccharide derived from chitin, a component of crustacean shells. It is known to have hemostatic and antibacterial properties, and is a common component in wound dressings. When combined with polymers such as poly(lactic-co-glycolic acid) (PLGA) and polyethylene glycol (PEG) in solvent, it forms a solution that can be easily airbrushed onto a number of surfaces and has potential for a self-adhering, easily administered wound dressing with healing properties.

The effects of these scaffolds on cell growth and healing were assessed by growing cells on samples of this material containing 0% to 10% dry weight of chitosan, and either 0% PEG or 15% PEG. Their growth and metabolic activity over a period of nine days were measured using a number of methods, including WST cell proliferation assays, PicoGreen assays, and RT-PCR. The antimicrobial properties of the scaffolds were assessed via ATCC method 100-2012, by inoculating samples with a culture of *Streptococcus mutans* and incubating for two hours. The number of living bacteria were then determined via a count of colony-forming units (CFU) from cultures of these samples grown on agar. A commercially available chitosan wound dressing was included for comparison as a positive control.

Initial results indicate that those sample groups containing chitosan or PEG do not exhibit increased cellular toxicity when compared to those without. Groups containing PEG do have visibly increased antibacterial properties compared to those without; however, these investigations will contribute to the development of this novel wound dressing by elucidating its effects on new tissue growth.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Joseph A. Lagrene	<b>Grant Number</b> 70NANB15H172
<b>Academic Institution:</b> University of Maryland, Baltimore County	<b>Major:</b> Chemical Engineering
<b>Academic Standing</b>	<b>Junior</b>
<b>(Sept. '15):</b>	<b>Senior</b>
<b>Future Plans</b>	I plan to attend grad school and earn a Master's Degree in Computer Science.
<b>(School/Career):</b>	
<b>NIST Laboratory,</b>	<b>NIST Laboratory,</b> NIST Information Technology Lab, Computer Security Division, Cryptographic Technology
<b>Division, and Group:</b>	<b>Division, and Group:</b> Group
<b>NIST Research</b>	Kerry McKay
<b>Advisor:</b>	
<b>Title of Talk:</b>	<b>Feasibility and Applications of RapidMiner 5 for Estimating the Entropy of an Entropy Source</b>
<b>Abstract:</b>	As our lives increasingly depend on technology and more data becomes publicly accessible, cybersecurity has become more important than ever. Random Number Generators (RNGs) play a critical role in the encryption of data, and it is important that one's RNGs be sufficiently unpredictable. We seek to design a plugin for RapidMiner 5, a data mining program which allows users to perform operations on data sets with relative ease through a simple drag-and-drop graphical user interface, which will attempt to answer the question, "How unpredictable is this data set?" Or, in other words, "What is the entropy of this data source?" Topics of discussion for this talk include some of the approaches we took towards estimating entropy, whether we can definitively estimate the entropy of a data source, and ultimately whether RapidMiner 5 is a feasible tool for prototyping and deploying entropy estimation methods.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
<b>Name:</b> Matthew Kovarek	<b>Grant Number</b> 70NANB15H172
<b>Academic Institution:</b> University of Maryland, Baltimore County	<b>Major:</b> Chemical Engineering
<b>Academic Standing</b>	<b>Senior</b>
<b>(Sept. '15):</b>	
<b>Future Plans</b>	I am planning to work in industry for a few years and then return to Graduate School after determining my specific field of interest
<b>(School/Career):</b>	
<b>NIST Laboratory,</b>	<b>NIST Laboratory,</b> Engineering Laboratory, Materials and Structural Systems Division, Structures Group
<b>Division, and Group:</b>	
<b>NIST Research</b>	Marc Levitan, DongHun Yeo
<b>Advisor:</b>	
<b>Title of Talk:</b>	<b>Dynamic Pressure Propagation in a Tubing System</b>
<b>Abstract:</b>	The behavior of wind is of interest to those involved in the construction of habitable structures as the wind loading needs to account for the additional forces that the building will be subjected to. Therefore, CFD (computational-fluid-dynamics) is of interest to model this behavior accurately. However, the CFD modeling of these types of structures is not well-documented and it is desirable to compare these simulations with actual data collected in a controlled manner in a wind-tunnel as this would lend validation to the accuracy of the simulations of this wind loading using CFD modeling. Due to sensor size, it is not possible to place the pressure transducers directly on the surface of the models in the wind-tunnel, generating a need for a tubing system to convey the induced pressure waves to the main sensor body. The propagation of these pressure waves inside a thin, circular tube generates distortion due to the acoustic and visco-thermal effects of the fluid media, boundary layer and the tubing material structure and dimensions. It is therefore desirable to predict and model this accurately before assembly and testing of the models. This is done by considering the inviscid Navier-Stokes Equations, thermodynamic behavior, wave propagation, and mass and energy conservation within a program constructed using the software MATLAB. This program will generate theoretical data that is then used to optimize a tubing system configuration, which is then tested against real data. The final tube construction will be used to construct the model system for use in the wind-tunnel. Results and conclusion are forthcoming, but based upon previous research the theoretical data should closely match the collected experimental results.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Stephen Lee
<b>Academic Institution:</b> University of Maryland, Baltimore County	<b>Grant Number</b> 70NANB15H172
<b>Academic Standing (Sept. '15):</b>	<b>Major:</b> Computer Science
<b>Future Plans (School/Career):</b>	Attend Graduate school to obtain a PhD in Computer Science
<b>NIST Laboratory, Division, and Group:</b>	Information Technology Laboratory, Computer Security Division, Secure Systems and Applications Group
<b>NIST Research Advisor:</b>	Michaela Jorga
<b>Title of Talk:</b>	Cloud Rubik's Cube: NIST's Cloud Security Reference Tool
<b>Abstract:</b>	Clean water is needed in many areas of life, but a shortage is already happening in some areas of the world. While pressure-driven separation (reverse osmosis) via a dense polyamide thin film composite is a viable approach for purifying seawater, it is not sufficiently energy efficient for many water-starved nations. This energy efficiency is linked to the extrinsic (thickness) and intrinsic property (polymer structure) of the polyamide layer. However, there is limited insight that commercial materials can provide to improve membrane design. To provide some insight into these polyamide materials, we use molecular layer-by-layer, a technique developed here at NIST, to fabricate model polyamide films with well-defined thicknesses ranging from 10 nm up to 70 nm. We study the water swelling of these model polyamide films using X-ray reflectivity in order to extract the polymer network parameters that governs water transport and determine how these parameters scale with film thickness.
<b>Name:</b> Matthew Landen	<b>Grant Number</b> 70NANB15H141
<b>Academic Institution:</b> University of Science and Technology of China	<b>Major:</b> Chemical Engineering
<b>Academic Standing (Sept. '15):</b>	<b>University of Minnesota, Sophomore</b>
<b>Future Plans (School/Career):</b>	Either a job in the private sector or graduate school
<b>NIST Laboratory, Division, and Group:</b>	Material Measurement Laboratory, Materials Science and Engineering Division, Functional Polymers Group
<b>NIST Research Advisor:</b>	Edwin Chan
<b>Title of Talk:</b>	Effect of film thickness on the network structure of polyamide water desalination membranes
<b>Abstract:</b>	Clean water is needed in many areas of life, but a shortage is already happening in some areas of the world. While pressure-driven separation (reverse osmosis) via a dense polyamide thin film composite is a viable approach for purifying seawater, it is not sufficiently energy efficient for many water-starved nations. This energy efficiency is linked to the extrinsic (thickness) and intrinsic property (polymer structure) of the polyamide layer. However, there is limited insight that commercial materials can provide to improve membrane design. To provide some insight into these polyamide materials, we use molecular layer-by-layer, a technique developed here at NIST, to fabricate model polyamide films with well-defined thicknesses ranging from 10 nm up to 70 nm. We study the water swelling of these model polyamide films using X-ray reflectivity in order to extract the polymer network parameters that governs water transport and determine how these parameters scale with film thickness.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Matthew Landen
<b>Academic Institution:</b> University of Science and Technology of China	<b>Grant Number</b> 70NANB15H141
<b>Academic Standing (Sept. '15):</b>	<b>Major:</b> Chemical Engineering
<b>Future Plans (School/Career):</b>	Either a job in the private sector or graduate school
<b>NIST Laboratory, Division, and Group:</b>	Material Measurement Laboratory, Materials Science and Engineering Division, Functional Polymers Group
<b>NIST Research Advisor:</b>	Edwin Chan
<b>Title of Talk:</b>	Effect of film thickness on the network structure of polyamide water desalination membranes
<b>Abstract:</b>	Clean water is needed in many areas of life, but a shortage is already happening in some areas of the world. While pressure-driven separation (reverse osmosis) via a dense polyamide thin film composite is a viable approach for purifying seawater, it is not sufficiently energy efficient for many water-starved nations. This energy efficiency is linked to the extrinsic (thickness) and intrinsic property (polymer structure) of the polyamide layer. However, there is limited insight that commercial materials can provide to improve membrane design. To provide some insight into these polyamide materials, we use molecular layer-by-layer, a technique developed here at NIST, to fabricate model polyamide films with well-defined thicknesses ranging from 10 nm up to 70 nm. We study the water swelling of these model polyamide films using X-ray reflectivity in order to extract the polymer network parameters that governs water transport and determine how these parameters scale with film thickness.
<b>Name:</b> Matthew Landen	<b>Grant Number</b> 70NANB15H172
<b>Academic Institution:</b> University of Maryland, Baltimore County	<b>Major:</b> Computer Science
<b>Academic Standing (Sept. '15):</b>	<b>University of Minnesota, Sophomore</b>
<b>Future Plans (School/Career):</b>	Either a job in the private sector or graduate school
<b>NIST Laboratory, Division, and Group:</b>	Information Technology Laboratory, Computer Security Division, Secure Systems and Applications Group
<b>NIST Research Advisor:</b>	Michaela Jorga
<b>Title of Talk:</b>	Cloud Rubik's Cube: NIST's Cloud Security Reference Tool
<b>Abstract:</b>	Cloud computing is a new approach to information systems which uses virtualization to provide scalable computational resources offered by dedicated companies as an utility that can be consumed as needed. Government agencies recognize the value of cloud services and are looking to adopt cloud-based solutions. Even though the tremendous benefits of cloud computing services make this new technology very attractive, the lack of control and visibility into the architecture is concerning. Agencies work with sensitive data and they question whether the data will be safe in the cloud because cloud-based systems send information through channels, leaving data vulnerable to cyber attacks if not properly secured. NIST is taking steps to develop guidance for government agencies to overcome these concerns and speed up adoption of cloud solutions.
	With support from the NIST Cloud Security Working Group, NIST created a security architecture that provides agencies with a methodology to adopting cloud. The basis is a list of functional capabilities of cloud services. NIST selected, for each capability, the security controls designed to protect the system and the data it contains. The overall goal of the architecture is to develop trust between consumers and providers of cloud services.
	Cloud Rubik's Cube is a tool that helps users analyze the data. The tool provides different ways to view the relationships between functional capabilities and security controls. Users want to analyze this data and display the correlations in different ways. My tool processes spreadsheets with aggregated data that identifies functional capabilities and the associated security controls necessary to secure these capabilities and organizes the data, populating the database. The program can then create different types of reports by extracting data. The Cloud Rubik's Cube aims to help government agencies perform their risk assessment and analyze the security data of particular cloud-based solutions.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
Name: Wa In Lee	Grant Number   70NANB15H14-1
Academic Institution: University of Maryland, College Park	Major: Secondary Education: Mathematics
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Graduate School, University of Maryland, College Park
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical Measurement Science Group
NIST Research Advisor:	Jeannie Brown Thomas
Title of Talk:	Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials
Abstract:	<p>Well-characterized reference materials and reliable analytical methods are needed in the food testing and nutrition communities to help facilitate compliance with nutritional labeling laws and improve the accuracy of nutrition information that is provided to assist consumers in making sound dietary choices. As a result of the Nutrition Labeling and Education Act (NLEA) of 1990, the National Institute of Standards and Technology (NIST) has developed a series of food-matrix Standard Reference Materials (SRMs) characterized for nutrient concentrations. The NLEA requires food processors to provide specific nutrition information on labels of products distributed in the United States. Information about vitamin C content is required on nutrition labels, thereby making certified reference materials with assigned values for vitamin C useful.</p> <p>Vitamin C concentrations will be determined in three new NIST food-matrix Standard Reference Materials (SRMs) using a liquid chromatographic (LC)-absorbance method developed at NIST. These SRMs include SRM 2252 Protein Drink Mix, SRM 3290 Dry Cat Food, and SRM 2386 Avocado Powder. The procedure used to extract vitamin C from the different matrices, a description of the LC method employed, and the results from the measurement of vitamin C in each material will be presented.</p>
Name: Joseph Lesniowski	Grant Number   70NANB15H186
Academic Institution: Mount St. Mary's University	Major: Chemistry
Academic Standing (Sept. '15):	Georgetown University, 1 <sup>st</sup> Year Graduate School
Future Plans (School/Career):	I am enrolled as a graduate student in chemistry at Georgetown University for the fall of 2015. After graduate school I would like to continue working at NIST or a similar national laboratory.
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group
NIST Research Advisor:	Dr. William Ratcliff
Title of Talk:	BLAND: A Stimulating Method for the Analysis of Diffraction Patterns
Abstract:	<p>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 called the Bayesian Library for Analysis of Neutron Diffraction (BLAND). 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 Rodriguez-Carvajal, which provides a wide range of neutron and x-ray diffraction specific calculations. The DREAM algorithm, which uses a combination of Markov Chain, Monte Carlo and Differential Evolution is used to perform Bayesian analysis in order to provide automated fitting. This algorithm allows for a thorough and automatic exploration of the parameter space and minimizes the <math>\chi^2</math> value for the model fit. Using this algorithm the pitfalls of traditional least-squares based refinements can be avoided. This avoids the need to painstakingly hand fit data. DREAM will not get stuck in local minima or diverge as other algorithms do. This approach also 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. This iteration of BLAND expanded the library adding the capability to resolve magnetic structures as well as the capability to fit single crystal data (in addition to powder data). Data from several example materials was used to test the effectiveness of the method. The limits and capabilities of the method were then explored using super-computing clusters.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
Name: Wa In Lee	Grant Number   70NANB15H14-1
Academic Institution: University of Maryland, College Park	Major: Secondary Education: Mathematics
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Graduate School, University of Maryland, College Park
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical Measurement Science Group
NIST Research Advisor:	Jeannie Brown Thomas
Title of Talk:	Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials
Abstract:	<p>Well-characterized reference materials and reliable analytical methods are needed in the food testing and nutrition communities to help facilitate compliance with nutritional labeling laws and improve the accuracy of nutrition information that is provided to assist consumers in making sound dietary choices. As a result of the Nutrition Labeling and Education Act (NLEA) of 1990, the National Institute of Standards and Technology (NIST) has developed a series of food-matrix Standard Reference Materials (SRMs) characterized for nutrient concentrations. The NLEA requires food processors to provide specific nutrition information on labels of products distributed in the United States. Information about vitamin C content is required on nutrition labels, thereby making certified reference materials with assigned values for vitamin C useful.</p> <p>Vitamin C concentrations will be determined in three new NIST food-matrix Standard Reference Materials (SRMs) using a liquid chromatographic (LC)-absorbance method developed at NIST. These SRMs include SRM 2252 Protein Drink Mix, SRM 3290 Dry Cat Food, and SRM 2386 Avocado Powder. The procedure used to extract vitamin C from the different matrices, a description of the LC method employed, and the results from the measurement of vitamin C in each material will be presented.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Jenny Esther Li
Academic Institution:	Binghamton University, State University of New York
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Career in Holographic Development or Robotics
NIST Research Advisor:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, CMOS and Novel Devices Group Lin You, Joseph Kopanski
Title of Talk:	COMSOL Simulation of Electromagnetic Test Structures
<b>Abstract:</b>	
<p>A new and promising method for increasing the functionality of circuits, 3D integrated circuits (3D-IC) has become a major focus of research. Moore's law predicts a limitation in size reduction of IC design, but 3D-ICs can overcome this limitation by stacking integrated circuits on top of each other. These novel designs have both reduced power consumption and parasitic capacitance. However, a lot of research is still necessary before this method is available for commercialization. As promising as 3D-ICs are for the future of semiconductor and electronics industry, the method is still novel and not without vulnerabilities to defects. Detecting these defects will be an important next step towards building a new reliability standard for this innovation. Scanning Microwave Microscopy (SMM) is one possible tool for the task. Its ability to produce high resolution images of subsurface geometry with non-invasive scanning makes it suitable for detecting defects. By sending microwave frequency waves (1–2GHz) through a nanometer wide tip that traces across the surface of the 3D-IC, the SMM will be able to detect hidden subsurface geometry based on the reflected wave amplitude and phase, denoted the s-parameters. Based on the amplitude and angle of the resultant s-parameter values, the occurrence and depth of subsurface geometry and defects can be recorded. For this SURF project, a simplified model of the SMM is to be created for comparison between experimental and simulated results. COMSOL Multiphysics will be used for this objective due to its powerful finite element analysis tools. A simulation of buried wires will be used as a representation of subsurface geometry in a 3D-IC. Matching experimental and simulation data has been achieved for models 20–70 times larger than experimental equipment. Simulation models of the same size as experimental equipment have been created and the generated data is currently being analyzed. A second simulation of frequency across microstrip lines and various samples is currently underway. Due to notable similarities between experimental and simulated results, it is encouraged that more models are to be built in the future to address different variations of subsurface geometries.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Daniel Lessoff
Academic Institution:	The College of New Jersey
Academic Standing (Sept. '15):	B.S. in Computer Science
Future Plans (School/Career):	Graduate school, career in Network/Computer Security
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Networks and Technology Division, Internet and Scalable Systems Metrology Group
NIST Research Advisor:	Oliver Borchert
Title of Talk:	Improvements in Routing Security: A BGPSEC Test System
<b>Abstract:</b>	
<p>The Border Gateway Protocol, or BGP, is one of the key components of the “backbone of the Internet” – It is the “Glue that hosts the Internet together”. BGP allows routers to exchange routing information needed to be able to send traffic from A to B. However, the way in which this capability is negotiated is not secure, and efforts to make it secure have not received wide support to date. BGPSEC, an extension of the existing BGP infrastructure, seeks to add an additional layer of security to the existing Border Gateway Protocol. BGPSEC modified the existing BGP protocol in such that it adds signatures to the propagated information to allow each participating BGP speaker / node to verify the correctness of the received routing path. This ‘signed path’ ensures that a given node (or Autonomous System, AS) has the ability to detect modifications in the path. This set of standards are under development at the IETF Secure Inter-Domain Routing group (SIDR) and in its final stage to become an official RFC.</p> <p>My task over the summer has to been to work on a set of testing tools to test BGPSEC deployment. These have consisted of continuing work on a Wireshark module to inspect BGPSEC packets, as well as continuing work on traffic generation tools such as SimpleBGP and Hoofprints, to allow the generation of BGP traffic as it is specified in the BGPSEC protocol definition. Over the course of my research, I have looked into dissecting the components of BGPSEC protocol into discrete pieces for easier analysis. Furthermore I analyzed currently available test tools to determine the best to be extended for BGPSEC traffic generation that will allow the generation of well-defined sample traffic for unified protocol testing.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Simón Lorenzo <b>Academic Institution:</b> Louisiana State University <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> Future Plans <b>(School/Career):</b> NIST Laboratory, Physical Measurement Laboratory, Sensor Science Division, Optical Radiation Group <b>Division, and Group:</b> NIST Research <b>Advisor:</b> Maritoni Litorja <b>Title of Talk:</b> Calibrating a Solid Tissue Phantom for use in Fluorescent Imaging
	<b>Name:</b> Akshay Lingayat <b>Academic Institution:</b> University Of Maryland, College Park <b>Major:</b> Mechanical Engineer <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> To attend graduate school studying nanotechnology. <b>(School/Career):</b> NIST Laboratory, Material Measurement Laboratory, Chemical Sciences Division, Inorganic Measurement <b>Division, and Group:</b> Science Group <b>Advisor:</b> Monique E. Johnson <b>Title of Talk:</b> The Gold-Worm Conundrum
	<p><b>Abstract:</b></p> <p>The incorporation of nanomaterials into consumer products we encounter in our everyday lives has resulted in a need to determine the effects such materials have on the environment, as well as on organisms. Due to their ability to disperse rapidly, exposure to nanoparticles is inevitable and thus must be investigated in order to prevent any detrimental effects. The research presented examines the uptake of gold nanoparticles by a model organism, <i>C. elegans</i>. A method was developed to identify transformations and effects due to nanoparticle uptake with the use of both conventional and single particle inductively coupled plasma mass spectrometry (ICP-MS). The use of gold nanoparticles helps establish and validate the methodology which can then be further applied to toxicology studies of the uptake of more toxic metallocnanoparticles. The protocol entails maintenance of both <i>C. elegans</i> and its food source (<i>E. coli</i>), extracting viable worms from the culture media and exposing viable nematodes to gold nanoparticles over a 24 hour time period. In previous studies, insufficient rinsing of the worm cuticle resulted in false positive nanoparticle uptake measurements; therefore, we developed a sophisticated gradient density sucrose method for separating <i>C. elegans</i> from free nanoparticles in solution and adhered to the worm cuticle. It was observed that through the gradient density sucrose method, worms tended to congregate between the salt and least dense sucrose layer interface enabling separation of exterior nanoparticles from the cuticle of the nematode. Following the validation of this new rinsing procedure, nematodes were exposed to 30 nm and 60 nm AuNPs (NIST) in liquid media for 24 h. Two procedures were established for the quantification of AuNP uptake; a microwave digestion procedure (using a mixture of concentrated acids to determine the total metal uptake within the dry worm pellet) and a base digestion procedure (using tetramethylammonium hydroxide (TMAH) to liberate and size internalized particles from the biological tissue). Nematodes in the control experimental condition contained a trace amount of Au, whereas for 30 nm AuNP-exposed and 60 nm AuNP-exposed nematodes consumed 11.536 ± 261.1 ng Au/g <i>C. elegans</i> and 21.881 ± 229.3 ng Au/g <i>C. elegans</i>, respectively. A zero hour and 24 hour experiment revealed that approximately 10% of the total gold concentration for each exposure condition could be attributed to particles absorbed to the cuticle.</p> <p><b>Abstract:</b></p> <p>When patients are diagnosed with breast and prostate cancer, as well as some other forms of cancer, standard medical practice involves removing lymph nodes for biopsy. Unfortunately, this leaves the patients with damaged lymphatic and compromised immune systems. Optical systems currently in development image the lymphatic system from outside the body using near-infrared fluorescent (NIRF) tracers. For now, this non-invasive process would use indocyanine green as it is the only approved molecular probe that emits in the infrared. Eventually, molecular probes that bind to tumor cells could quantify metastasis without removing lymph nodes.</p> <p>The Food and Drug Administration (FDA) requires (when applicable) performance descriptions using The International System of Units (SI) units, for all approved medical measuring devices. For drug and device combinations such as the NIRF imager, this would also allow any user to evaluate the usefulness of the technology or improve it. To date, there exists no such quantitative characterization for cameras used with NIRF despite their growing role in static cancer imaging. These cameras as capture light indicative of fluorescent probe concentrations within a patient. However, responses to the emitted light vary across camera manufacturers, presenting a barrier for medical professionals attempting to compare measurement results. Measurement traceability in SI units would allow for comparable imaging data and help build benchmarks in quantifying metastasis. To help FDA examination of these devices, a solid tissue phantom could serve as an SI calibration source for all NIRF imaging systems. Illuminated by a similar near-infrared light as applied to the patient, the phantom (polyurethane with embedded TiO<sub>2</sub> and quantum dots) would mimic fluorescing human tissue. This calibration source should have a constant radiance value (W/m<sup>-2</sup>/sr) for a given incident laser irradiance and wavelength. Cameras with different electrical components could then be compared to the source, and as a result, to each other. Additionally, the phantom should approximate a Lambertian emitter to large angles from the normal at distances typical in an operating room. This would allow for practical use by a medical technician without undue optical alignment during surgery. The goal of the 2015 SURF internship lies in investigating whether a prototyped tissue phantom exhibits the above properties in a reproducible and repeatable fashion. If so, the techniques for determining these properties and the resulting radiometric values will be documented in SI units. Furthermore, transportable equipment for taking NIRF camera measurements in the clinic will be purchased/prototyped in a manner conducive to data acquisition in SI units.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Akshay Lingayat <b>Academic Institution:</b> University Of Maryland, College Park <b>Major:</b> Mechanical Engineer <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> Future Plans <b>(School/Career):</b> NIST Laboratory, Material Measurement Laboratory, Chemical Sciences Division, Inorganic Measurement <b>Division, and Group:</b> Science Group <b>Advisor:</b> Monique E. Johnson <b>Title of Talk:</b> The Gold-Worm Conundrum

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Adam Macata <b>Academic Institution:</b> Worcester Polytechnic Institute <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>Future Plans (School/Career):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>NIST Laboratory, Division, and Group:</b> Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Group <b>NIST Research Advisor:</b> Erik Johnsson <b>Title of Talk:</b> The Effect of Wind-Driven Fires Along Fences on Homes in the Wildland-Urban Interface
<b>Name:</b> Kurt Lynn <b>Academic Institution:</b> Savannah State University <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> I plan to commission in the United States Navy in Spring of 2017 as a Nuclear Officer <b>Future Plans (School/Career):</b> I plan to commission in the United States Navy in Spring of 2017 as a Nuclear Officer <b>NIST Laboratory, Division, and Group:</b> NIST Center for Neutron Research, Operations and Engineering Group <b>NIST Research Advisor:</b> Mike Middleton <b>Title of Talk:</b> Characterizing Radiation Induced Faults in Microprocessors	<b>Name:</b> Adam Macata <b>Academic Institution:</b> Worcester Polytechnic Institute <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>Future Plans (School/Career):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>NIST Laboratory, Division, and Group:</b> Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Group <b>NIST Research Advisor:</b> Erik Johnsson <b>Title of Talk:</b> The Effect of Wind-Driven Fires Along Fences on Homes in the Wildland-Urban Interface

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Kurt Lynn <b>Academic Institution:</b> Savannah State University <b>Academic Standing:</b> Junior <b>(Sept. '15):</b> I plan to commission in the United States Navy in Spring of 2017 as a Nuclear Officer <b>Future Plans (School/Career):</b> I plan to commission in the United States Navy in Spring of 2017 as a Nuclear Officer <b>NIST Laboratory, Division, and Group:</b> NIST Center for Neutron Research, Operations and Engineering Group <b>NIST Research Advisor:</b> Mike Middleton <b>Title of Talk:</b> Characterizing Radiation Induced Faults in Microprocessors
	<b>Name:</b> Adam Macata <b>Academic Institution:</b> Worcester Polytechnic Institute <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>Future Plans (School/Career):</b> Master's in Fire Protection Engineering at Worcester Polytechnic Institute <b>NIST Laboratory, Division, and Group:</b> Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Group <b>NIST Research Advisor:</b> Erik Johnsson <b>Title of Talk:</b> The Effect of Wind-Driven Fires Along Fences on Homes in the Wildland-Urban Interface

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
	
Name: Theodora Martin	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Chemical Engineering, with focus on Bioengineering
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Graduate School	School: Master's degree
(School/Career):	Career: Pharmaceutical industry, drug synthesis and manufacture
NIST Laboratory, Division, and Group: Center for Nanoscale Science and Technology, NanoFab Operations Group	
NIST Research Advisor: Jessie Zhang and Robert Newby	
Title of Talk: Process Development of Polydimethylsiloxane (PDMS) Films for Microfluidic Device Fabrication	
Abstract:	
<p>The CNST NanoFab has recently established a soft lithography laboratory dedicated to microfluidic device fabrication and soft polymer based research. Polydimethylsiloxane (PDMS) is a two part polymer that is readily available in soft lithography lab. A process database related to PDMS is in demand for the lab. This work is to support this purpose and has been focused on (1) understanding the effect of PMDS-to-hexane ratio and spin speed on PDMS film thickness and (2) effect of plasma intensity, plasma exposure time, and working pressure on the bond strength between PDMS and glass. For the first study, five different PDMS-to-hexane ratios and six different spin speeds were selected. PDMS film thickness with various spin speeds and hexane dilutions were measured using the Dektak XT profilometer. Results show that increasing spin speeds and decreasing PDMS-to-hexane dilution ratios produce thinner PDMS films. For the second study, three plasma power settings, three working pressures along with six plasma exposure times were selected. The strongest bonds occurred in samples exposed to high plasma intensities for long periods of time and at low pressures. The data collected from both studies are summarized in tables and plots, and will be added to the process database for the soft lithography lab.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Alexander Mandarino	Grant Number 70NANB15H096
Academic Institution: Appalachian State University	Major: Applied Physics
Academic Standing Senior	
(Sept. '15):	
Future Plans Graduate School	
(School/Career):	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Applied Electrical Metrology Group	
NIST Research Advisor: Jason Underwood	
Title of Talk: Simulation of pulse-driven Josephson junction dynamics.	
Abstract:	
<p>The ac Josephson voltage standard (ACJVS) is one of several quantum-based systems that are intended to supersede artifact electrical standards. Beyond the important goal of improving calibration uncertainties, these new quantum standards are also critical to the proposed redefinition of the SI in terms of fixed physical constants, such as the speed of light. The ACJVS converts weakly-defined input current pulses into precisely defined voltage pulses with voltage-time areas of <math>\hbar/2e</math> where <math>\hbar</math> and <math>e</math> are fundamental constants, thus making it an ideal quantizer. Quantum-accurate waveforms can then be synthesized by precisely controlling the timing and density of the input microwave pulses to the Josephson junction (<math>J_J</math>) array. The dynamical behavior of the <math>J_J</math> array has been examined via simulations based on the resistively-shunted junction (RSJ) model and compared with experimental measurements of the ACJVS at NIST-Gaithersburg. This talk will cover the motivation for this project, the physics behind the Josephson effect, as well as the challenges involved in modeling <math>J_J</math> dynamics and in assessing systematic errors of the ACJVS.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Joshua E. Massey
	<b>Academic Institution:</b> University of Maryland, Baltimore County (UMBC)
<b>Academic Standing</b> <i>(Sept. '15):</i>	<b>Grant Number</b> 70NANB15H142 <b>Major:</b> Materials Science and Engineering and Physics
<b>Future Plans</b> <b>(School/Career):</b>	<b>Future Plans</b> Graduate School <b>(School/Career):</b> Management Resources
<b>NIST Laboratory,</b> <b>Division, and Group:</b> <b>NIST Research</b>	<b>NIST Laboratory,</b> Management Resources <b>Division, and Group:</b> Information Services Office, Digital Services and Publishing Group <b>Advisor:</b> Kimberly A. Tryka
<b>Title of Talk:</b> Harmonizing Standards: Reviewing Military and Law Enforcement PPE Performance Standards	<b>Title of Talk:</b> The MML Data Management Plan Tool: Understanding and Reporting Data About Data
<b>Abstract:</b>	
	<p>In the Spring of 2015, the Office of Data Informatics (ODI) of the NIST Material Measurement Laboratory (MML) released a data management planning (DMP) tool to provide a uniform method and location for MML researchers to store information about data related to their projects (title, description, keywords, instruments used, where the data can be obtained, et cetera). This tool also allows MML management to stay up-to-date on the data-related activities of their respective groups. Since the release of the DMP tool a few months ago, over 200 total records have been submitted.</p> <p>This summer, I worked with staff in the Information Services Office (ISO), as well as ODI staff, to better understand what information is typically entered into this tool and how users interact with it. I first explored the dataset, becoming familiar with its structure and contents. I then wrote a Python algorithm to query the tool's MySQL database, compute statistics about the data, and output basic reports. After discussing the initial results with ODI staff, I revamped the algorithm to be more flexible – including more detailed reports and allowing parameters to be specified.</p> <p>In this talk, I will briefly describe the DMP tool and the resulting Python algorithm, as well as show a few sample reports generated from the data in the tool. In the future, this algorithm will be further developed by the ODI and integrated into the DMP tool.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Jose Martinez
	<b>Academic Institution:</b> Northwestern University
<b>Academic Standing</b> <i>(Sept. '15):</i>	<b>Grant Number</b> 70NANB15H142 <b>Major:</b> Materials Science and Engineering and Physics
<b>Future Plans</b> <b>(School/Career):</b>	<b>Future Plans</b> TBD
<b>NIST Laboratory,</b> <b>Division, and Group:</b> <b>NIST Research</b>	<b>NIST Laboratory:</b> Associated Director of Laboratory Programs, Standards Coordination Office, Standards Division, and Group: Services <b>Advisor:</b> Cassandra Robinson
<b>Title of Talk:</b> Harmonizing Standards: Reviewing Military and Law Enforcement PPE Performance Standards	<b>Title of Talk:</b> Performance Standards are critical to emergency management and response practitioners and help to ensure that the equipment they use performs as expected in the field. Every day military and law enforcement go out to protect fellow Americans accepting the unexpected with their only protection being their training and personal protective equipment (PPE). In most cases, the PPE is ballistic-resistant body armor compliant with either the National Institute of Justice or US Army standards. Having two standards, with varying tests methods and criteria, result in inconsistencies and uncertainty in both the measurements and decisions. An effort to harmonize the standards is underway, and several aspects of the standards are being reviewed, including pretest conditioning, measurement methods, testing instruments, and test range configuration, as well as the detail and coherence of the standards. Through the observation and inquiry of testing laboratories and their technicians, federal agency personnel, end users, and manufacturers, one learns the nuances of performing a conditioning procedure, a test, or a measurement; the thoughts officers have about wearing body armor; as well as the managing official's thought process when choosing body armor. A cohesive set of standards is being coordinated that not only meet the needs of those using them but more importantly creates reliability in the ballistic-resistant body armor that military and law enforcement use every day. A second type of PPE routinely used is helmets. ASTM is developing a new standard for "Ballistic resistant head protection for law enforcement applications". Support for this work involved reviewing existing procedures (where applicable), providing relevant input, and assisting in drafting the standards.
<b>Abstract:</b>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Kamala Mayo	Grant Number   70NANB15H185
Academic Institution: University of the District of Columbia	Major: Information Technology
Academic Standing (Sept. '15): May 2015 Graduate – Bachelor of Science in Information Technology	
Future Plans (School/Career): Graduate School – University of Maryland and Career in Cyber Security	
NIST Laboratory, Division, and Group: Information Technology Laboratory, Software and Systems Division, Software Quality Group	
NIST Research Advisor: Vadim Okun and Aurelien Delaitre	
Title of Talk: Testing Wireshark Protocols for Vulnerabilities using Fuzzed Data	
<b>Abstract:</b>	Wireshark is a network protocol analyzer that uses many independent protocol dissectors to capture and analyze network traffic. People use Wireshark for network monitoring and troubleshooting software, communications protocol development and various other reasons. Its large attack surface and the fact that it often runs with extra privileges makes Wireshark an excellent test case for static analysis tool assessment. Static analyzers are tools designed to detect bugs in software. NIST is developing testing methods for these tools to assess their efficiency. To determine if a tool can find defects, we need to feed it software that contain some. The goal of this project is to find bugs in Wireshark using a fuzzer and use them as test cases for static analyzers. Our work consisted of developing the fuzzer designed to trigger bugs in Wireshark. In particular, I will present the module that takes random data as input and generates network packets as output to feed Wireshark and attempt to crash it. The data obtained from this crash will identify the bugs in Wireshark and be used as test data for static analysis tools.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Robert McAllister	Grant Number   70NANB15H160
Academic Institution: University of Delaware	Major: Chemical Engineering
Academic Standing (Sept. '15): Junior	
Future Plans (School/Career): Graduate School or a job concerned with sustainable energy	
NIST Laboratory, Division, and Group: NIST center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor: Dr. Katie Weigandt	Shooting Neutrons at Soap: Orientation of Wormlike Micelles Under Extensional Flow
<b>Abstract:</b>	Wormlike micelles are involved in multiple practical applications including oil recovery, ink-jet printing, personal and home cleaning products, and drag reduction for turbulent flow in cogeneration. They are semi-flexible macromolecules that are a product of surfactant self-assembly, giving them the ability to break and reform unlike semi-flexible polymer solutions. Both shear and extensional flow are very common in areas ranging from hypodermic needles to polymer processing, but extensional flow is difficult to study because shear flow tends to dominate in experimental scenarios. In this work we studied the alignment of wormlike micelles in extensional flow using a cross-slot flow cell with a solution of 75mM cetylpyridinium chloride (CPyCl) / 45mM sodium salicylate (NaSal) in D <sub>2</sub> O which forms wormlike micelles at room temperature. Small angle neutron scattering (SANS) measurements were used to determine the amount of orientation of the wormlike micelles. The values of the nematic order parameter ( $S_{nl}$ ), and Maier-Saupe degree of order parameter ( $S_{ml}$ ) were compared and shown to be equal measures of alignment, but the nematic order parameter proved to be the easiest value to use. Time resolved measurements as well as steady state measurements were made in order to better understand how the orientation of these micelles evolves as a function of time for different extensional strain rates. Cross-slots of different neutron pathlengths were used in order understand the effect that aspect ratio can have on the flow type, shear or extensional occurring at the stagnation point. We were able to measure the changes in the orientation at the stagnation point as the flow transitions from symmetric, purely extensional strain to a more complex shear-extensional flow combination associated with higher flow rates and asymmetric flow.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Jessica Meisinger-MacDonald
Academic Institution:	University of New Haven
Academic Standing:	Senior
(Sept. '15):	Plan on graduating and entering the work force.
Future Plans:	Plan on graduating and entering the work force.
(School/Career):	NIST Laboratory, Engineering Laboratory, Fire Research Division, Fire Fighting Technology Group
Division, and Group:	NIST Research
Advisor:	Daniel Madrykowsky, Michelle K. Donnelly
Title of Talk:	The Effects of High Temperatures on Radio Speaker Microphones
Abstract:	<p>Firefighters and other first responders use many electronic devices to aid their responses and tactics when answering an emergency call. Portable handheld radios are essential to the communication of emergency personnel while responding to and working to mitigate an emergency. This presentation will focus on the Remote Speaker Microphones (RSMs) attached to the portable radios used by firefighters. Using a breakdown of the thermal environments commonly found in structural firefighting operations that the radios will be expected to operate in, the performance of the RSMs were tested in three thermal classes for electronic equipment defined in NIST Technical Note 1477 (Donnelly, et al. 2006). The RSMs will be tested in a flow loop that will expose them to an elevated temperature for a prescribed time period. These tests will establish if the current equipment is capable of surviving long enough to provide adequate operation in structural firefighting situations. The testing will include three different RSM models, and each model will be tested to each of the three thermal classes and repeated to verify findings. The results from these tests will aid the National Fire Protection Association (NFPA) in establishing RSM standards and provide recommendations for future standards.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Natalie McDonald
Academic Institution:	University of Maryland, Baltimore County
Academic Standing:	Senior
(Sept. '15):	I would like to pursue a career in biomedical research.
Future Plans:	I would like to pursue a career in biomedical research.
(School/Career):	NIST Laboratory, Material Measurement Laboratory (MML), Biomolecular Measurement Division, Bioprocess Measurement Group
Division, and Group:	NIST Research
Advisor:	Dr. Jeffrey Hudgens
Title of Talk:	Statistical Analyses of Data Obtained from the NIST Hydrogen/Deuterium Exchange Mass Spectrometry Inter-laboratory Comparison Project
Abstract:	<p>The pharmaceutical industry is always looking for better ways to measure properties of its researched materials during the drug development and approval process. Biosimilar industry that wants to make generic forms of biologic medical products is seeking techniques to effectively demonstrate the similarity of its products to the FDA-approved innovator. Over the last few decades, proteolytic fragmentation Hydrogen-Deuterium Exchange Mass Spectrometry (HDX-MS) has become an influential instrument for studying the dynamical structure of proteins and protein interactions. HDX-MS has been identified as a key physicochemical technique that allows us to gain a better understanding of higher order structure characterizations of proteins.</p> <p>HDX-MS is a method for determining the dynamical behavior of proteins by observing the relative exchange rates of hydrogen-for-deuterium along the protein amide backbone during deuterium labeling experiments. In proteins, hydrogen atoms that are ionically bound partially to adjacent atoms swap protons with the solvent. The exchange of hydrogen-deuterium at a specific rate due to the function of protein structure and solvent accessibility. The hydrogen bonds that are bound in beta sheets and alpha helices exchange more slowly. When immersed in D<sub>2</sub>O, the protein will gain weight through the exchange, which can be measured by mass spectrometry. Thus, their exchange rates of hydrogen-for-deuterium along the protein amide backbone are a reflection of structure and structural stability of the protein.</p> <p>In the future, HDX-MS data may be used in commerce to establish the acceptability of biotherapeutics, mainly via comparability studies between test and reference protein. Unfortunately, we do not know what the reproducibility of the measurements are. Therefore, we do not know what the reliability of the data is.</p> <p>The objective of the study is to determine the reproducibility of the HDX-MS measurements. NIST has developed a reference standard kit that can determine the precision of the HDX-MS measurements. The Test Kits have been distributed to 18 laboratories in the University, biopharmaceutical, government, and other non-profit sectors. Participating laboratories measured HDX-MS patterns for prescribed D<sub>2</sub>O immersion intervals and reported their data sets back to NIST.</p> <p>During my tenure at NIST this summer, I have been assigned to conduct the statistical analysis of data obtained from the NIST inter-laboratory comparison of HDX-MS measurements. NIST will statistically analyze the report results to determine the uncertainty component of the inter-laboratory reproducibility and evaluate the results for variance due to different realizations of the HDX-MS methodology. Also, we will be able to determine the bias that could possibly arise from chemical properties of peptide sequences, such as hydrophobicity and molecular weight. I am currently working on seven (7) data sets that have been reported by participants, which will eventually expand up to 12 data sets. The project might comprise as much as 32,000 measurements as more data sets get reported back to NIST. The present study is an ongoing project. Thus, NIST will report analyses of HDX-MS precision in scientific paper that will be published in a refereed archival science journal.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Rahul Menon	Grant Number   70NANB15H163
Academic Institution: University of Maryland – College Park	Major: Aerospace Engineering
Academic Standing   Sophomore	
(Sept. '15): Future Plans   Private Aerospace Industry or Engineering Consulting	
(School/Career): NIST Laboratory, Materials and Structures Division, Structures Group	
NIST Research Division, and Group: Engineering Laboratory, Materials and Structures Division, Structures Group	
Advisor: Dat Duthinh	
Title of Talk: Developing MATLAB Functions to Analyze Wind Pressure Coefficients on Building Envelopes	
<b>Abstract:</b>	
<p>This project developed computer tools to analyze wind velocity pressure coefficients from wind tunnel tests performed by the University of Western Ontario under the sponsorship of NIST. The work is part of an effort to update wind design standards in the US, which are currently based on 30-year to 50-year old data that have been considerably enlarged in the last couple of decades. I developed a series of Matlab functions that (1) plot 2D and 3D contour maps of the maxima and minima of pressure taps distributed unevenly on the surface of the building model; (2) select individual time series of pressure to analyze; and (3) provide an alternative to the method currently available in the NIST Database-Assisted Design to estimate the peak wind pressure with a given probability of exceedance. Peak wind pressures follow a Type I Extreme Value Distribution (EV1) and I applied the Best Unbiased Linear Estimator method (BLUE, developed at NIST) to evaluate the parameters of location and scale of EV1 that fits the measurements. I applied these Matlab functions to several low-rise building wind tunnel tests as examples.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Rohan Mittal	Grant Number   70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Materials Science and Engineering
Academic Standing   Senior	
(Sept. '15): Future Plans   Graduate school immediately after Undergraduate, or acquire work experience first.	Graduate school is definitely in the future, however, still considering whether or not to enter Graduate school immediately after Undergraduate, or acquire work experience first.
(School/Career): NIST Laboratory, Material Measurement Laboratory, Special Programs Group Division 643 in the Materials Division, and Group: Measurement laboratory	Material Measurement Laboratory, Special Programs Group Division 643 in the Materials Division, and Group: Measurement laboratory
NIST Research Advisor: Dr. Amanda L. Forster	
Title of Talk: Characterization of High-strength Fibers used in Soft Body Armor	
<b>Abstract:</b>	
<p>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 vest failed in the 30 year history of the National Institute of Justice (NIJ) Body Armor Standard. The National Institute of Standards and Technology (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.</p>	
<p>The objective of my work this summer is to extend the group's research on the artificial aging properties of high strength fibers used in body armor. One material that has been extensively studied in this research group is ultra-high molar mass polyethylene fibers. This material is prepared by starting with a polymer with a molar mass between 3 and 5 million, and then dissolving it in a solvent to form a gel. This gel is extruded to form a fiber and then highly oriented, between 50x to 100x its original length. The result is a highly crystalline (over 85 %) highly oriented fiber that can be successfully used to defeat ballistic threats. One major question that has been asked of research to use elevated temperatures to artificially age this material is the role of shrinkage and relaxation in the fiber due to its initial, highly stressed state. One of my major projects was to characterize this shrinkage at temperatures relevant to the aging protocol.</p>	
<p>A second major thrust for my research this summer was a comparison of existing two different samples of artificially aged polyaramid fiber tensile strengths with a known kinetic model for degradation of this material at two different preparation conditions and four temperatures. I compared both tensile strength and strain to failure of the material with the model at these conditions and made recommendations for how to improve procedures for performing artificial aging for the future. Finally, I explored the use of several different analytical methods, such as Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), and Scanning Electron Microscopy (SEM) to detect changes in high strength fiber materials after aging.</p>	
These results will be further discussed in my presentation.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Nusrat Molla
Academic Institution:	University of California, Berkeley
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Graduate School in Environmental Engineering and Development Engineering
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Control Group
Advisor:	Amber Pertzborn, Glen Glaeser
Title of Talk:	Turning Up the Heat: Simulating Outdoor Air Temperatures in the Intelligent Agents Laboratory
<b>Abstract:</b>	
Commercial buildings account for an increasing portion of US energy use, creating the need to improve the efficiency of the building systems, especially heating, ventilating, and air conditioning (HVAC) that make up the majority of their energy usage. Intelligent agents are combinations of hardware and software that have the potential to reduce energy consumption, maximize comfort, and cut the cost of operation of building systems using existing equipment by learning the performance of the systems they monitor, and communicating and collaborating with other agents. To provide realistic and reproducible conditions for testing prototypes, the Intelligent Agents Laboratory, consisting of a typical commercial HVAC system, was recently constructed and is in the process of having its data acquisition system tested, sensors wired, and control algorithm written. As a part of commissioning the laboratory, my project focused on controlling the outdoor air unit that conditions the incoming air to the desired inlet conditions for the HVAC system to ensure the reproducibility of the system. Since the cooling condenser being used to condition the air contains its own proprietary control algorithm, a method for communicating the zone temperature and setpoint to the microprocessor, as a thermostat does, needed to be devised. This was done using two digital potentiometers that can output variable resistances that are sent to the condenser's microprocessor where it is then interpreted into its corresponding temperature. These potentiometers are programmed using LabVIEW and a digital output module, allowing for easy and automated control of the incoming air temperature. The range and reproducibility of the inlet conditions will be tested and the resulting unit used for future tests.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Adeolu Mojibola
Academic Institution:	Morgan State University
Academic Standing (Sept. '15):	First year Graduate Student
Future Plans (School/Career):	Graduate School at the University of Maryland, College Park
NIST Laboratory, Division, and Group:	Material Measurement Laboratory
NIST Research Advisor:	Ella Mihalescu
Title of Talk:	Structural Studies of an Inactivating Peptide of Ion Channels in Phospholipid Bilayers
<b>Abstract:</b>	
In biological membranes, Voltage-gated (VG) transmembrane ion channels function to regulate electrical signaling via controlling the flow of ions ( $K^+$ , $Na^+$ ) in the membrane by opening and closing in response to membrane polarity. An important event in the functional cycle of VG channels is fast inactivation: soon after activation the channels enter into an inactivated state (open, but non-conducting). Inactivation of ion channels limits the duration of channel openings and is essential in shaping and regulating cellular excitability. This process is dependent on the membrane environment. In this regard, we examined the structural interactions of an inactivating peptide with zwitterionic and charged lipid membranes, by employing structural and spectroscopic techniques such as X-ray and Neutron diffraction, Circular Dichroism and Fourier Transform Infrared Spectroscopy. We found that the inactivating peptide interacts more strongly with charged lipid membranes compared to neutral membranes. Moreover, we propose that the inactivating peptide conforms to a $\beta$ -sheet structure when incorporated in the charged lipid bilayer, due to an interplay between hydrophobic and polar interactions. Our results may provide the foundation for understanding the mechanistic details for channel inactivation.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Zora Moore
	<b>Academic Institution:</b> Hampton University
	<b>Grant Number</b> 70NANB15H134
	<b>Major:</b> Computer Information Systems
<b>Academic Standing</b>	<b>Academic Standing</b>
Junior	Sophomore
<b>(Sept. 15):</b>	<b>(Sept. 15):</b>
Future Plans:	At the moment I have the desire to attend Law School after I obtain my undergraduate degree
(School/Career):	
NIST Laboratory, Division, and Group:	NIST Laboratory, Information Technology Laboratory, Computer Security Division, Secure Systems & Applications Group
NIST Research Advisor:	Vincent Hu
<b>Title of Talk:</b>	<b>Title of Talk:</b> Access Control Rule Logic Circuit Simulation: Immediate Fault Detecting System
<b>Abstract:</b>	<b>Abstract:</b> Access control (AC) is a very important component in computer security. Systems often utilize access control to control which users have access to which resources based on the particular system's policies. The set of rules that allow access to specific pieces of information are based on three variables: subjects, actions, objects, and the environment conditions of the protected systems. A rule assigns permission which is either a grant or denial of specific actions on the objects to authorized subjects under environment variables. Detecting faults in the rules can be complicated especially when the AC rules are intricately covering duplicated variables to a high degree of complexity. The reason for the complexity is due to the fact that some faults may not be caused by one specific rule but by multiple rules. In this project, access control policy scenarios were tests for the AC Rule Logic Circuit Simulation (ACRLCS) technique, for example, in a hospital AC policy, the manager is granted access to all the patient's files except for their private files and the doctors are only allowed access to their specific patient's files including their private files. A doctor happens to be the manager and a conflict occurs when the manager is denied access to a patient's private file but the doctor is granted access. To rectify the issue, ACRLCS enables the AC authors to detect a fault when the fault-causing AC rule is added to the policy. The error can be identified in real time before the addition of new rules clouds the detection process. There are two new features added to the ACRLC simulation. Users are able to save the project, meaning that after all the rules are entered they can save it and access it at a later date if desired, as well as an option to update and delete rules that have been previously entered. Optionally, one more feature will be added to allow the user to specify the environment condition variables in the policy.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Katelyn Montgomery
	<b>Academic Institution:</b> University of Maryland, College Park
	<b>Grant Number</b> 70NANB15H141
	<b>Major:</b> Computer Science
<b>Academic Standing</b>	<b>Academic Standing</b>
Junior	Junior
<b>(Sept. 15):</b>	<b>(Sept. 15):</b>
Future Plans:	Grad School in the field of Human Computer Interaction (HCI)
(School/Career):	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division
NIST Research Advisor:	Nicholas Dagalakis
<b>Title of Talk:</b>	<b>Title of Talk:</b> Simulation of a Robot Tool Dynamic Impact on Human Skin and Soft Tissue Bio-simulant Artifacts Based on the NIST DITCI Instrument Simulator Test Data
<b>Abstract:</b>	<b>Abstract:</b> In the past 15 years, manufacturing has moved to countries where companies can find labor at a lower cost. This shift has influenced the development of robots that can work with people to combine the intelligence and dexterity of humans with the strength, repeatability and endurance of industrial robots. The field of Human-Collaboration-Robots is relatively new and because robots are very powerful programmed machines, the safety of workers working with and around these robots must be considered and has become a top priority. The development of safety standards will provide guidance for a comprehensive risk assessment of the robot arm, its tools, its controller, and the operating workspace as a whole. For the project, bio simulant materials mimic human skin and soft tissue, specifically the abdomen. These bio simulant materials will be used for the construction of disposable Human-Collaboration-Robotics safety testing artifacts. These artifacts will be used to measure the damage of a possible robotic impact and the severities of the injuries caused by the robot including both static and impact pressure. To test and calibrate the artifacts, a Dynamic Impact Testing and Calibration Instrument (DITCI) was constructed. Data has been collected from these tests using a high speed camera and various sensors. My role in the project is to create a computer model that will replicate the damage caused by the impact of the robot tool on the bio simulant artifacts. ANSYS Finite Elements Modeling (ANSYS-FEM) software was used for the model and the simulation was based on real test data obtained from the NIST DITCI. The project maps the maximum stress and strain data inside the artifact. The computer model provides more information than the physical model can alone. Specifically we are interested to know if there is more stress and strain near the edges of the tool which could make the impact unsafe even if the average pressure is within the recommended guidelines.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Sawyer Morgan	Grant Number 70NANB15H143
Academic Institution: Purdue University	Academic Institution: Purdue University
Academic Standing 1 <sup>st</sup> year PhD student, University of Washington (Sept. '15):	Academic Standing 1 <sup>st</sup> year PhD student, University of Washington (Sept. '15):
Future Plans University of Washington; eventually industry research (School/Career):	Future Plans University of Washington; eventually industry research (School/Career):
NIST Laboratory, Materials and Structural Systems Division, Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group	NIST Laboratory, Materials and Structural Systems Division, Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group
Division, and Group: Polymeric Materials Group	Division, and Group: Polymeric Materials Group
NIST Research Advisor: Xiaohong Gu	NIST Research Advisor: Xiaohong Gu
Title of Talk: Degradation Study of PV Polymeric Materials during Accelerated Laboratory Testing	Title of Talk: Degradation Study of PV Polymeric Materials during Accelerated Laboratory Testing
<b>Abstract:</b>	
Solar photovoltaic (PV) electricity has shown rapid growth in adoption around the world, but PV modules must be able to last for over 20 years to be more cost-effective. Protection of the solar cells and electrical connections is commonly performed by encapsulants made of polymers. These polymeric materials, however, degrade under years of weathering from the effects of ultraviolet radiation, humidity, and temperature, which can result in the reduced performance of PV modules and safety concerns. This study investigates the degradation of polymeric backsheets system using commercial PPE (polyethylene terephthalate (PET)/PET/ethylene-vinyl acetate) backsheets film. Exposure of samples to three different temperatures, four levels of ultraviolet (UV) irradiance, and four UV spectral wavelengths is conducted in the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) under accelerated weathering conditions. Characterization of chemical, physical, and optical property changes are conducted with UV-visible spectroscopy, and Fourier transform infrared spectroscopy (FTIR) mechanisms of backsheets failures observed in the field.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Adriana Morales Miranda	Grant Number 70NANB15H171
Academic Institution: University of Puerto Rico, Rio Piedras Campus	Major: Mathematics
Academic Standing Senior	
(Sept. '15):	
Future Plans Grad School, Ph.D. in Mathematics	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Computer Security Division, Security Testing, Validation and Measurement Group	
Division, and Group: Validation and Measurement Group	
NIST Research Advisor: Allen Roginsky	
Title of Talk: Counting Large Prime Numbers	
<b>Abstract:</b>	
Large prime numbers are a basic element of keys for digital signature standards such as RSA, which has been standardized by NIST. However, the primes chosen for the RSA digital signature must satisfy a different set of restrictions. The problem arises when trying to generate those large primes with given (fixed) number $L$ of bits and for them to suffice the conditions so they are secure enough to withstand a cryptanalytic attack. Are there enough primes available for the purpose of the RSA? What if more conditions are added? The prime numbers are counted under various assumptions and then the results are expressed as an estimate of the number of the primes as a function of the parameters established by Federal Information Processing Standard (FIPS) 186-4. The results are analyzed to see to what extent these new requirements reduce the already small pool of available primes and if more conditions can be added.	

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4–6, 2015



Name: Matthew T. Mosley

Academic Institution: Hampton University

Grant Number: N/A

Major: Forensic Chemistry

Academic Standing (Sept. '15): Senior

Future Plans: Continue on to Graduate School at University of Maryland, Baltimore County. Pursue a Career in Forensics under the Department of Law Enforcement

(School/Career): NIST Laboratory, Material Measurement Laboratory, Chemical Sciences Division, Organic Chemical Division, and Group: Measurement Science Group

Advisor: Dr. Jeanita Pritchett, Dr. Bruce Benner, Dr. Mimi Young

Title of Talk: The Application of Gas Chromatography – Mass Spectrometry

### Abstract:

For many years, the separation and quantification of organic chemical species has become essential to a wide range of areas in which analytical chemistry is applied. One of the most efficient and robust methods for separation and identification is gas chromatography – mass spectrometry (GC-MS). This analytical technique separates the often complex sample using a narrow bore fused silica capillary column with a gas (helium or hydrogen) mobile phase. The separated organic species are subsequently ionized, identified by known fragmentation patterns of the ionized chemical species (mass spectra), and quantified based on the intensities of the resulting signals. GC-MS is commonly used in the various forensic and environmental applications. As GC-MS can function to provide many quantitative measurements, it was used to generate calibration methods for the analysis of volatile compounds, to determine of phthalates in polyvinyl chloride (PVC) materials, and to develop a method for assigning values for Tobacco-Specific Nitrosamines (TSNAs) in Candidate Standard Reference Material (SRM) 3222, Tobacco Filler. Brief descriptions of these three GC-MS applications are below.

The initial focus of this project targeted understanding the vapor profiles of energetic materials found in C4-solutions. Calibration methods were investigated for the headspace analysis of volatile compounds associated with explosive materials. Quantitation of vapors was accomplished by preparing standard solutions containing volatiles associated with C-4 explosives, including cyclohexanone and 2-ethyl-1-hexanol with their respective deuterated compounds as internal standards. This allows for the quantitation of vapors from headspace analysis and evaluate the figures of merit.

The second aspect of this work focused on the analysis of target phthalate compounds found in PVC material at concentrations of 0.1% (mass fraction), which is the upper limit of phthalate concentrations allowed in PVC-based children's toys. Sample preparation as well as extraction techniques were optimized in order to examine the plasticized material through GC-MS. During the screening of the PVC material, six phthalates were identified including dibutyl phthalate, di-(2-ethylhexyl) phthalate, benzyl butyl phthalate, diisonyl phthalates, and diisodecyl phthalate.

The final phase focused on using a targeted GC-MS method for the analysis of TSNAs found in tobacco filler material. Tobacco-Specific Nitrosamines are extremely carcinogenic and can be harmful to the health of cigarette users. GC-MS was utilized to analyze two of the main TSNAs, N'-Nitrosomonicotine (NNN), and 4-(methylnitrosoamino)-1-(3-pyridyl)-1-butanolone (NNK), found in the candidate reference material.

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 5–7, 2014



Name: Khanh Nguyen

Academic Institution: University of Maryland, College Park

Grant Number: 70NANB15H168

Major: Mathematics, Computer Science  
(Sept. '15): Senior

Future Plans: Undetermined beyond graduation  
(School/Career):

NIST Laboratory, Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainability Group.  
Division, and Group: Energy and Sustainability Group.

NIST Research Advisor: Dr. Sara Barron

Title of Talk: Materials Informatics for Combinatorial Thin Film Libraries

### Abstract:

Recently, machine learning has gained popularity in many fields thanks to its versatile uses. In materials science, machine learning proves itself a great tool to automate the analysis of large data sets. One important example is materials structure data since material structure is predictive of other material properties.

X-ray powder diffraction (XRD) is an analytical technique used to identify the phase of a crystalline material. The data to be analyzed is X-ray diffraction spectra from a combinatorial thin film library of many different chemical compositions. In this project, we focus on clustering, that is a machine learning technique that puts data objects of similar types in the same cluster. Applying it to a library of thin film samples with diverse spectra, the purpose of the project is to partition spectra with similar patterns into clusters, and then identify the composition (or location) of those samples on the wafer. The ultimate goal is to figure out the crystal structure based on finding the peaks of a few representative spectra rather than all spectra. The first algorithm is a stability algorithm which determines how many clusters should be chosen to make this partitioning stable by comparing the instability scores from different clustering methods such as k-means and spectral clustering. The second one is an ensemble algorithm which is about finding the best combination of all clustering results from various clustering algorithms. By using these machine learning algorithms, identifying material structure can be automated more robustly based on the information about the number of clusters that should be chosen and the best combination of different algorithms.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Nicolas Nikoloutsos	Grant Number   70NANB15H149
Academic Institution: Lamar University	Major: Electrical Engineering, Physics
Academic Standing   Junior	
(Sept. '15):	
Future Plans   PhD in Bioengineering	
(School/Career):	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Semiconductor and Dimensional Metrology, Nanoscale Metrology Group	
NIST Research Advisor:	Darwin Hernandez-Reyes, Kiran Bhadriraju
Title of Talk: Single Molecule Fluorescence Imaging of DNA-SWCNTs	
<b>Abstract:</b>	
<p>Single-walled carbon nanotubes (SWCNTs) have been shown to be capable of forming composites with single-stranded deoxyribonucleic acid (ssDNA) wrapped around them known as DNA-SWCNTs. The combination of these two important molecules represents a breakthrough in many fields including biotechnology and nanomedicine as DNA-SWCNTs have the potential to be used as biomedical probes, drug or gene therapy delivery systems, and for various other biological applications. However, fluorescence imaging, the most common method of microscopy in the biosciences, of DNA-SWCNTs remains a difficult task due to their size and optical properties. We investigated the combination of total internal reflection fluorescence microscopy (TIRFM) and OliGreen, an ssDNA binding fluorescent dye, to visualize DNA-SWCNTs.</p>	
Name: Yvonne Niyonzima	Grant Number   70NANB15H131
Academic Institution: East Carolina University	Major: Chemistry, Mathematics
Academic Standing   Senior	
(Sept. '15):	
Future Plans   My interest is in Chemistry and Biochemistry. My current goal is to obtain a Bachelor's degree in Chemistry BS and Mathematics BA. I plan to attend graduate school in Chemistry then medical school afterwards. My ultimate career goal is to become a medical doctor and do research.	
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group	
NIST Research Advisor:	Dr. Tom Allison, Dr. Karl Irikura and Dr. Peter Linstrom
Title of Talk: Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	
<b>Abstract:</b>	
<p>The NIST Chemistry WebBook is a popular reference database for researchers, engineers, and students. It contains theoretical and experimental information such as molecular structure, thermodynamics and spectral data on approximately 130,000 molecules. Our primary focus this summer was to optimize 3-dimensional (3D) molecular structures for compounds in the Webbook. Our secondary focus was to utilize the vibrational frequencies and intensities that were computed by developing a web application to display the infrared (IR) spectrum in a user-friendly manner.</p>	
<p>The 3D structures were optimized using an efficient multi-step process. Starting with a classical molecular mechanics (MM2) approach, we refined initial structures created from 2D structural drawings. Quantum chemistry methods implemented in the Gaussian09 software package were used to produce accurate structures using the PM6 semi-empirical and B3LYP density functional theory (DFT) methods. DFT is more computationally expensive, but has a reputation for yielding molecular structures that are in good agreement with experimental results. Before uploading to the WebBook, we checked the structures for accuracy and consistency with existing WebBook information.</p>	
<p>The web application is constructed in JavaScript using the plotting package Flot to interactively display the IR spectrum of the molecule. The spectrum plot is linked to a 3D representation of the molecule that can be visualized through the JSMol package. Users can select individual frequencies to see the corresponding normal mode molecular vibrations. We hope this functionality will be included in the next release of the WebBook.</p>	
<p>3D structures and IR spectra are important in areas such as drug discovery, experimental simulation, and communication to non-chemists. We were able to optimize more than 20,000 molecules this summer, ensuring that the WebBook remains a valuable resource for scientists and educators.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Nicolas Nikoloutsos	Grant Number   70NANB15H149
Academic Institution: Lamar University	Major: Electrical Engineering, Physics
Academic Standing   Junior	
(Sept. '15):	
Future Plans   PhD in Bioengineering	
(School/Career):	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Semiconductor and Dimensional Metrology, Nanoscale Metrology Group	
NIST Research Advisor:	Darwin Hernandez-Reyes, Kiran Bhadriraju
Title of Talk: Single Molecule Fluorescence Imaging of DNA-SWCNTs	
<b>Abstract:</b>	
<p>Single-walled carbon nanotubes (SWCNTs) have been shown to be capable of forming composites with single-stranded deoxyribonucleic acid (ssDNA) wrapped around them known as DNA-SWCNTs. The combination of these two important molecules represents a breakthrough in many fields including biotechnology and nanomedicine as DNA-SWCNTs have the potential to be used as biomedical probes, drug or gene therapy delivery systems, and for various other biological applications. However, fluorescence imaging, the most common method of microscopy in the biosciences, of DNA-SWCNTs remains a difficult task due to their size and optical properties. We investigated the combination of total internal reflection fluorescence microscopy (TIRFM) and OliGreen, an ssDNA binding fluorescent dye, to visualize DNA-SWCNTs.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Elizabeth Orrick <b>Academic Institution:</b> Hobart and William Smith Colleges <b>Academic Standing:</b> Graduated college in Spring 2015; Plan to attend graduate school in Fall 2016 <b>(Sept. '15):</b> <b>Future Plans</b> Graduate school in Fall 2016 <b>(School/Career):</b> <b>NIST Laboratory,</b> Engineering Laboratory, Materials and Structural Systems, Materials and Structural <b>Division, and Group:</b> <b>NIST Research Advisor:</b> Erica Kuligowski <b>Title of Talk:</b> Community-wide Disaster Recovery: The Choices that Divide Us
	<b>Abstract:</b> <p>The term <i>disaster</i> refers to ‘a serious disruption of the functioning of a community or a society causing widespread human, material, economic or environmental losses which exceed the ability of the affected community or society to cope using its own resources’ (National Science and Technology Council 2005). After an impact, households are faced with various decisions concerning whether they remain in their home and/or community or travel elsewhere (temporarily or permanently). The purpose of this project was to develop a comprehensive understanding of household recovery decision-making. Over 50 publications, including journal articles and research reports, were analyzed to create an annotated bibliography. The bibliography includes publications on various disaster recovery-related topics, such as disaster mobility decision making, household recovery, business recovery, non-disaster migration, international studies of disaster mobility and decision making, social capital, and governmental influence. The annotated bibliography highlighted the following for each publication reviewed: the type of disaster event described and a description of the event, the theoretical framework, the study’s methodology, and results/conclusions. The conceptual model was then developed based upon the results and conclusions of the publications. Results indicate that along socio-economic and race distinctions, people do not experience disasters equally, and as a result, the decision making process varies along class lines. Other factors such as the functionality of the community systems, including businesses, within the affected area as well as access to governmental aid and policy changes influence not only mobility but who is able to migrate or stay. This research is preliminary, and it is crucial that more research be conducted to make disaster recovery and decision-making more equitable.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Cody O'Meara <b>Academic Institution:</b> West Virginia Wesleyan College <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> <b>Future Plans</b> Obtain a Master's in Electrical Engineering with a focus on Power Systems and Renewable Energy. <b>(School/Career):</b> <b>NIST Laboratory,</b> Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, <b>Division, and Group:</b> Dimensional Metrology Group <b>NIST Research Advisor:</b> Dr. K Meghan Shilling <b>Title of Talk:</b> 3D Laser Scanner Performance Test Development
	<b>Abstract:</b> <p>The Dimensional Metrology Group (DMG) at NIST is participating in the development of a standard for the volumetric performance of large scale 3D laser scanners. It is desirable to characterize the performance of these systems by testing them in methods that are sensitive to the instrument errors. A number of other factors may influence the results of testing, including the user-selected scan density. This project involves designing experiments to examine this potential influence, followed by data collection and manipulation using the laser scanner software, and data analysis, including sphere fitting, in Matlab. These results will be shared with the working group that is developing the standard.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Zee Park	Grant Number 70NANB15H133 Major: Computer Science
Academic Institution: Georgetown University	
Academic Standing (Sept. '15): Junior	
Future Plans Undecided	
(School/Career):	
NIST Laboratory, Division, and Group: Information Technology Laboratory, Applied and Computational Mathematics Division, Computing and Communications Theory Group	
NIST Research Advisor: Brian Cloteaux	
Title of Talk: Generating Random Graphs	
<b>Abstract:</b>	
Large random graphs generated from degree sequences can be used to model networks and determine the number of graphs possible for a given sequence. While many algorithms already exist to generate random graphs, most suffer from issues including lack of speed, excessive memory usage, or no termination guarantee. We implemented a new algorithm to generate random graphs that uses majorization faster runtimes by reducing the time spent selecting a new edge to add to the random graph. We also improved an existing algorithm by Blitzstein and Diaconis by using the properties of graphical degree sequences to optimize their identification of possible new edges. Our algorithms were written in both Python and C++. All of the algorithms we explored offered significant improvements over existing implementations, reducing generation time and guaranteeing termination while using a relatively small amount of memory.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Maria J. Pascale	Grant Number 70NANB15H168 Major: Materials Science and Engineering
Academic Institution: University of Maryland at College Park	
Academic Standing (Sept. '15): Junior	
Future Plans Research in nerve regeneration or biomedical materials, Graduate School, or Industry	
(School/Career):	
NIST Laboratory, Division, and Group: NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor: Nicholas Butch	
Title of Talk: Control your Spin: Using Chemistry and Pressure to Regulate Magnetic Order	
<b>Abstract:</b>	
The knowledge and understanding of magnetic properties has allowed technology to expand from the implementation of superconductors, to magnetic levitation (Maglev) trains, to creating smaller storage devices and faster processing chips. $\text{Au}_2\text{Mn}$ has a fascinating and unusual magnetic structure. Every layer of the $\text{Au}_2\text{Mn}$ crystal is ferromagnetic, and is offset from the layers above and below it by a spin angle, creating a helical magnetic structure in the crystal. As pressure on the $\text{Au}_2\text{Mn}$ crystal is increased, the spin angles decrease slowly to about 40 degrees before ultimately collapsing, causing the crystal to transition from a paramagnetic state to a ferromagnetic state. In order to map out the full temperature and pressure dependence of the spiral, we are working to synthesize single crystalline $\text{Au}_2\text{Mn}$ , which has not previously been accomplished, so that we may analyze and understand its behavior using resistivity, susceptibility, x-ray diffraction, and neutron scattering. These studies will tell us more about the interactions between the spins in the crystal.	
We are also examining $\text{Pd}_{1-x}\text{Ni}_x$ . Nickel is naturally ferromagnetic, and it is known that doping paramagnetic palladium with small fractions of nickel can cause the alloy to become ferromagnetic. We are growing and studying $\text{Pd}_{1-x}\text{Ni}_x$ to see how low of a percentage of Ni will cause a ferromagnetic transition to occur. Our goal is to study how the onset of magnetic order by chemical tuning differs from the conventional ferromagnetic transition caused by temperature. I will present new information on the quantum phase transitions in $\text{Au}_2\text{Mn}$ and $\text{Pd}_{1-x}\text{Ni}_x$ based on our measurements and discuss the potential implications for future technological advancements.	

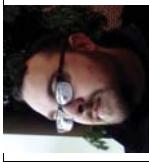
<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
Name: Madeleine D. Pasco	Grant Number   70NANB15H153
Academic Institution: Rose-Hulman Institute of Technology	Major: Biology, Biochemistry and Molecular Biology
Academic Standing   Sophomore	
(Sept. '15):	
Future Plans   Graduate school, PhD in Synthetic Biology	
(School/Career):	
NIST Laboratory, Material Measurement Laboratory,	
Division, and Group:	
NIST Research Advisor:	Samuel P. Farry and Nancy J. Lin
Title of Talk:	Reproducible, Multispecies, Microbial Biofilms
Advisor:	
Abstract:	<p>Biofilms, communities of microorganisms adherent to a surface, appear in a range of conditions, from the environment to ourselves (e.g., the human mouth). The microbes in biofilms secrete extracellular polymeric substance (EPS) that is difficult for antibiotics and other drugs to penetrate, and hard to disperse. Naturally occurring biofilm communities typically contain hundreds or thousands of different strains of bacteria interacting and competing with each other. In order to study these systems in a laboratory setting and to acquire reliable results, it is important to have validated methods for generating model multispecies biofilms.</p> <p>This summer we developed a protocol that improves the reproducibility of single- and multispecies biofilms. We first characterized several ways to quantifying the numbers of bacteria used to inoculate biofilms. We also characterized the resulting biofilms by their metabolic activity and the amount of DNA they contained. These measurements were applied to various culture conditions to identify key parameters influencing microbial growth and to define a methodology that produces reproducible multispecies biofilms with predictable behaviors.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Daniel Paseltiner	Grant Number   70NANB15H153
Academic Institution: Bates College	Major: Physics
Academic Standing   Senior	
(Sept. '15):	
Future Plans   Planning to pursue AMO Physics in graduate school.	
(School/Career):	
NIST Laboratory, Physical Measurement Laboratory, Quantum Measurement Division, Fundamental Electrical	
Division, and Group: Measurement Group	
NIST Research Advisor:	Dean Jarrett
Title of Talk:	Design, Construction and Calibration of a Temperature Monitoring System for Resistance Standards
Abstract:	<p>The ongoing Metrology of Ohm Project is responsible for maintaining resistance standards and measurement systems in order to provide resistance calibrations to US industry and government agencies, as well as continuing to develop new resistance measurement techniques with greater accuracy. The expanded uncertainties (<math>k=2</math>) associated with these calibrations range from <math>0.04 \mu\Omega/\Omega</math> to <math>100 \mu\Omega/\Omega</math> over 20 decades of resistance. When measuring resistance to these uncertainty levels, temperature variations, even on the order of <math>20 \text{ mK}</math> can have a significant impact. In light of this, while resistance standards are measured, their temperature is held stable in one of several oil or air baths. Previously no systems existed to continuously monitor the temperature of all these critical locations, and provide notification if they deviated from their allowable temperature range. This talk will describe the design, construction, and calibration of the instrumentation and software for such a system. The system supplies a constant current to thermistor temperature probes and measures the voltage across them. These voltages are then compared to the voltage, due to the same constant current, across a reference resistance standard in order to determine the resistance of the probes. To reduce systematic errors these voltage measurements are taken with the supplied current flowing in both directions. Finally, using the Steinhart-Hart model the probe resistances are converted into temperatures that are recorded locally as well as to a secure networked drive. If at any time a probe reads a temperature outside of the desired temperature range for its location, the software will send an email alert to all the staff who work in lab. An additional message will be sent to facility services if the probe is measuring the lab temperature.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: William Paulson	Grant Number   70NANB15H166
Academic Institution: Binghamton University	Major: Mechanical Engineering
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	PhD in Mechanical Engineering; Entrepreneurship in Manufacturing
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group
NIST Research Advisor:	Monter Helu
Title of Talk:	Data Requirements to Characterize Machine Utilization
Abstract:	<p>Smart manufacturing systems (SMS) combine advanced manufacturing capabilities and digital technologies to create products faster, cheaper, and greener. SMS enables manufacturers to collect data and information to support informed decision making. For example, data and information on machine utilization can support scheduling, requests for proposals, and resource budgeting. Solution providers offer machine utilization measurement and reporting tools, such as System Insights Vizmania, TechSolve ShopViz, and FORCAM Factory Framework. Greater detail in the measurement of machine utilization and contextualizing these measurements with process and operations information is crucial to allow manufacturers to understand the reasons driving machine utilization and support decision making to improve efficiency. The goal of this research is to determine the data and information needed to calculate and contextualize machine utilization. Specific machine tool states are defined and the information needed to identify these states are determined. A system model of a machine tool and its surrounding systems is also created to provide the holistic perspective needed to contextualize machine utilization. Based on this research, data and information requirements are defined so that manufacturers have an approach to monitor and characterize machine utilization on the shop floor.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
Name: Zachary Pollock	Grant Number   70NANB15H140
Academic Institution: Miami University	Major: Physics
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	Graduate from Miami, attend grad school for physics
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Dosimetry Group
NIST Research Advisor:	Dr. Ronald Tosh
Title of Talk:	Interferometry for Calorimetry of Medical Radiotherapy Beams
Abstract:	<p>Dosimetry—measuring the dose, in energy per unit mass, absorbed by irradiated matter—is key to proper treatment during radiation therapy. Within the realm of treatment planning, quality assurance procedures (in clinics and hospitals), and calibration metrology, this is typically done using a phantom, something used to represent human tissue; dose absorbed by the phantom is measured with a variety of instruments. The national primary standard for radiation dose at NIST is based on water calorimetry; thus, a calorimeter vessel is submerged in a water phantom, and dose is obtained by measuring temperature changes induced in the water by absorption of ionizing radiation. Water is a simple, readily available material for a phantom that is a good stand-in for tissue in terms of radiation absorption. It is also transparent at optical wavelengths, thus it is conceivable that a sensitive optical probing technique, such as interferometry, might also be made to work as a remote sensor for dosimetric applications by measuring small, temperature-induced variations of the index of refraction. Interferometry compares two beams of light that travel over different paths, one of which passed through the irradiated phantom, later combining to form an interference pattern whose characteristics vary with the changes in the index of refraction of the phantom. The objective of this work is to design an interferometer with sufficient resolution that changes in the index of refraction that correspond to microkelvin changes in temperature can be resolved. We set out to develop a system using standard optics that would achieve this resolution. This process involved comparing different types of interferometers in terms of stability and practicality, investigating causes of instabilities, and developing programs to correct for these while executing data analysis.</p>



<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Daniel J. Rabiega
	<b>Academic Institution:</b> Millersville University
	<b>Academic Standing:</b> Graduate with Bachelor's Degree
	<b>(Sept. '15):</b> Applying to Graduate Schools in the Fall
	<b>Future Plans:</b> Future Plans / career in research
	<b>(School/Career):</b> NIST Laboratory, Information Technology Lab, Applied and Computational Mathematics Division, Mathematical Analysis and Modeling Group
	<b>NIST Research:</b> Michael Mascagni
	<b>Advisor:</b>
	<b>Title of Talk:</b> Walk-On-GPU: Implementing Monte-Carlo Algorithms on GPU
	<b>Abstract:</b>
	The insatiable consumer demand for more powerful graphics cards has provided the scientific community with a class of computing hardware with highly cost efficient computational throughput. Only certain classes of algorithms with high levels of inherent parallelism are able to take advantage of this capacity, however. Monte Carlo solving techniques are especially friendly to this paradigm of computation. We created a Graphics Processing Unit (GPU) implementation of the Walk-on-Spheres technique for determining the capacitance of a molecule. Because optimization concerns in GPU algorithms are much more complex than those of traditional, Central Processing Unit (CPU) based implementations, the effectiveness of various optimization methods is described and compared.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> Ben Price
	<b>Academic Institution:</b> University of Maryland, Baltimore County
	<b>Academic Standing:</b> Major: Physics/Philosophy
	<b>(Sept. '15):</b> Junior
	<b>Future Plans:</b> Graduate School for Physics / career in research
	<b>(School/Career):</b> NIST Laboratory, Physical Measurements Laboratory, Sensor Science Division, Infrared Technology Group
	<b>NIST Research:</b> David Allen, Joe Rice
	<b>Advisor:</b>
	<b>Title of Talk:</b> Evaluating sensors with the Hyperspectral Image Projector
	<b>Abstract:</b>
	Hyperspectral imagers produce images in which each pixel provides dozens, or even hundreds, of adjacent spectral bands. The small size of these bands allows a continuous spectrum to be created for each pixel; this provides more information than the human eye perceives and can be used to identify and characterize materials without physical contact. Hyperspectral imagers have many potential uses, including medical imaging, law enforcement, and environmental monitoring. In each of these applications there is a burning question: How well can it be measured. NIST is currently developing a Hyperspectral Image Projector (HIP) which can project hyperspectral images that can be used to evaluate the performance of hyperspectral imagers. As input data for the HIP, first collected a variety of spectral signatures from the NIST campus. Then I used the HIP to re-produce these spectral signatures in the lab, with the goal of determining how well the HIP can match these spectra. These spectral signatures provide real world measurements that are valuable in evaluating some key performance parameters of the system, including noise, stability, and repeatability. Characterizing and potentially refining the HIP performance will in turn facilitate better characterized hyperspectral imagers intended to address societal needs.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Enan Rahman	Grant Number   70NANB15H187
Academic Institution: University of New York	Major: Computer Science
Academic Standing   Senior	
(Sept. '15):	
Future Plans   I am aiming to get a job as a Software Engineer. Then in a year or two I'm considering going to graduate school.	
(School/Career):	
NIST Laboratory, Division, and Group: Engineering Laboratory, System Integration Division, Life Cycle Engineering	
NIST Research	Guodong Shao, Yan Lu
Advisor:	
Title of Talk:	A Case Study of Implementing ISO 15746 Standard for Chemical Process Optimization

**Abstract:**  
 Integrating heterogeneous advanced process control and optimization (APC-O) functions for manufacturing system is very important. Due to the diversity of development environments and the variety of demand focus, the analytical and control solutions from various suppliers are isolated and relatively independent. Each tool is designed for a different task such as control, simulation, and optimization. Modeling with each tool typically requires specialized data representation, as a result, instead of being modeled uniformly only once, the same manufacturing process and system knowledge is often modeled multiple times using different specialized abstractions. In this project, ISO 15746 (Integration of advanced process control and optimization capabilities for manufacturing systems) is studied, Extensible Markup Language (XML) schema for the APC-O information models and XML instances for a chemical process case study have been developed. The created XML files can be used as input for difference analysis and control tools. Initial effort has also been performed on integrating the standard XML with optimization programming language metamodel for deriving optimal solution for the case study.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2015	
	
Name: Swaksha Rachuri	Grant Number   70NANB15H188
Academic Institution: University of Maryland	Major: Biochemistry
Academic Standing   Junior	
(Sept. '15):	
Future Plans   Medical School/Graduate School (Biochemistry)	
(School/Career):	
NIST Laboratory, Division, and Group: Molecular Measurement Division, Biomolecular Structure and Function Group	
NIST Research	Prasad Reddy
Advisor:	
Title of Talk:	Characterization of an Eukaryotic Factor that activates a Secreted Adenylyl Cyclase Exoy from <i>Pseudomonas aeruginosa</i>
<b>Abstract:</b>	
<p>Adenylyl Cyclase (AC) is an enzyme with key roles in cellular regulation. All classes of AC catalyze the conversion of adenosine triphosphate (ATP) to cyclic AMP (cAMP). cAMP is utilized in many organisms for intercellular signal transduction which is a critical process controlling cellular response and function. Four major classes of AC exist in nature: class I, II, III and IV. The human pathogen <i>Pseudomonas aeruginosa</i> (Pa) is an opportunistic, nosocomial pathogen that infects those with weakened immune function. Genome sequence analysis of <i>P. aeruginosa</i> revealed three genes within the genome that code for the expression of AC Class I, II and III. One of these genes, codes for a Class II AC that is secreted into eukaryotic cells, called Exoy. Exoy is activated two to three orders of magnitude by an unknown eukaryotic factor to produce very high level of cAMP in eukaryotic cells. Our aim is to localize and identify the Exoy activation factor and study its properties. We performed activity measurements to understand how the Exoy protein is regulated, eventually aiming to localize the activation factor in eukaryotic cells. Analysis of Exoy activation by subcellular protein fractions suggests that the activator is a peripheral membrane protein. Efforts are currently underway to identify the Exoy activation factor and to purify the protein using different chromatography techniques such as ion exchange (specifically anion) chromatography, gel filtration (size exclusion) chromatography, or by any other protein purification technique deemed necessary.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Zachary Ratliff	Grant Number: 70NANB15H036
Academic Institution: McLennan Community College	Major: Computer Science
Academic Standing: Junior	
(Sept. '15): Tarleton State University, Junior	
Future Plans: Graduate school at Texas A&M or Baylor University. I want to pursue a career in cybersecurity or software engineering.	
(School/Career): NIST Laboratory, Information Technology Laboratory, Computer Security Division, Security Components and Mechanisms Group	
NIST Research: Rick Kuhn	
Advisor: Rick Kuhn	
Title of Talk: The Relationship Between Software Bug Type and Number of Factors Involved in Failures	
<b>Abstract:</b>	
In this talk we consider the relationship between different types of software bugs and the average t-way interaction involved in triggering them. Previous studies have defined different types of software bugs based on their complexity and reproducibility. Simple bugs, which involve only direct factors and are often easy to reproduce, are considered Bohrbugs. Complex bugs, which always involve at least one indirect factor and are generally much more difficult to reproduce, are known as Mandelbugs. Locating Mandelbugs in software is often difficult and expensive during the development phase due to their complexity. Other previous research has investigated the number of factors involved in software failures, showing that most failures are induced by single factor faults or by the joint combinatorial effect (interaction) of two factors, with progressively fewer failures induced by interactions between three or more factors. This SURF project brings together these two lines of research.	
	After analyzing hundreds of bugs reported from the open source database software MySQL, we have determined how understanding the complexity of Mandelbugs can naturally make combinatorial testing much more effective in locating them. Analysis of the MySQL bugs show that Mandelbugs have a significantly higher interaction strength when triggering their faults. This suggests that there is a good chance that direct factors, alongside the indirect factor(s), will many times play a role in triggering the fault. By using combinatorial testing methods, we can have high assurance of locating Mandelbugs as long as the indirect factors are present at the time of testing.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Brett Rastatter	Grant Number: 70NANB15H175
Academic Institution: Virginia Tech	Major: Chemical Engineering
Academic Standing: Senior	
(Sept. '15): Graduate school in chemical engineering / process engineering	
Future Plans: Material Measurement Laboratory, Biomolecular Measurement Division, Bioanalytical	
(School/Career): NIST Laboratory, Material Measurement Laboratory, Biomolecular Measurement Division, Bioanalytical	
Division, and Group: Science Group	
NIST Research: Dr. John Schiel	
Advisor: Dr. John Schiel	
Title of Talk: Optimizing HPLC-Based Biopharmaceutical Analysis using Design of Experiments	
<b>Abstract:</b>	
The current trend in the pharmaceutical industry is toward the use of biopharmaceuticals, particularly monoclonal antibodies, for the development of new therapeutics. Biopharmaceuticals offer a few key benefits over traditional small molecule drugs such as increased specificity and the potential to target otherwise unmet indications. However, because they are derived from biological sources, their production and subsequent quality control are increasingly complex. A common problem in the manufacturing of biopharmaceuticals is the unintended production of aggregates. Aggregates are large agglomerations of proteins that may negatively affect the immunogenicity of the desired product. They may be formed as a result of both upstream and downstream processes. To ensure detection and removal of aggregates from the final product, careful process and quality control measures are implemented. One commonly used method for detecting aggregates is size exclusion chromatography. The method separates samples based on their relative sizes, with larger species (aggregates) being eluted first and smaller species (monomer) being eluted later. Ultra-violet lamps are employed to detect variations in absorbance of the eluent in order to determine the presence of a species. Factors such as the buffer concentration, pH, salt concentration, eluent flow rate, column temperature, and injection volume can potentially impact the resolution of the peaks and subsequent detection of aggregates in the sample. A fractional factorial design of experiments was developed in order to determine the critical factors as well as the optimum values for producing the best peak resolution. A $2^{5-1}$ fractional factorial design was chosen as it did not result in confounding main effects with either 2-factor, 3-factor, or 4-factor interactions. The sample used for testing was the NISTmAb IgG1k, which is intended to be used as a standard reference material for the biopharmaceutical industry. The resultant optimized method resulted in an information rich platform for monitoring monomeric purity and stability of the NISTmAb.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Jeffrey Register
Academic Institution:	Princeton University
Academic Standing:	Sophomore
(Sept. '15):	
Future Plans (School/Career):	Graduate school
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Functional Polymers Group
NIST Research Advisor:	Jacob Tarver
Title of Talk:	X-ray and Neutron Reflectivity Studies of Nanoimprinted Polystyrene Bilayers
Abstract:	<p>Nanoimprint lithography (NIL) is a low-cost, high-throughput technique for nanofabrication that involves imprinting a polymer layer with a mold at high temperature and pressure. This imprinting process can cause defects in the imprinted polymer. Low molecular weight polymers flow well into the imprint mold, but develop fractures due to high stress at the corners of the imprint. On the other hand, high molecular weight polymers do not develop such fractures, but also do not flow as well into the imprint mold. One possible solution to these defects is to imprint a bilayer of different molecular weight polymers, with the lower molecular weight polymer on the top, rather than a single layer of one molecular weight polymer.</p> <p>X-ray and neutron reflectivity provide a high-resolution and nondestructive method for characterization of the imprinted polymer. X-ray reflectivity can determine the overall shape and thickness of the imprinted polymer. If one layer is deuterated, there will be contrast between the deuterated and hydrogenated layers in neutron reflectivity, and the composition of the imprinted polymer can be determined from this.</p> <p>In this research, bilayers of different molecular weight polystyrene were examined before and after imprinting using X-ray and neutron reflectivity. From this we were able to extract the thickness, cross-sectional shape, and the composition of the imprinted polystyrene.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
Name:	Carroll Reed III
Academic Institution:	Bowie State University
Academic Standing:	Junior
(Sept. '15):	
Future Plans (School/Career):	I plan to go on to graduate school after earning my bachelor's degree. I plan to stay in school until I obtain my doctorate and work in industry or with the government while I am in school.
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Electron Physics Group
NIST Research Advisor:	Dylan L. Klomparens
Title of Talk:	Development of Cross Platform Apache Web Server Authentication Modules using the Kerberos Network Authentication Protocol
Abstract:	<p>In recent years there has been a major surge in the number of cyberattacks perpetrated against many governments, business, and personal computer networks. These attacks can result in the theft of sensitive data and incur significant cost due to fraud or network downtime. Our project intends to improve network security by developing a network authentication module utilizing Kerberos, "a computer network authentication protocol which works on the basis of tickets" to allow [computers] communicating over a non-secure network to prove their identity to one another in a secure manner".<sup>1</sup> Work is ongoing to examine the existing apache security module "mod_auth_kerb" as a reference and then write a new module with improved testability, documentation, and adhering to the philosophy of the kerberos network authentication protocol.</p> <p>[1] <a href="http://en.wikipedia.org/w/index.php?title=Kerberos&amp;oldid=5800000">http://en.wikipedia.org/w/index.php?title=Kerberos&amp;oldid=5800000</a></p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Grant Reynolds	Grant Number 70NANB15H095 Major: Electrical Engineering
Academic Institution: Bucknell University	
Academic Standing Senior	
(Sept. '15):	
Future Plans (School/Career):	I plan to have a career somewhere within the power electronics industry.
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, CMOS and Novel Devices Group
NIST Research Advisor:	Jason Ryan
Title of Talk:	Building Test Structures for the Massively Parallelized Reliability Test System
Abstract:	<p>Accurate prediction of semiconductor device reliability relies heavily on the statistical analysis of device-level accelerated testing. However, traditional semiconductor device reliability testing is expensive and time consuming and obtaining enough data to ensure a statistically accurate lifetime projection is simply unfeasible. The massively parallel reliability system (MPRS) described herein is a measurement platform that can perform long term reliability tests on thousands of devices, simultaneously. The MPRS thereby provides a solution to the inefficiencies of the traditional testing methodologies and permits cost effective and accurate reliability predictions.</p> <p>The MPRS apparatus accomplishes this by integrating thirty, 100 probe pin mini probe stations, all running independently in parallel and each with individual control. Each of these mini-probe stations are controlled by a printed circuit board (PCB) designed to perform different modes of electrical stresses on a semiconductor device, while also measuring device lifetime performance. The PCB's have an on board microcontroller that communicates with several on board devices that implement the actual voltage conditioning. Each DUT (device under test) constantly has a stress voltage, but only one device is measured at a time.</p> <p>Currently each PCB is connected to a computer with one USB cable in order to communicate with a main LabVIEW program that allows the user to specify certain variable testing conditions and connection to the board. The current research has been to develop different PCB cards that are either improved or can run other modes of reliability tests. The current research involves programming the PIC firmware so that it can talk to each on board device while getting its commands from a large LabVIEW program. Many test structures must be made in order for LabVIEW to send and receive information to and from the PIC firmware through a DLL (dynamic link library) and USB communication.</p> <p>The end goal is to provide a universal standard reliability platform that can test for all the degradation modes in semiconductor devices.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	
Name: Corey Rhodes	Grant Number 70NANB15H179 Major: Applied Physics
Academic Institution: West Virginia Wesleyan College	
Academic Standing Senior	
(Sept. '15):	
Future Plans (School/Career):	Planning to pursue a graduate degree in electrical engineering
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, CMOS and Novel Devices Group
NIST Research Advisor:	Joseph Kopanski
Title of Talk:	Testing and Characterizing a Charge-Based Capacitance Measurement Circuit for interfacing with an Atomic Force Microscope
Abstract:	<p>Measuring the properties of devices, such as capacitance, becomes increasingly difficult as the scale of the devices shrink. Knowledge of such properties is critical to ensuring that computer simulations of these devices match closely with real-world operation. In the case of capacitance, traditional measurement techniques become ineffective for nanoscale devices due to the parasitic capacitance of the cables overcoming the capacitance to be measured. In order to measure the femto-farad intrinsic capacitance of these nanoscale devices, the charge-based capacitance measurement (CBCM) method is employed. This technique produces a reference signal and a signal from the device being tested that varies slightly from the reference. The differential between these signals can be extracted with the use of a differential amplifier, allowing for the capacitance of the device in question to be determined.</p> <p>Testing of the current differential amplifier design revealed that this implementation lacked the necessary precision and had an insufficient frequency response to be used for this application. To attempt to correct the problem, the differential amplifier that was implemented by a single operational amplifier, will be substituted for a design that incorporates three operational amplifiers. This configuration separates the gain and common-mode rejection into two distinct stages, which should improve the precision and frequency response problems seen in the previous implementation. In addition, the CBCM portion of the circuit will be fully tested and verified to be functioning correctly. Once the CBCM circuit is confirmed to be operating normally, the final goal is to implement the CBCM in a custom integrated circuit package, so that it can be mounted on a printed circuit board and combined with the differential amplifier to interface with an atomic force microscope for nanoscale device capacitance measurement.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> James Rogers
	<b>Academic Institution:</b> Towson University
	<b>Grant Number</b> 70NANB14H
	<b>Major:</b> Molecular Biology, Biochemistry, and Bioinformatics (MBBB) major specializing in Biochemistry, double major Chemistry
<b>Academic Standing</b> <b>(Sept. '15):</b>	5 <sup>th</sup> year senior (graduating in December 2015)
<b>Future Plans</b>	Laboratory research in biochemical studies
<b>Scholar/Career:</b> <b>NIST Laboratory, Division, and Group:</b>	Associate Director of Laboratory Programs (ADLP), 601, Standards Coordination Office
<b>NIST Research</b>	Clare Allocca
<b>Advisor:</b>	
<b>Title of Talk:</b>	Development of Standards within ISO/TC 276-Biotechnology
<b>Abstract:</b>	<p>In modern cryptography, effective encryption schemes are specified by mathematical algorithms, which can be proven to have desired properties. However, in order to use these algorithms they must be implemented in a machine-readable language; these implementations must then have their equivalence verified to be fully trusted. In the past such verification has been done via statistical sampling, a technique that is useful but still insufficient for implementations with rarely triggered cases.</p> <p>In order to address this deficiency one may use symbolic evaluation, running circuit representations of the programs using symbols that verify all possible inputs instead of just sample values. This method is particularly well-suited to languages like Cryptol, a domain-specific cryptographic language that strongly adheres to the functional paradigm.</p> <p>While functional languages are simpler to formally verify, the process can be extended to traditionally state-dependent languages using tools such as the Software Assurance Workbench (SAW). SAW has the ability to run scripts which use automated theorem provers to symbolically verify Cryptol code, Java Bytecode, and the LLVM bitcode that can be generated from a C file.</p> <p>In order to investigate the potential limitations of SAW in this use, a test suite was written in C consisting of modifications to a simple function that represented a range of common inputs, mid-routine statements, and outputs. This suite was then evaluated using the LLVM conversion, for completion and correctness of evaluation.</p> <p>To further examine the efficiency of SAW when given longer functions, multiple differing C implementations of lightweight cryptographic algorithms such as SIMON and SPECK were analyzed for equivalence to reference implementations written in Cryptol. Various modifications were made in the implementations, inspired by techniques used in code obfuscation, to determine the ability of SAW to correctly evaluate obfuscated code and the relative resource cost incurred by analyzing obfuscated code.</p>
<b>Title of Talk:</b>	Practical Proof Potential: Examining the Algorithm Verification Ability of the Software Assurance Workbench
<b>Abstract:</b>	<p>In modern cryptography, effective encryption schemes are specified by mathematical algorithms, which can be proven to have desired properties. However, in order to use these algorithms they must be implemented in a machine-readable language; these implementations must then have their equivalence verified to be fully trusted. In the past such verification has been done via statistical sampling, a technique that is useful but still insufficient for implementations with rarely triggered cases.</p> <p>In order to address this deficiency one may use symbolic evaluation, running circuit representations of the programs using symbols that verify all possible inputs instead of just sample values. This method is particularly well-suited to languages like Cryptol, a domain-specific cryptographic language that strongly adheres to the functional paradigm.</p> <p>While functional languages are simpler to formally verify, the process can be extended to traditionally state-dependent languages using tools such as the Software Assurance Workbench (SAW). SAW has the ability to run scripts which use automated theorem provers to symbolically verify Cryptol code, Java Bytecode, and the LLVM bitcode that can be generated from a C file.</p> <p>In order to investigate the potential limitations of SAW in this use, a test suite was written in C consisting of modifications to a simple function that represented a range of common inputs, mid-routine statements, and outputs. This suite was then evaluated using the LLVM conversion, for completion and correctness of evaluation.</p> <p>To further examine the efficiency of SAW when given longer functions, multiple differing C implementations of lightweight cryptographic algorithms such as SIMON and SPECK were analyzed for equivalence to reference implementations written in Cryptol. Various modifications were made in the implementations, inspired by techniques used in code obfuscation, to determine the ability of SAW to correctly evaluate obfuscated code and the relative resource cost incurred by analyzing obfuscated code.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
	<b>Name:</b> James Robertson
	<b>Academic Institution:</b> Towson University
	<b>Grant Number</b> 70NANB14H
	<b>Major:</b> Molecular Biology, Biochemistry, and Bioinformatics (MBBB) major specializing in Biochemistry, double major Chemistry
<b>Academic Standing</b> <b>(Sept. '15):</b>	5 <sup>th</sup> year senior (graduating in December 2015)
<b>Future Plans</b>	Laboratory research in biochemical studies
<b>Scholar/Career:</b> <b>NIST Laboratory, Division, and Group:</b>	Associate Director of Laboratory Programs (ADLP), 601, Standards Coordination Office
<b>NIST Research</b>	Clare Allocca
<b>Advisor:</b>	
<b>Title of Talk:</b>	Development of Standards within ISO/TC 276-Biotechnology
<b>Abstract:</b>	<p>Standards play a foundational role in the translation of innovative research into competitive products—a strong U.S. presence in standards development can position U.S. industry for increased success in the global marketplace. The Biotechnology sector is poised to benefit from standards development to enable more reliable, higher quality, better understood, and globally competitive products. To address this need, ISO has formed a technical committee (TC276) for the identification of standardization gaps and development of new standards. My contributions to efforts in the Standards Coordination Office (SCO) and Material Measurement Laboratory (MML) provide:</p> <ul style="list-style-type: none"> <li>• Valuable analysis that strengthens TC276's ability to identify and address key terminology issues</li> <li>• Significant data to support validation of cell counting methods that are the subject of the first standards to be produced by this committee.</li> </ul> <p>My SCO work is assisting the TC276 working group on Terminology by redesigning and developing a biotechnology terminology compendium based on collected information, and supplementing it to address specific terms that will be active in TC276-developed standards. This compendium, including terms and definitions from existing standards, roadmaps, and other key documents, ensures that current knowledge is considered and not duplicated while determining definitions to be employed by TC276 in its work.</p>
<b>Title of Talk:</b>	My MML work supports the development of standards for cell counting. Through experimental design and statistical analysis, investigated the contribution of sample preparation methods to the variability observed in cell count measurements. These studies, conducted using a Coulter Counter, were benchmarked on polymeric beads, and will be tested on prepared NIH 3T3 fibroblast cells. Additionally, I investigated the variability in cell counts by monitoring cell growth profiles of NIH 3T3 cultures grown according to data obtained by the hemocytometer and Coulter Counter. My contributions included: maintaining cell cultures, designing and conducting bead and cell counting experiments, and analyzing count data.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Alicia Ross	Grant Number 70NANB15H085
Academic Institution: California Polytechnic State University, San Luis Obispo	Major: Chemistry
Academic Standing (Sept. '15): Senior	
Future Plans PhD in Chemistry	
(School/Career):	
NIST Laboratory, Materials Measurement Lab, Materials Science and Engineering Division, Polymers and	
Division, and Group: Complex Fluids	
NIST Research Advisor: Kathryn Beers	
Title of Talk: Quantifying the Amount of Diffusion Between 3D Printed Layers	
<b>Abstract:</b>	
	Electronic cigarettes (ECs) consist of a heating element, cartridge and battery. Power generated by the battery is delivered to the heating element where a solution (e-liquid) in the cartridge becomes aerosolized. Generally, e-liquid contains various ratios of propylene glycol, nicotine and other flavoring agents. So far, misleading, inconsistent and contradicting EC research results have polarized researchers, policy makers and the general public, leaving them with little scientific fact to evaluate the potential health risks. Current gaps that are critical for understanding biological and chemical effects of EC aerosol exist in part due to lack of e-liquid RM (Reference Material), a highly reproducible EC device, a practical metrology to evaluate aerosol, and a physiologically relevant biological <i>in-vitro</i> model.
	To address this issue, we developed high-quality molecular grade e-liquid. Next we built a standard testing EC device that generates aerosol in a consistent manner and uses accurate smoking topology. Using our standardized testing parameters, we characterized chemical and physical properties of the e-liquid. We found that 50mL aerosol volume generated by 2 sec puff / 30 sec interpuff intervals was physiological sound and follows established EC smoking topography. We treated oral epithelial cells with our standard EC aerosol and found that EC aerosol induces DNA double-strand breaks (DSBs) which was measured by H2AX Immunofluorescence microscopy. Additionally, we used spectrometry to measure cell viability and metabolic activity (toxicology and cell proliferation assays). Our preliminary data indicate that EC aerosol increases DNA Double-Strand Breaks (DSBs) and apoptosis; and decreases metabolic activity in oral epithelial cells.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Nicole Sabatelli	Grant Number 70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Bioengineering
Academic Standing Junior	
(Sept. '15):	
Future Plans Finish Bachelor's Degree and pursue Graduate School	
(School/Career):	
NIST Laboratory, Material Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials	
Division, and Group: Group	
NIST Research Jeffrey Kim	
Advisor:	
Title of Talk: Developing Standards to Assess Biological Effects of Electronic-Cigarettes	
<b>Abstract:</b>	
	3D printing has become a common practice in industry, research and development, and even in some private homes. Because 3D printing is relatively new, there are still many aspects of a printed objects that are being studied and characterized. An extrusion deposition printer, one which heats up a selected plastic and extrudes it in thin lines to build the desired 3D object, will be the focus of this paper. It is known that the interface between these thin extruded lines are a weak point in printed objects - reducing the strength of printed parts. We developed a labeled molecule, whose chemistry is matched to the printed line, but has a fluorescent dye (or fluorophore) attached to it, to see if we could observe molecules moving across the interface into the hot printed line. Fluorophores are molecules which fluoresce when they are exposed to a certain wavelength of light. They can be detected using a fluorescence confocal microscope. A model polymer, polycaprolactone (pCL), with coumarin dye attached to it was used to develop a proof-of-concept experiment. This fluorophore-pCL sample was deposited onto a clear surface, and a line of pCL was extrusion deposited from a 3D printer onto it. When this printed sample was observed using a confocal microscope, it was possible to see the diffusion pattern from the labeled layer into the printed pCL layer. The purpose behind this research is to demonstrate that it is possible to quantify the amount of diffusion between printed layers of polycaprolactone. This can be used to compare the amount of diffusion between different speeds, temperatures, and other print variables.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name:	Sa/AdiVishnu Sanigepalli
Academic Institution:	CUNY: City College of New York
Academic Standing	Grant Number
(Sept. '15):	70NANB15H187
Future Plans	Major: Mechanical Engineering
(School/Career):	Sophomore
NIST Laboratory,	
Division, and Group:	Engineering Laboratory, Systems Integration Division,
NIST Research	Information Modeling and Testing Group
Advisor:	Donald Libes
Title of Talk:	Real-Time Data Analytics for Smart Manufacturing Systems Project
Abstract:	<p>Data analytics is becoming increasingly attractive for manufacturers. This is motivated by several factors. First, increasing amounts of data (often referred to as "big data") from models, sensors, etc., enables new approaches (algorithmic, visualization, etc.) that produce novel conclusions. This in turn creates a second factor -- an increasingly competitive environment. Manufacturers who do not use data analytics will not be competitive with manufacturers that do. While this competition drives prices down, increasing costs for resources and additional regulation provides an additional factor for finding savings wherever possible. Thus, data analytics can be expected to play a critical role in smart manufacturing in the future.</p>
	<p>For this project, we created a virtual factory model that generates virtual data as close to real-life data as possible. Using AnyLogic software, a simulation modeling system, we made a model of a factory cell to generate and visualize the data that can be used in a neural network, a machine learning algorithm, to optimize time, power consumption, etc. The virtual model will not only serve for this specific project but also can help other researchers analyze and test their own data analytics algorithms on manufacturing data.</p>

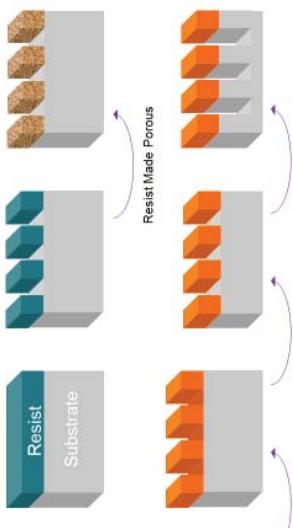
<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5–7, 2014	
Name:	Tyler Alyssa Saunders
Academic Institution:	University of the District of Columbia
Academic Standing	Grant Number
(Sept. '15):	70NANB14H
Future Plans	Major: Mechanical Engineering
(School/Career):	Sophomore
NIST Laboratory,	
Division, and Group:	Innovation and Industry Services/Technology Partnerships Office (40/401.00)
NIST Research	Undecided
Advisor:	Jack Pevenstein
Title of Talk:	An Analysis of Economic Ecosystems and the Circumstances Leading to Their Evolution
Abstract:	<p>Economic ecosystems drive innovation. It is access to materials and external expertise that speed up technological growth by acting as an incubator for these sorts of environments. Ecosystems develop due to a composition of factors including: the economic atmosphere of the area, whether something monumental has happened in the nation that sparked inspiration in its citizens; the local resources, a local source of a desirable mineral or substance can greatly influence whether an industry develops and stays in a particular area; infrastructure, accessibility by railroad or cargo ship; any significant change in the industry itself such as the streamlining of a manufacturing process making it easier and cheaper to supply goods. Discussed here are some of the world's biggest ecosystems and the factors that contributed to their evolution.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4–6, 2015
Name: Austin Scherbarth	Grant Number   70NANB15H143 Major: Materials Science Engineering
Academic Institution: Purdue University Academic Standing: Graduate School, Virginia Tech	
Academic Standing (Sept. '15): (School/Career):	
Future Plans NIST Laboratory, Division, and Group:	Graduate School or at a National Lab NIST Center for Neutron Research, Neutron Condensed Matter Science Group
NIST Research Advisor:	Jeffrey J. Richards
Title of Talk: Applications	Synthesis and Characterization of Conducting Composite Nanoparticles for Flow Battery Applications
Abstract:	The increasing demand for renewable energy has created a need for improved energy storage technologies that are able to cope with the unpredictable energy generation associated with renewables. The flow battery is one promising solution that can address the need for scalable and inexpensive grid-scale storage. A typical flow battery consists of a flow-cell through which two electrochemically active substances are pumped, separated by an ion-permeable membrane. In this way, the battery's capacity is limited only by the size of external storage tanks, not its packaging. Semi-Solid flow batteries (SSFBs), a sub-class of flow batteries, are of particular interest because of their high energy density and well established electrochemistry. In order to achieve these high energy densities, SSFBs replace the traditional soluble electrolytes with electroactive metal oxide particles. Carbon black (CB) is then added as a filler to maintain electrical percolation and high conductivity. Unfortunately, along with this electrical percolation comes mechanical percolation, which leads to an increased viscosity and undesirable flow properties. In order to avoid these high viscosities, we look to replace CB by synthesizing composite nanoparticles consisting of metal oxide particles with a poly(3,4-ethylenedioxythiophene)-polystyrene sulfonate (PEDOT:PSS) surface layer. We hypothesize that this polymer surface layer will allow for electrical and ionic conductivity without the undesirable rheological properties associated with CB. In this work, we use a variety of characterization tools, including dynamic light scattering (DLS), transmission electron microscopy (TEM), electrophoresis and small angle neutron scattering (SANS) to better understand the relationship between the structural properties of the PEDOT:PSS layer and the electrical properties of the entire particle network.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4–6, 2015
Name: Charles Scott	Grant Number   70NANB15H144 Major: Physics
Academic Institution: Rowan University Academic Standing: Senior	
Academic Standing (Sept. '15): (School)/Car for a masters degree in the process	
• Future Plans Graduate school and/or a job in the aeronautics/aerospace industry and potentially going elsewhere;	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development and Thermodynamics and Kinetics Groups
NIST Research Advisor:	Carelyn Campbell, Yannick Congo, and Laura Espinal
Title of Talk:	Data curation software for reproducible results in the FACT Lab
Abstract:	The goals of the MGI to reduce the time and cost of the deployment of new materials by 50% have increased the need to share experimental and computational data. Concurrent with the increased need to share data, the materials science community has increased the emphasis on the data reproducibility as well. To enable the ability to share data and provide reproducible data, a variety of data curation tools are being developed. One of these curation tools is the NIST Information Technology Laboratory, Materials Data Curation System. This data curation tool is a Python/MongoDB/Django Web-based system that provides a means for capturing, sharing, and transforming data. This is being used to develop a data curation protocol for high pressure CO <sub>2</sub> adsorption isotherms measured at 20 °C on the NIST reference material RM-8852 (zeolite ZSM-5) using state-of-the-art instruments in the Facility for Adsorbent Characterization and Testing (FACT Lab), a laboratory commissioned to establish testing procedures and provide reliable material property data. We aim to build a validation workflow to address the effectiveness of the testing procedures and the reliability of the material property data. The data is converted directly from Excel into a JSON and XML format using a python script. The XML formatted data can then be entered into the curator using the application programming interface (API). Once the data are entered into the MDCS, the data can be searched and shared with other users. The result of this workflow will help refine standards of how the experimental results are gathered and curated to the MDCS, while also improving how other scientists should use these results in the best way to improve reproducibility across further computations.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Jamshaid Shahir	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Mathematics/Applied Statistics
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Graduate School in Applied Mathematics	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Systems and Software Division, Information Systems	
Division, and Group: Group	
NIST Research Joe Chalfoun	
Advisor:	
Title of Talk: Quantify differences between image feature extraction tools	
<b>Abstract:</b>	
Over the past several decades, microscopy has been one of the main tools in cell biology. Digital assessment of microscopy images has continued to serve a major role in cell biology, where biologists analyze cell state and expression via software-based image measurements of cellular regions of interest. With the increasing amount of microscopy image data during biological experiments, qualitative visual inspection of images has to be replaced with quantitative automated image-based measurements in order to derive knowledge about cells with high confidence. Automation of software-based image measurements (image features) has led to a plethora of implementations. While software libraries contain thousands of implementations, many of them implement the same image measurements and sometimes result in a different numerical value. This poses a challenge for deriving knowledge about cells and for reproducing scientific results.	
<b>Abstract:</b>	
What if there was a service that allowed a user to store any important information to be used at any place and at any time? With breaches becoming increasingly prevalent on the news, securing data has become sought out now more than ever. Personal Data Stores (PDS) will allow users to have more control over who controls their data, what their data is being used for, and, most importantly, where that data is being stored.	
This cloud service's main benefit is the convenience of having secure access to important personal information wherever needed. However, there are important problems that need to be addressed in this field. For instance, how will a user be ensured that the service is as secure as it needs to be, will PDS providers have access to the information being stored, and how will PDS providers ensure of information termination after disclosure? These are all important questions that must be addressed before these services can be provided.	
In order for Personal Data Stores to be possible, clear requirements and guidelines must be in place. For instance, describing the importance of using client side encryption versus server side encryption. These would demonstrate the ideal functions that are needed for a successful PDS, and, in short, would allow for a more defined and consistent approach for all PDS providers to follow.	

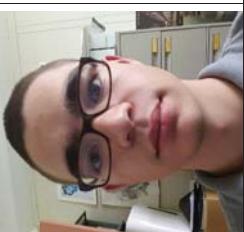
<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Jamshaid Shahir	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Mathematics/Applied Statistics
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Graduate School in Applied Mathematics	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Systems and Software Division, Information Systems	
Division, and Group: Group	
NIST Research Joe Chalfoun	
Advisor:	
Title of Talk: Quantify differences between image feature extraction tools	
<b>Abstract:</b>	
Over the past several decades, microscopy has been one of the main tools in cell biology. Digital assessment of microscopy images has continued to serve a major role in cell biology, where biologists analyze cell state and expression via software-based image measurements of cellular regions of interest. With the increasing amount of microscopy image data during biological experiments, qualitative visual inspection of images has to be replaced with quantitative automated image-based measurements in order to derive knowledge about cells with high confidence. Automation of software-based image measurements (image features) has led to a plethora of implementations. While software libraries contain thousands of implementations, many of them implement the same image measurements and sometimes result in a different numerical value. This poses a challenge for deriving knowledge about cells and for reproducing scientific results.	
<b>Abstract:</b>	
The overall goal of this project is to quantify the differences between image features computed by several feature extraction tools. Extracted features can be classified into 3 main categories: (1) shape features, such as the circularity, perimeter, area etc., (2) intensity features, such as the mean, standard deviation, skewness, entropy, etc., and (3) texture feature, such as the contrast, energy, homogeneity, etc. Our approach is to identify implementations of the same image features across multiple software packages, extract numerical values of image features, and compute statistical variance of image features. We analyze the following software packages: ImageJ, CellProfiler, Protein Subcellular Location Image Database (PSUD) from the Murphy Lab in Carnegie Mellon University, and our NIST feature extraction tools in MATLAB, Java, and Python. A Python script is written to read the features calculated by these software libraries, execute the feature extraction algorithms, and compute variances for all common image features. All commonly found image features will be rank-ordered based on the variances to assist biologists in achieving repeatability of image measurements.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
	
Name: Michelle Shiu	Grant Number 70NANB15H130
Academic Institution: University of Virginia	Major: Chemical Engineering
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Graduate School	
(School/Career):	
NIST Laboratory, Center for Nanoscale Science and Technology, Nanofab Operations Group	
Division, and Group:	
NIST Research Lei Chen	
Advisor:	
Title of Talk: High-Aspect-Ratio Nanostructure Fabrication	
Abstract:	
 <p>The diagram illustrates the sequential steps of nanostructure fabrication. It starts with a 'Resist' layer on a 'Substrate'. This is followed by 'ALD' (Atomic Layer Deposition) where orange ALD precursors are deposited onto the resist. After ALD, the structure undergoes 'Etching' to remove the resist, leaving a porous structure. Finally, the 'Resist Made Porous' stage shows the resulting high-aspect-ratio nanostructure.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Vivienne Shaw	Grant Number 70NANB15H170
Academic Institution: Wellesley College	Major: Computer Science
Academic Standing Senior	
(Sept. '15):	
Future Plans To pursue a career in software development and interaction design.	
(School/Career):	
NIST Laboratory, Engineering Laboratory, Intelligent Systems Division,	
Division, and Group: Manipulation and Mobility Systems Group	
NIST Research Jeremy Marvel	
Advisor:	
Title of Talk: Context Awareness for Adaptive Human-Robot Interaction	
Abstract:	
<p>As the role of robots in the manufacturing industry grows, so do the safety risks posed to human operators and robot technicians. Furthermore, current methods of human-robot interaction, such as the teach pendant, are inefficient and unintuitive to modern operators. To facilitate both efficient and safe human-robot collaboration, this project focuses on developing a contextually aware robotic system using commercially available smart devices. This research implements conceptual principles from the “Internet of Things”, or networked embedded systems that are able to adapt to the needs of users.</p> <p>We present a smart robotics system integrating a Microsoft Kinect, Android tablet, and Pebble smartwatch in addition to a Universal Robots UR10. Within this system, three virtual zones are generated in front of the robot with associated levels of risk. Upon detection of unrecognized users in these zones, the robot will slow down and stop or perform a designated task for a recognized user. Robot operators are also notified of these intrusions via smartwatch notifications and an Android tablet interface that also provides live robot process and task information. Finally, operator responses via the watch or tablet produce motion commands to reposition the robot to a “presentation pose” for part inspection. Projected test results find robot response speed is sufficient to deal with unrecognized disturbances in the work setting, and interface design provides ample situational awareness for both the operator and the robot system.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
<b>Name:</b> Brian Sim	<b>Grant Number</b> : 70NANB15H162
<b>Academic Institution:</b> University of Massachusetts Amherst	<b>Major:</b> Chemical engineering
<b>Academic Standing</b>	<b>Graduate school</b>
(Sept. '15):	Senior
<b>Future Plans</b>	Graduate school
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b>	Materials Measurement Science Division, Nano Materials Research Group
<b>NIST Research Advisor:</b>	Stacey Louie
<b>Title of Talk:</b>	Effects of environmental photo-oxidants on the stability of polymeric coatings on nanoparticles
<b>Abstract:</b>	
<p>Gold nanoparticles (AuNPs) are being more commonly considered for medical applications and there are increasing concerns on the fate and transport of these released nanoparticles (NPs) in the environment. The environmental exposure and toxicity risks of nanomaterials can depend significantly on the presence and properties of adsorbed macromolecular coatings. Little work has been done on the stability of these coatings on AuNPs under environmental conditions (e.g. sunlight exposure). The goal of this project was to assess the effects of environmental photo-oxidants (e.g. nitrate, dissolved iron, and hydrogen peroxide) on the rate of coating transformation.</p>	
<p>AuNPs were coated with methoxy polyethylene glycol thiol (mPEG-SH) and then exposed to UVA radiation with the different photo-oxidants. Samples were collected at zero, three, and six hours and measured for size using dynamic light scattering (DLS) and zeta-potential using laser Doppler micro-electrophoresis. For nitrate, the size of the coated AuNPs decreased over time while for the dissolved iron, the size increased over time. The zeta-potential of the coated AuNPs with both nitrate and dissolved iron became more negative over time. Compared to deionized water, the photo-oxidants had no significant effect on size or zeta-potential. The results were also compared to the behavior seen using a colorimetric assay with ultraviolet-visible spectroscopy (UV-VIS) to distinguish reactivity of the AuNP-sorbed versus dissolved mPEG-SH in the photo-oxidants. The implication of the results can provide guidance regarding sample preparation for photochemical studies and the effect of environmental conditions on NP fate in the environment.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
<b>Name:</b> Alexander Silver	<b>Grant Number</b> : 70NANB15H142
<b>Academic Institution:</b> Northwestern University McCormick School of Engineering	<b>Major:</b> Materials Science & Engineering
<b>Academic Standing</b>	<b>Junior</b>
(Sept. '15):	Northwestern University McCormick School of Engineering
<b>Future Plans</b>	Graduate School or career in aerospace
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b>	Materials Measurement Science and Engineering Division, Nano Functional Polymers Group
<b>NIST Research Advisor:</b>	Jonathan Downing
<b>Title of Talk:</b>	Measuring Aggregation in Organic Photovoltaic Solutions
<b>Abstract:</b>	
<p>Organic photovoltaic cells are an important developing technology which could enable the creation of robust, flexible and low-cost solar panels. The key part of these devices is the bulk heterojunction (BHJ), which is typically made of a blend of polymer and fullerene molecules in solution. The performance of a BHJ device is dependent on how the polymer chains interact in solution. The polymers can be considered to conform to two general states: aggregated and non-aggregated. Configuration is dependent on the solution properties and temperature. Since aggregated areas interact with incident light to create absorption peaks, the general configuration can be observed by measuring the UV-visible absorption spectrum of the solution. A profile of absorption as a function of temperature was created for various materials by observing absorption spectra at various temperatures. This profile can then be used to determine a processing temperature when constructing the organic solar cells which maximizes the effectiveness of the device. It is hoped that this will allow construction of organic photovoltaic cells with an efficiency of 10% or greater.</p>	



**SURF Student Colloquium**

NIST – Gaithersburg, MD

August 4–6, 2015

Name: Joseph A. Smiga	Grant Number   70NANB15H168
Academic Institution: University of Maryland, College Park	Major: Physics, Math
Academic Standing (Sept. '15): Sophomore	
Future Plans (School/Career): Grad School for PhD in theoretical physics	
NIST Laboratory, Division, and Group: Physical Measurement Lab, Quantum Measurement Division, Atomic Spectroscopy Group	
NIST Research Advisor: Yuri Raichenko	
Title of Talk: LMO dielectronic resonance in highly charged bismuth	

**Abstract:**

Dielectronic resonances from high-Z elements are important for the analysis of high temperature plasmas. Thus, the extreme ultraviolet spectra of highly charged bismuth were measured using the NIST electron beam ion trap at beam energies ranging from 8.7 keV to 9.2 keV. The measured intensity ratios between forbidden magnetic-dipole lines in Bi<sup>6+</sup> and Bi<sup>5+</sup> indeed show strong resonance features. The experimental data were then compared to theoretical predictions from a large-scale collisional-radiative model and a good agreement was found that allowed us to identify the observed resonance features as the LMO inner-shell dielectronic resonances. These resonances occur when an electron in the L-shell (i.e.,  $n=2$ ) is excited to the M-shell ( $n=3$ ) of an ion while a free electron is captured in the O-shell ( $n=5$ ). Additionally, the effects of bismuth escape rates were analyzed.



**SURF Student Colloquium**

NIST – Gaithersburg, MD

August 4–6, 2015

Name: Erika M. Spangler	Grant Number   70NANB15H1835
Academic Institution: University of the District of Columbia	Major: Mechanical Engineering
Academic Standing (Sept. '15): Senior	
Future Plans (School/Career): Study Materials Science in Grad School	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Semiconductor and Dimensional Metrology, Nanoscale	
NIST Research Advisor: Kate Klein, András Vadár	
Title of Talk: Understanding Focused Helium Ion Beam Milling through Cross-Sectional Imaging	

**Abstract:**

The ability to machine materials on the nanometer scale has many applications ranging from nanoelectronics and integrated circuit editing to the creation of nanopore sensors and optical devices. The Orion helium ion microscope (HiM), with a typical probe size of less than 1 nm, offers a unique method for nanofabrication at a scale currently unattainable by conventional gallium-based focused ion beam (FIB) processing. However, the slow material removal rate (low sputter yield) and helium implantation damage present challenges to this technique. In this study, we seek to find optimal conditions for helium ion nanomachining of thin film and bulk substrates. Using previous results from a partnership with Intel, which explored helium ion beam interaction with Silicon substrates, a methodology for quantifying beam-sample interactions via cross-sectional imaging has been developed. This methodology was then applied to study milling in Gold substrates. SRIM (Stopping and Range of Ions in Matter) simulation software (using a Monte Carlo method), was employed to explore trends in sputter yield as a function of substrate material, thickness and beam energy as well as verify experimental outcomes. The results of this study will provide optimal nanomachining conditions at the lowest dose feasible.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Sara Stoudt	Grant Number   70NANB15H145 Major: Mathematics and Statistics
Academic Institution: Smith College	
Academic Standing   UC Berkeley, first year graduate student	
(Sept. '15):	
Future Plans   Complete my Ph.D. in Statistics at UC Berkeley and go on to work in a government lab or in industry	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis & Modeling Group	
Division, and Group:	
NIST Research Advisors: Antonio Possolo & Tom Bartel	Doug Thomas
Advisors:	
Title of Talk: "Big Force" Calibrations: An Errors-in-Variables Approach	Title of Talk: Mapping Vulnerability of Regional Economies to Natural Disasters Using Input-Output Data

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Mara Stutzman	Grant Number   70NANB15H177 Major: Economics (Statistics & China Studies)
Academic Institution: St. Olaf College	
Academic Standing   Senior	
(Sept. '15):	
Future Plans   I plan to work for a couple years before attending graduate school. I hope to find a career (School/Career): that allows me to combine my passion for analytics with my Mandarin language skills.	
NIST Laboratory, Engineering Laboratory, Office of Applied Economics	
Division, and Group:	
NIST Research Advisor:	Doug Thomas
Advisor:	
Title of Talk: "Big Force" Calibrations: An Errors-in-Variables Approach	Title of Talk: Mapping Vulnerability of Regional Economies to Natural Disasters Using Input-Output Data

**Abstract:** Hurricanes, earthquakes, and other disasters devastate cities across the United States every year. While the physical damage these disasters impose is great, the destruction to the economy in the form of business interruptions and critical infrastructure losses can be equally crippling. The New Orleans economy is still recovering from Hurricane Katrina, which made landfall ten years ago; Superstorm Sandy caused record-setting power outages which spanned 21 states; and the New Madrid fault threatens Memphis and St. Louis, which are, largely, not designed to withstand an earthquake. This project proposes a method to determine how susceptible local economies are to future disasters.

Existing research on regional economies and their ability to withstand natural and man-made disasters focuses on impact analysis and economic loss estimation. This presentation seeks to understand an economy's vulnerability to disasters based upon the susceptibility of its critical infrastructure systems, such as utility lifelines. Specifically, we focus on the inputs required to maintain these systems and whether those inputs originate in the region or outside of it. The study analyzes the economies of nine metropolitan statistical areas, which are all located in regions of the United States especially prone to either hurricanes or earthquakes. Relative vulnerability is determined through comparisons with national-scale data.

**Abstract:** Measuring forces is key to commerce (weighing truck loads at truck scales), to manufacturing (shaping automotive body panels using presses), and to transportation (thrust of aircraft jet engines). Forces are measured using devices called *force transducers*, which convert an applied force to the deflection of an indicating mechanical pointer, or to an electrical signal (also called a *deflection*, by analogy). These devices are elastic, in the sense that they return to their original condition once the force is removed. Calibrating such a device means establishing a mapping between applied forces and instrumental indications. NIST uses machines with large weights to calibrate transducers capable of measuring forces of up to 4.5 million newton (the weight of 180 Humvees!). NIST calibrates force transducers by applying known forces that the earth's gravity exerts upon very large stainless steel disks, and relating these forces to the corresponding deflections using a *calibration curve*. When the force transducer is used in practice, the user observes a deflection and uses the calibration curve to determine the corresponding force.

Currently, an ordinary least squares method is used to fit a curve (usually a polynomial of low degree) to the calibration data. However, this method does not account for the uncertainty in the applied forces, which can bias the fit. I have developed and implemented an alternative errors-in-variables (EIV) method that takes into account uncertainties in both the applied forces and the deflections. In my presentation, I will describe this method and will also discuss a procedure for uncertainty quantification that produces a confidence band for the entire curve. Both this EIV method and the procedure for the evaluation of measurement uncertainty are currently being incorporated into the NIST force calibration services.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Lindsay Thornton	Grant Number 70NANB15H131
Academic Institution: East Carolina University	Major: Mathematics and Physics
Academic Standing Senior	
(Sept. '15): Future Plans Graduate School – looking to combine her previous degree in Environmental Studies and Biology with her current studies to do research that will positively impact the current state of the world's environmental health. Specific interest in the Chesapeake Bay Watershed.	Future Plans Graduate School pursuing a PhD in physics. Eventual career in atomic physics studying light matter interaction.
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Science and Engineering Division, NIST Research	NIST Laboratory, Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group
Advisor: Dr. Carelyn Campbell	Dr. Gillian Nave
Title of Talk: Can you see my data now?: The Materials Genome Initiative and building data infrastructure	Title of Talk: Line analysis of singly ionized titanium (Ti II)
Abstract:	
<p><b>Abstract:</b> New material development, from idea to industry, typically takes 10–20 years. The Materials Genome Initiative is an effort to develop infrastructure to accelerate this process. The acceleration of this process will mean a more competitive manufacturing sector as well as economic growth in the United States.</p> <p>One of the major factors slowing the development of new materials is the lack of data sharing options. Data sharing tools are needed to allow scientists and engineers at all stages of development ways to locate and then access data in a variety of systems and repositories associated with different institutions located here in the U.S. Specifically, having access to phase-based property data allows for accurate and efficient models for the calculation of phase-based material properties, which, in turn, is critical to the acceleration of new material development. This includes data such as thermodynamic properties, diffusion mobilities, elastic constants, and thermal expansion coefficients. As current access to phase-based data is still limited, scattered across both real and virtual space, it makes it difficult to locate, access, and use data efficiently.</p> <p>As a part of this initiative, the Materials Data Curation System (MDCS) being created here at NIST allows for the curation of such data into a repository using XML-based data schemas. Data can be imported and exported into the curation system via the Application Programming Interface (API) as well as manual use of a pre-defined template. The MDCS allows a user not only to import and export data, but also to search and share data. This project included creating XML-based data schemas for two types of data: raw instrument data and literature data. The schemas were then used in beta-testing the curator, which involved importing, searching, and sharing and exporting data, both manually and via the API using a python script.</p>	
Name: Keeley Irene May Townley-Smith	Grant Number 70NANB15H149
Academic Institution: Lamar University	Major: Physics and Electrical Engineering
Academic Standing Senior	
(Sept. '15): Future Plans Graduate School pursuing a PhD in physics. Eventual career in atomic physics studying light matter interaction.	Future Plans Graduate School pursuing a PhD in physics. Eventual career in atomic physics studying light matter interaction.
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group	NIST Laboratory, Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group
NIST Research	Dr. Gillian Nave
Advisor:	
Title of Talk:	
Abstract:	
<p><b>Abstract:</b> Atomic spectroscopy is the analysis of light emitted from a hot plasma and is used to determine atomic properties and composition. There is an on-going project in the Atomic Spectroscopy Group at NIST to obtain comprehensive spectral data for all of the singly ionized iron group elements and acquire more accurate energy levels and wavelengths. The heavy abundance of the iron group elements in stellar objects makes them of interest for astrophysical observations.</p> <p>The last published study of Ti II in the vacuum ultraviolet (VUV) region, which ranges from 300–2000 Å, was Huldt et al. in 1982 [1]. They report wavelength uncertainties of 0.02 Å and identified 1,240 lines from 1,100–11,000 Å. We believe that we can obtain better resolved VUV spectra using the 10.7 normal incidence spectograph here at NIST with SWP Kodak photographic plates and reduce wavelength uncertainties by at least an order of magnitude. We base this claim on a similar comparison that was already been done for Fe I using the same instrument and methodology. Using a Ti high current hollow cathode lamp (HCL), we collected grating spectra from approximately 800 to 3,500 Å. A Pt HCL was used for calibration of our spectra. From these plates, we see lines that have never been observed here, as well as lines below 1,100 Å. We are preparing a comprehensive line list to publish and contribute to NIST's Atomic Spectral Database.</p>	
<p>[1] Huldt, Sven; Johansson, Sveneric; Lützen, Ulf; Wyart, Jean-François. The Spectrum and Term System of Singly Ionized Titanium, Ti II. <i>Phys. Scr.</i> <b>25</b>: 401, 1982.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Lindsay Thornton	
Academic Institution: East Carolina University	
Academic Standing Senior	
(Sept. '15): Future Plans Graduate School – looking to combine her previous degree in Environmental Studies and Biology with her current studies to do research that will positively impact the current state of the world's environmental health. Specific interest in the Chesapeake Bay Watershed.	
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Science and Engineering Division, NIST Research	
Advisor: Dr. Carelyn Campbell	
Title of Talk: Can you see my data now?: The Materials Genome Initiative and building data infrastructure	
Abstract:	
<p><b>Abstract:</b> New material development, from idea to industry, typically takes 10–20 years. The Materials Genome Initiative is an effort to develop infrastructure to accelerate this process. The acceleration of this process will mean a more competitive manufacturing sector as well as economic growth in the United States.</p> <p>One of the major factors slowing the development of new materials is the lack of data sharing options. Data sharing tools are needed to allow scientists and engineers at all stages of development ways to locate and then access data in a variety of systems and repositories associated with different institutions located here in the U.S. Specifically, having access to phase-based property data allows for accurate and efficient models for the calculation of phase-based material properties, which, in turn, is critical to the acceleration of new material development. This includes data such as thermodynamic properties, diffusion mobilities, elastic constants, and thermal expansion coefficients. As current access to phase-based data is still limited, scattered across both real and virtual space, it makes it difficult to locate, access, and use data efficiently.</p> <p>As a part of this initiative, the Materials Data Curation System (MDCS) being created here at NIST allows for the curation of such data into a repository using XML-based data schemas. Data can be imported and exported into the curation system via the Application Programming Interface (API) as well as manual use of a pre-defined template. The MDCS allows a user not only to import and export data, but also to search and share data. This project included creating XML-based data schemas for two types of data: raw instrument data and literature data. The schemas were then used in beta-testing the curator, which involved importing, searching, and sharing and exporting data, both manually and via the API using a python script.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4-6, 2015
	
Name: Victor Manuel Trujillo Jr	Grant Number 70NANB15H083
Academic Institution: Texas A&M University	Major: Electrical Engineering
Academic Standing Senior	
(Sept. '15):	
Future Plans Attend graduate school and pursue a degree in applied physics	
(School/Career):	
NIST Laboratory, Engineering Laboratory, Intelligent Systems Division,	
Division, and Group: Cognition and Collaboration Systems Group	
NIST Research William Harrison II	
Advisor:	
Title of Talk: Virtual Fusion: Human Presence in Manufacturing Simulation	
<b>Abstract:</b>	
Augmented Reality is a technology that has been presented to us by movies and TV series. Until recently, Augmented Reality (AR) was an idea that seemed out of reach, but with the emergence of Virtual Reality (VR) it is now close at hand. With AR close at hand, manufacturing companies can invest in this technology and use it for process simulations and diagnostics of future components and layouts. More specifically, they can simulate manual workstations where the user is able to interact with virtual components while in the real world. The Virtual Fusion project addresses the ability to capably simulate objects in mixed reality (virtual and real) within a manufacturing environment. The end goal of the project is to develop a methodology that can aid the manufacturing industry in improving process downtime and system deployment. To achieve this, existing VR technology is leveraged to create a low cost open source AR system. The AR system that was created consists of the Oculus Rift, external cameras and the Leap motion sensor. The cameras project the video feed and the virtual object through the Oculus rift, allowing the user to see virtual objects in their current environment. The leap motion sensor allows the user to interact with the virtual objects. This system is designed to simulate an interactive manufacturing environment in the real world. Manufacturing components can be added and removed from the environment at any given time allowing for system validation and process planning. Leveraging this technology will help optimize how manufacturers operate in the future.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4-6, 2015
	
Name: Catherine Train	Grant Number 70NANB15H182
Academic Institution: Hood College	Major: Mathematics, Minor in Economics and Women's Studies
Academic Standing Senior	
(Sept. '15):	
Future Plans Career in Applied Mathematics	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Applied and Computational Mathematics Division, Division, and Group:	
NIST Research Mathematical Software Group	
Advisor:	
Title of Talk: Howard Cohl	
<b>Abstract:</b>	
Verification and Search for Generating Functions for Orthogonal Polynomials in the Askey Scheme	
This talk continues the presentation of my joint summer project with co-SURF student Isabelle Berger on the verification and search for generating functions for orthogonal polynomials in the Askey scheme. Whereas Isabelle described the algorithms behind our experiential mathematics verification and search, I will describe the results of how well our derived algorithms fared. I will summarize (1) the full parameter space in which we searched for new generating functions; (2) where and why particular choices failed; (3) where particular choices succeeded; (4) and deficiencies in existing algorithms and ideas for future improvements.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Tareq Uddin	Grant Number   70NANB15H141
Academic Institution: Montgomery College	Major: Mechanical Engineering
Academic Standing (Sept. '15):	University of Maryland , Junior
Future Plans (School/Career):	Graduate School, University of Maryland
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biosystems and Biomaterials Division, biomaterials Group
NIST Research Advisor:	Carl Simon, Nathan Hotaling, Harl Iyer
Title of Talk:	Quantitative Prediction of Biodegradable Nanofiber Diameter for use in Tissue Engineering: A Therapy for Age-Related Macular Degeneration
<b>Abstract:</b>	<p>Age Related Macular degeneration (AMD) is the most common cause of blindness in people over the age of 50. It is a disease where the macula deteriorates and is unable to support the photoreceptor cells of the retina. One possible cure for this disease is to use induced pluripotent stem cells (iPSCs) which can be turned into retinal cells and insert the retinal cells with a biodegradable nanofiber structural support into an AMD patient. The nanofiber is critical because it needs to mimic and act as the native extracellular matrix (ECM). In order to replace the ECM, the nanofibers need to have a specific diameter, spacing and other characteristics, but currently, this is hard to do because there isn't a model that can be used to accurately predict fiber diameter. We used electrospinning to produce PLGA (poly lactic-co-glycolic acid) fibers and analyzed the diameters of PLGA fibers produced.</p> <p>Electrospinning is a method used to create nanofibers in which high voltage electricity is applied to polymer solution flowing out of syringes and creating an electric potential between the solution and a collector plate placed some distance away. As a result, the polymer solution is pulled down in a very thin fiber which deposits on the grounded collector plate. We measured the changes in fiber diameter as we varied 7 electrospinning conditions (molecular weight, concentration of the polymer, needle gauge, flow rate, needle tip to collector plate distance, voltage and the relative humidity) by taking scanning electron microscope (SEM) images over three settings (low, medium and high). Due to the large parameter space (<math>3^7 = 2187</math>), an optimally selected 3<sup>7</sup> fractional factorial "Design of Experiments" strategy was used to screen 108 treatments. A custom, validated program called DiameterJ was used to analyze SEMs to determine the frequency of fiber diameters in each condition. Results from the fractional factorial design will be presented and discussed.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	
Name: Sam Underwood	Grant Number   70NANB15H193
Academic Institution: Reed College	Major: Chemistry
Academic Standing (Sept. '15):	Senior
Future Plans (School/Career):	Graduate school (PhD)
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Nanomaterials Research
NIST Research Advisor:	Justin Gorham
Title of Talk:	Preparation and Characterization of Silver Nanoparticle-loaded Fabrics as Test Materials
<b>Abstract:</b>	<p>Silver has long been known to exhibit anti-microbial properties through the generation of Ag<sup>+</sup> as a result of surface oxidation. Due to their high surface area to volume ratio, silver nanoparticles (AgNPs) are ideally suited for the generation of Ag<sup>+</sup>. Many take advantage of the desirable properties of AgNPs by loading them onto textiles and other commercial products. Researchers concerned with nanomaterial environmental health and safety issues have discussed the need for characterizing these AgNP-loaded consumer products and identifying their nano-silver component. To that end, this work outlines a method designed to load 30 nm to 50 nm silver nanoparticles into various fabrics to be employed as validation materials.</p> <p>AgNPs were synthesized in the presence of cotton or nylon fabric in boiling water from silver nitrate, with citrate acting as a reducing agent. These test materials were prepared at varying AgNP concentration by varying starting Ag<sup>+</sup> concentration. The AgNP-loaded textiles were then characterized using X-ray photoelectron spectroscopy, scanning electron microscopy, energy dispersive X-ray spectroscopy, and inductively coupled plasma mass spectrometry.</p> <p>For cotton textiles, the data revealed that a maximum surface silver concentration is reached when employing a 0.7 mmol/L Ag<sup>+</sup> solution. SEM shows that particles 30 nm to 100 nm in size coat the surface of cotton test materials, with some particle aggregation observed. Results from nylon-loaded test materials, as well as ICP-MS results, will also be presented.</p>

## SURF Student Colloquium

NIST – Gaithersburg, MD

August 4-6, 2015

<b>SURF Student Colloquium</b>	
	NIST – Gaithersburg, MD
	August 4-6, 2015
Name: Robert Valdillez	Grant Number 70NANB15H174
Academic Institution: North Carolina State University	Major: Physics
Academic Standing Junior	
(Sept. '15):	
Future Plans Graduate School	
(School/Career):	
NIST Laboratory Physical Measurements Laboratory, Radiation Physics Division, Neutron Physics Group	
Division, and Group:	
NIST Research Hans Pieter Mumm	
Advisor:	
Title of Talk: Can One Build A Global Neutron Surface Spectrum Map?	
Abstract:	
Free neutrons contribute an important background when conducting searches for illicit special nuclear material, during radiation monitoring, and in fundamental nuclear physics research. This talk discusses the degree of success one can hope to achieve in building a global neutron surface spectrum map. Pressure, the solar cycle, humidity, column water vapor, and soil moisture all affect this spectrum. Since the previous literature focused on each of these effects separately there was a need to compile the research. To validate created models, one of NIST's pre-existing neutron detectors was upgraded. The necessary repairs and upgrades to the detector will be discussed as will the methods and models used to analyze the data.	
Name: Kimberly Van Dongen	Grant Number 70NANB15H175
Academic Institution: Virginia Polytechnic Institute and State University	Major: Biochemistry
Academic Standing Senior	
(Sept. '15):	
Future Plans Medical school	
(School/Career):	
NIST Laboratory Materials Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials	
Division, and Group:	
NIST Research Group	
Advisor: Dr. Jirun Sun	
Title of Talk: Resistance of Next Generation Dental Resin to Biological Challenges in an Oral Environment	
Abstract:	
The traditional dental resins used in dentist offices today has been in use for over fifty years. They contain ester groups, which are readily broken apart by enzymes in saliva and cariogenic bacteria. In an effort to create more durable dental resins, ether-based instead of ester-based resins are created to fight against biological challenges including enzymatic and cariogenic challenges. These new materials will provide a dental restorative material with a longer service life to improve dental patient care.	
In order to compare the resistance of biodegradation between traditional and new resins, it is essential to understand the enzymatic activity, bacterial growth, and the chemical breakdown of ester-based and ether-based compounds. We tested the activity of two enzymes, Cholesterol esterase (CE) and Pseudocholine esterase (PCE). High performance liquid chromatography (HPLC) was used to assess the pathway of compound degradation under enzymatic challenges. We also evaluated the interaction of bacteria with new and traditional resins. These preliminary experiments help us understand our materials as we move forward to determine their resistance to biodegradation.	

<b>SURF Student Colloquium</b>	
	NIST – Gaithersburg, MD
	August 4-6, 2015
Name: Robert Valdillez	Grant Number 70NANB15H174
Academic Institution: North Carolina State University	Major: Physics
Academic Standing Junior	
(Sept. '15):	
Future Plans Graduate School	
(School/Career):	
NIST Laboratory Physical Measurements Laboratory, Radiation Physics Division, Neutron Physics Group	
Division, and Group:	
NIST Research Hans Pieter Mumm	
Advisor:	
Title of Talk: Can One Build A Global Neutron Surface Spectrum Map?	
Abstract:	
Free neutrons contribute an important background when conducting searches for illicit special nuclear material, during radiation monitoring, and in fundamental nuclear physics research. This talk discusses the degree of success one can hope to achieve in building a global neutron surface spectrum map. Pressure, the solar cycle, humidity, column water vapor, and soil moisture all affect this spectrum. Since the previous literature focused on each of these effects separately there was a need to compile the research. To validate created models, one of NIST's pre-existing neutron detectors was upgraded. The necessary repairs and upgrades to the detector will be discussed as will the methods and models used to analyze the data.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5-7, 2014	
Name:	Matthew Wade
Academic Institution:	Care Western Reserve University
Academic Standing:	Junior
(Sept. '15):	Ph.D. in either Chemical Engineering or Materials Science
Future Plans (School/Career):	NIST Laboratory, Materials Measurement Laboratory
Division, and Group:	Polymers and Complex Fluids
NIST Research Advisor:	Thomas Rosch
Title of Talk:	Calculation of Radial Distribution Functions for Polymer Nanocomposites using Parallel Processing on a Graphical Processing Unit
Abstract:	<p>Polymer nanocomposites (PNCs) are a class of materials that consist of nanoparticles dispersed throughout a polymer matrix. These hybrid materials are known to enhance certain characteristics of the polymer base while still retaining many of the properties that make the base polymer incredibly useful. The extent to which a polymer's viscosity, yield strength, elasticity, thermal conductivity, etc. is improved by the addition of nanoparticles depends on whether or not the nanoparticles are evenly distributed throughout the polymer matrix. To better understand the mechanisms that govern the dispersion of nanoparticles in a PNC, a number of research groups have turned to molecular dynamics and coarse grained simulations. Position and energy obtained from these simulations can be used to calculate the second virial coefficient (<math>B_2</math>) which can be used as a means to determine the extent to which nanoparticles are dispersed. A positive <math>B_2</math> value is indicative of a good dispersion, while a negative value indicates clumping or phase separation. This study focused on the use of Radial Distribution Functions (RDFs) as a means to determine <math>B_2</math>. RDFs represent the probability of locating a given atom type at a certain distance, thus providing information concerning the spacing of particles within a system. Typical calculations of an RDF involve comparing every single particle within the system to every other possible particle. As such, these calculations can be exceedingly slow when analyzing large systems. To ensure that data could be gathered and processed within a reasonable time, code to calculate a RDF, and though that the value of <math>B_2</math>, was written utilizing the parallel processing capabilities of a Graphical Processing Unit (GPU). Programming for the GPU has presented a number of challenges when attempting to make the program applicable to a wide variety of systems. Current efforts have led to a reduction in computation time by approximately one order of magnitude when compared to RDF calculations that use serial processing. This increase in speed makes it possible to calculate the RDF and <math>B_2</math> for larger and more complex systems.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Cecilia Vollbrecht
Academic Institution:	Centre College
Academic Standing:	Junior at Centre College
(Sept. '15):	Graduate School
Future Plans (School/Career):	Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group
NIST Laboratory, Division, and Group:	NIST Research Jeff Gilman, Muzhou Wang
Advisor:	
Title of Talk:	Synthesis and Characterization of Activatable Dyes for Integration into Polymer Systems
Abstract:	<p>Activatable dyes are an important class of molecules due to their ability to indicate changes in environment by their change in fluorescence and absorbance. Activation can occur through several methods, including acid, base, ultraviolet light and visible light. Mechanophores are a subclass of activatable dyes that become fluorescent with mechanical activation or force. In one type of mechanophore, application of force breaks a chemical bond within the molecule, shifting the equilibrium from a non-fluorescent to a fluorescent isomer. The ability to detect the deformation within a polymer is important to prevent its failure. Integration of these molecules into polymers would allow for the important identification and localization of mechanical stress and damage in a polymer via the visible fluorescence of the stressed dye molecule. The goal of this project is to synthesize and characterize several mechanophore dyes and incorporate them into polymers. The dyes being focused on are synthesized derivatives of spiropyran and rhodamine. Characterization of these dyes is done through absorbance, fluorescence and calculation of a relative quantum yield value. In addition other forms of activation, such as ultraviolet light, acid, base and visible light, for these dyes was studied. These dyes are then integrated into a polymer which can be tension tested, during which the dye should become visibly fluorescent in the polymer.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Andrew T. Wang <b>Academic Institution:</b> University of Maryland, College Park <b>Academic Standing:</b> Sophomore <b>(Sept. '15):</b> Graduate School <b>Future Plans:</b> Graduate School <b>(School/Career):</b> Information Technology Laboratory, Software and Systems Division, Information Systems <b>NIST Laboratory, Division, and Group:</b> Group <b>NIST Research Advisor:</b> Peter Bajcsy <b>Advisor:</b> Peter Bajcsy
<b>Title of Talk:</b> Characterization of Nanofiber Scaffolds	<b>Abstract:</b> Human cells change their 3D shapes and biological states depending on their environment. Currently, there is a lack of measurements of such changes, specifically how different types of scaffolds affect the cells placed on them. In order to establish such a relationship, confocal laser scanning microscopes can be used to acquire 3D images of human bone marrow stem cells. Imaging hundreds of cells on at 63x magnification yields several thousands of files. The objective of this project is to extract cell-scaffold contact points and create scaffold digital models. The challenges of this project lie in designing an automated segmentation algorithm and evaluating its accuracy, precision, and efficiency.
	<b>Name:</b> Peter Walecki <b>Academic Institution:</b> Florida Atlantic University <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> The pursuit of a career in the development of robust metrology systems for use in extreme environments. <b>(School/Career):</b> Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, <b>NIST Laboratory, Division, and Group:</b> Surface and Nanostructure Metrology Group <b>NIST Research Advisor:</b> Dr. George Orji <b>Advisor:</b> Dr. George Orji
<b>Title of Talk:</b> Development of Magnetic Contrast in Critical Dimension Atomic Force Microscopy	<b>Abstract:</b> There are a range of contrast mechanisms used in Atomic Force Microscopy (AFM) and many variants on the basic scanning probe technology. One of these is commonly referred to as Magnetic Force Microscopy (MFM), which incorporates information about the magnetic field surrounding a sample into the measurement. The technology required to perform MFM measurements using a conventional AFM platform has existed for several decades. However, this has not been extended to Critical Dimension microscopes (CD-AFMs), because of the added complexity of tip-sample control in two axes compared with the single axis methods of conventional AFM.  In order to use AFMs as dimensional metrology instruments, their performance and accuracy needs to be characterized. This involves evaluating the scale errors in all three axes, and their corresponding angular errors. Other aspects of the evaluation include drift and tip shape characterization. Part of the work involves learning the principles of AFMs as well as evaluation of the data. Software for evaluating the metrological performance of the AFM was implemented in MATLAB and used for the analysis.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Peter Walecki <b>Academic Institution:</b> Florida Atlantic University <b>Academic Standing:</b> Senior <b>(Sept. '15):</b> The pursuit of a career in the development of robust metrology systems for use in extreme environments. <b>(School/Career):</b> Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, <b>NIST Laboratory, Division, and Group:</b> Surface and Nanostructure Metrology Group <b>NIST Research Advisor:</b> Dr. George Orji <b>Advisor:</b> Dr. George Orji
<b>Title of Talk:</b> Development of Magnetic Contrast in Critical Dimension Atomic Force Microscopy	<b>Abstract:</b> There are a range of contrast mechanisms used in Atomic Force Microscopy (AFM) and many variants on the basic scanning probe technology. One of these is commonly referred to as Magnetic Force Microscopy (MFM), which incorporates information about the magnetic field surrounding a sample into the measurement. The technology required to perform MFM measurements using a conventional AFM platform has existed for several decades. However, this has not been extended to Critical Dimension microscopes (CD-AFMs), because of the added complexity of tip-sample control in two axes compared with the single axis methods of conventional AFM.  In order to use AFMs as dimensional metrology instruments, their performance and accuracy needs to be characterized. This involves evaluating the scale errors in all three axes, and their corresponding angular errors. Other aspects of the evaluation include drift and tip shape characterization. Part of the work involves learning the principles of AFMs as well as evaluation of the data. Software for evaluating the metrological performance of the AFM was implemented in MATLAB and used for the analysis.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Ryan Weller
	<b>Academic Institution:</b> University of Colorado Boulder
<b>Academic Standing</b>	<b>Grant Number</b>
(Sept. '15): Senior	70NANB15H094
<b>Future Plans:</b> Graduate Studies in Atomic Physics	<b>Major:</b> Physics and Computer Science
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b> Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group	<b>(School/Career):</b> Information Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Software Group
<b>NIST Research Advisor:</b> Dr. Gillian Nave	<b>NIST Research Advisor:</b> Stephen Langer
<b>Title of Talk:</b> Vacuum Ultraviolet Wavelengths of Fe V and Ni V for Measuring the Gravitational Dependence of the Fine-Structure Constant	<b>Title of Talk:</b> Designing 3D GUI Widgets for OOF
<b>Abstract:</b>	
	The recent publication [1] tests for a potential variation in the fine-structure constant in the presence of high gravitational potentials through the spectral analysis of a white-dwarf star. The spectrum of the white-dwarf star studied in the paper, G191-B2B, has prominent Fe V and Ni V spectral lines, which were used to determine any variation in the fine-structure constant via observed shifts in the wavelengths of Fe V and Ni V in the vacuum ultraviolet region. The results of the paper suggest that refined laboratory values for the observed wavelengths could greatly reduce the uncertainty associated with the paper's findings. An investigation of Fe V and Ni V spectra in the vacuum ultraviolet region has been conducted to reduce wavelength uncertainties currently limiting modern astrophysical studies of this nature. The analyzed spectra were produced by a sliding spark light source with electrodes made of Invar, an iron nickel alloy, at peak currents of 1500 A. The use of Invar ensures that systematic errors in the calibration are common to both species. The spectra were recorded with the NIST Normal Incidence Vacuum Spectrograph on phosphor image plate and photographic plate detectors. Calibration was done with a Pt II spectrum produced by a Platinum Neon Hollow Cathode lamp.
	I will report on the new wavelength values of approximately 350 spectral lines. From these lines, all of the Fe V and Ni V lines used in the previously mentioned paper are identified, along with new values for an additional approximately 200 lines.
	[1] J. C. Berengut, V. V. Flambaum, A. Ong, et al Phys. Rev. Lett. 111, 010801 (2013).
	<b>Abstract:</b>
	OOF-3D (Object-Oriented Finite Elements) is a computer application for finite element (FE) analysis of material properties. It solves equations for physical quantities (like stress or temperature) that vary across a 3D physical structure. This structure can have one or more regions which differ by material composition. The user provides OOF3D with 3D image data in which the color of a given region indicates what material that region is composed of. Then, the user determines the boundaries between these regions using OOF3D's 3D image analysis tools. Knowing these boundaries allows a suitable mesh (a subdivision of space into smaller parts) to be generated for the FE analysis.
	In working with both the image and the mesh, the user must be able to visualize and select portions of 3D data. I developed several features for OOF3D that enable the user to do these things more easily.
	One such feature is the interactive adjusting of clipping planes. A clipping plane is a plane that cuts through 3D objects, and hides ("clips away") any portions of those objects that lie to a particular side of the plane. It lets the user look at the insides of 3D objects, rather than just at their outsides. In the new feature, the user clicks and drags a 2D widget to rotate and move a selected clipping plane around in 3D space.
	A second such feature is the interactive selecting of groups of voxels, the 3D pixels which comprise an image. In this new feature, the user clicks and drags the mouse to select all the voxels within a desired type of region (a rectangular prism, a sphere, etc.).
	I will discuss how I approached various challenges in developing these new features in C++ and Python, including the challenge of interpreting 2D mouse movements as 3D transformations.

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
	<b>Name:</b> Jacob Wolfgang Ward
	<b>Academic Institution:</b> Arizona State University
<b>Academic Standing</b>	<b>Grant Number</b>
(Sept. '15): Senior	70NANB15H094
<b>Future Plans:</b> Graduate Studies in Atomic Physics	<b>Major:</b> Physics and Computer Science
<b>(School/Career):</b>	
<b>NIST Laboratory, Division, and Group:</b> Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group	<b>(School/Career):</b> Information Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Software Group
<b>NIST Research Advisor:</b> Dr. Gillian Nave	<b>NIST Research Advisor:</b> Stephen Langer
<b>Title of Talk:</b> Vacuum Ultraviolet Wavelengths of Fe V and Ni V for Measuring the Gravitational Dependence of the Fine-Structure Constant	<b>Title of Talk:</b> Designing 3D GUI Widgets for OOF
<b>Abstract:</b>	
	The recent publication [1] tests for a potential variation in the fine-structure constant in the presence of high gravitational potentials through the spectral analysis of a white-dwarf star. The spectrum of the white-dwarf star studied in the paper, G191-B2B, has prominent Fe V and Ni V spectral lines, which were used to determine any variation in the fine-structure constant via observed shifts in the wavelengths of Fe V and Ni V in the vacuum ultraviolet region. The results of the paper suggest that refined laboratory values for the observed wavelengths could greatly reduce the uncertainty associated with the paper's findings. An investigation of Fe V and Ni V spectra in the vacuum ultraviolet region has been conducted to reduce wavelength uncertainties currently limiting modern astrophysical studies of this nature. The analyzed spectra were produced by a sliding spark light source with electrodes made of Invar, an iron nickel alloy, at peak currents of 1500 A. The use of Invar ensures that systematic errors in the calibration are common to both species. The spectra were recorded with the NIST Normal Incidence Vacuum Spectrograph on phosphor image plate and photographic plate detectors. Calibration was done with a Pt II spectrum produced by a Platinum Neon Hollow Cathode lamp.
	I will report on the new wavelength values of approximately 350 spectral lines. From these lines, all of the Fe V and Ni V lines used in the previously mentioned paper are identified, along with new values for an additional approximately 200 lines.
	[1] J. C. Berengut, V. V. Flambaum, A. Ong, et al Phys. Rev. Lett. 111, 010801 (2013).

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Shira Winston
Academic Institution:	University of Maryland – College Park
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	My future plans include going to graduate school and getting a job in bioengineering
NIST Laboratory, Division, and Group:	Material Measurement Laboratory; Biomolecular Measurement Division, Applied Genetics Group
NIST Research Advisor:	Kevin Klesler, Nate Olson
Title of Talk:	STRviz - An informatics pipeline for visualizing Next Generation Sequencing data of Short Tandem Repeats (STRs) of DNA
<b>Abstract:</b>	
Short tandem repeats (STRs) are short sequences of DNA that are repeated consecutively within the genome. The number of repeats varies from person to person, which makes them very useful for identity analysis in forensic cases and paternity testing. Typically STRs are analyzed by capillary electrophoresis (CE) to evaluate STR polymorphisms in the length of polymerase chain reaction (PCR) fragments. Next Generation Sequencing (NGS) is an umbrella term used to define many types of modern sequencing techniques, in contrast to traditional methods, such as Sanger sequencing. The benefit of NGS technologies is that they can generate large quantities of sequence data, which is similar in accuracy to traditional methods. The quantity of sequence generated allows for additional marker types such as SNPs and mitochondrial DNA to be included in a single analytical workflow, preserving limited forensic evidence and enabling analysis of highly degraded DNA.	
The purpose of my project is to create understandable, practical information summaries on STRs amplified from a sample of DNA and sequenced on an NGS platform. The pipeline starts by inputting a FASTQ file, which is the output of the NGS sequencer, into STRailrazor, a perl script for detecting and sorting STRs. Then my pipeline analyzes and summarizes the data. This was done by calculating summary metrics such as stutter and genotype as well as creating several visualization tools using the statistical package, "R". R is especially useful in analyzing very large sums of data, which is necessary for my project. The final product of this project would be a single pipeline that inputs a FASTQ file, and outputs an interactive web-based report with all the desired information.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name:	Wendell Foyet, Yann S.
Academic Institution:	McDaniel College
Academic Standing (Sept. '15):	Junior
Future Plans (School/Career):	Graduate school
NIST Laboratory, Division, and Group:	Material measurement laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group
NIST Research Advisor:	Ao Geyou
Title of Talk:	Carbon Nanotube Purification by Specific DNA Sequences
<b>Abstract:</b>	
Single-wall carbon nanotubes (SWCNTs) have been considered as fundamental building blocks for electronics and biomedical applications due to their remarkable electrical, thermal, mechanical, and optical properties. In light of their potentials, polydispersity of as synthesized SWCNT materials has been one of the major challenges limiting their fundamental research and technological development. Polymer aqueous two-phase (ATP) extraction has been recently demonstrated as an effective technique to sort polydisperse nanotube material. The spontaneous partition of single-stranded DNA-wrapped SWCNTs in a given ATP system is strongly sequence-dependent and can be further modulated by salt and polymer additives to efficiently isolate single nanotube structures. In this project, a specific 12-mer DNA sequence pattern was explored to disperse and separate SWCNTs in an ATP system. Effects of SWCNTs:DNA mass ratio, oxidation and surfactant exchange reactions of dispersed SWCNTs on their subsequent separation in an ATP system were also investigated.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Shiran Winston	Grant Number   70NANB15H168
Academic Institution: University of Maryland – College Park	Major: Bioengineering
Academic Standing   Junior	
(Sept. '15): Future Plans   My future plans include going to graduate school and getting a job in bioengineering	
(School/Career): NIST Laboratory, Biomolecular Measurement Division, Applied Genetics	
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group	
NIST Research Advisor: Kevin Kiesler, Nate Olson	
Title of Talk: STRviz - An informatics pipeline for visualizing Next Generation Sequencing data of Short Tandem Repeats (STRs) of DNA	
<b>Abstract:</b>	
Short tandem repeats (STRs) are short sequences of DNA that are repeated consecutively within the genome. The number of repeats varies from person to person, which makes them very useful for identity analysis in forensic cases and paternity testing. Typically STRs are analyzed by capillary electrophoresis (CE) to evaluate STR polymorphisms in the length of polymerase chain reaction (PCR) fragments. Next Generation Sequencing (NGS) is an umbrella term used to define many types of modern sequencing techniques, in contrast to traditional methods, such as Sanger sequencing. The benefit of NGS technologies is that they can generate large quantities of sequence data, which is similar in accuracy to traditional methods. The quantity of sequence generated allows for additional marker types such as SNPs and mitochondrial DNA to be included in a single analytical workflow, preserving limited forensic evidence and enabling analysis of highly degraded DNA.	
The purpose of my project is to create understandable, practical information summaries on STRs amplified from a sample of DNA and sequenced on an NGS platform. The pipeline starts by inputting a FASTQ file, which is the output of the NGS sequencer, into STRraitor, a perl script for detecting and sorting STRs. Then my pipeline analyzes and summarizes the data. This was done by calculating summary metrics such as stutter and genotype as well as creating several visualization tools using the statistical package, "R". R is especially useful in analyzing very large sums of data, which is necessary for my project. The final product of this project would be a single pipeline that inputs a FASTQ file, and outputs an interactive web-based report with all the desired information.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5–7, 2014	
	
Name: Sarah Wollman	Grant Number   70NANB15H175
Academic Institution: Virginia Polytechnic Institute and State University	Major: Chemistry
Academic Standing   Junior	
(Sept. '15): Future Plans   Graduate school and then pursuing a career in chemistry research	
(School/Career): NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group	
NIST Research Advisor: Thomas Allison, Karl Irikura, Peter Linstrom	
Title of Talk: Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	
<b>Abstract:</b>	
The NIST Chemistry WebBook is a popular reference database for researchers, engineers, and students. It contains theoretical and experimental information such as molecular structure, thermodynamics and spectral data on approximately 130,000 molecules. Our primary focus this summer was to optimize 3-dimensional (3D) molecular structures for compounds in the Webbook. Our secondary focus was to utilize the vibrational frequencies and intensities that were computed by developing a web application to display the infrared (IR) spectrum in a user-friendly manner.	
The 3D structures were optimized using an efficient multi-step process. Starting with a classical molecular mechanics (MM2) approach, we refined initial structures created from 2D structural drawings. Quantum chemistry methods implemented in the Gaussian99 software package were used to produce accurate structures using the PM6 semi-empirical and B3LYP density functional theory (DFT) methods. DFT is more computationally expensive, but has a reputation for yielding molecular structures that are in good agreement with experimental results. Before uploading to the WebBook, we checked the structures for accuracy and consistency with existing WebBook information.	
The web application is constructed in JavaScript using the plotting package Flot to interactively display the IR spectrum of the molecule. The spectrum plot is linked to a 3D representation of the molecule that can be visualized through the JSMol package. Users can select individual frequencies to see the corresponding normal mode molecular vibrations. We hope this functionality will be included in the next release of the WebBook.	
3D structures and IR spectra are important in areas such as drug discovery, experimental simulation, and communication to non-chemists. We were able to optimize more than 20,000 molecules this summer, ensuring that the WebBook remains a valuable resource for scientists and educators.	

**SURF Student Colloquium**  
NIST – Gaithersburg, MD  
August 4–6, 2015



<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	August 4–6, 2015
	
Name: Celestine Wong	Grant Number 70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Computer Science, Social Work
Academic Standing Sophomore	
(Sept. '15):	
Future Plans Hope to graduate with a B.S. in Computer Science and a B.A. in Social Work. After earning an undergraduate degree, I hope to attend graduate school and bridge the two fields in using software to address the needs of the disadvantaged.	
(School/Career):	
NIST Laboratory, Information Technology Laboratory, Software and Systems Division, Software Quality	
Division, and Group: NIST Research Group	
Advisor: Vadim Okun, Aurelien Delaitre	
Title of Talk: Developing Programs with Hard Coded Passwords to Test Static Analysis Tools	
<b>Abstract:</b>	
The objective of the Software Assurance Reference Dataset (SARD) is to provide users, researchers, and software assurance tool makers with a set of known security flaws. SARD has over 148,000 test cases, covering over 200 common weaknesses types. Test cases are programs with flaws. We produce test cases for an important weakness type, Hard Coded Password. The weakness occurs when software uses hard coded password to communicate with an external component. By specifically focusing on Hard Coded Passwords, we can look at how software becomes vulnerable and the consequences of such practices. Different test cases will address different environments and technologies for which Hard Coded Passwords can be/are used and exposed. We will look at real-life examples of how the use of Hard Coded Passwords has affected system administration on small and large scopes. We will further discuss potential mitigations to prevent this authentication failure. The use of Hard Coded Passwords is only one of many mistakes common programmers make. Ultimately, SARD encapsulates the common weaknesses which need to be detected by software-checking tools in order to improve and protect our software.	
<b>Abstract:</b>	
This project seeks to quantify the error resulting from using discrete measurement points within a variety of flow distributions. Polar functions representing flow distributions arising from different pipe geometries were taken from the literature and generated in Matlab. The distributions were then continuously integrated to compute the true volume flow rate, the reference flow rate with which all other estimates could be compared. Simulating the traversal of a point velocity probe within a cross section consisted of creating a varying number of chords with measurement points on each. Different combinations of number of radii and number of points per radii were tested to determine the discretization error. Commonly used numerical integration methods including Trapezoidal Rule, Simpson's Rule, Centroid of Equal Area Method, and Gaus-Legendre Method were tested.	
<b>Abstract:</b>	
Our results show that given the same measurement data the Gaus-Legendre Method gives the best accuracy and is only narrowly more accurate than the Centroid of Equal area method. Increasing the number of radii provides a wider interrogation of the cross section and therefore reduces the range of possible error. Results show that there is a drastic decrease in the range of error when increasing the number of radii from two to four. Less of a decrease was observed when using more than four radii, unless the flow distribution was very complicated or contained high gradient regions. The compiled results of this study can be used as a tool to establish a measurement strategy based on the flow distribution and the required level of accuracy.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Sean Ye	Grant Number 70NANB15H142
Academic Institution: Northwestern University	Major: Mechanical Engineering & Cognitive Science
Academic Standing Sophomore	(Sept. '15): Future Plans
(School/Career):	Earn B.S. Degree in Chemical Engineering
NIST Laboratory, Division, and Group:	NIST Laboratory, Materials Measurement Lab, Chemical Sciences Division, Chemical Process Measurements Group
NIST Research Advisor:	Chris Zangmeister
Title of Talk:	Characterizing Aerosols Absorption Using Photoacoustic Spectroscopy
Abstract:	<p>Aerosols are solid or liquid particles suspended in a gas that impact the amount of radiation absorbed or scattered in the Earth's atmosphere. Depending on their size (nano- or micro-scale), composition (carbonaceous versus inorganic materials), and location (over snow, water, urban center, etc.), aerosol particles can either warm or cool the local atmosphere; these processes are the greenhouse and whitehouse effects, respectively. Currently, research laboratories around the globe are working to fully assess the impact of aerosols on climate. However, no standard reference materials exist for instrument calibration, which results in large variations between measurement platforms thereby enhancing uncertainties. Therefore, NIST is now working towards calibration standards for aerosol optical properties by focusing on materials and instrumentation development.</p> <p>My talk focuses on new metrology involving photoacoustic spectroscopy (PAS), which operates based on the principle of the conversion of absorbed light energy to heat to pressure (i.e., sound). A new method developed at NIST uses PAS to measure an aerosol absorption spectrum across the visible and near-infrared range. This summer, I used this technique to measure aerosol absorption spectra for various systems, and I will discuss these results and their potential relevance.</p>
Title of Talk:	Sensor-Based Diagnostics of CNC Linear Axes
Abstract:	<p>Computer Numerical Control (CNC) Linear axes lie at the heart of machine tools which enable them to fabricate parts for a wide range of products. Degradation of linear axes impact the parts produced by manufacturers but degradation patterns are often too time consuming to determine. Diagnosing the motion errors of a single axis can cause large disruptions to production, so it is often inefficient to use traditional approaches. Our project aims to reduce the amount of time for diagnosis of linear axis degradation through use of a relatively cheap sensor box. The box contains two inclinometers, a triaxial rate gyroscope, and three accelerometers. This setup was tested on a linear axis test-bed that contains a servo motor (for position control) and a commercial laser-based system (for purposes of validation and verification).</p> <p>Our linear axis test-bed relies on LabVIEW* software to interface with the sensors and motors. The main challenge was to achieve different sampling rates simultaneously for each sensor along with control of the servomotor. This process involved writing LabVIEW field programmable gate array (FPGA) code so that data could have different sampling rates for each sensor and hardware setup. One challenge was the rate gyroscope, which is a digital device that required special data conversion and supervision of its data packets. All data was formatted so that it could be easily analyzed within MATLAB®. Finally, experiments with controlled degradation patterns were performed using ball bearings with varying diameters to simulate degradation. Data was then analyzed to ensure that the new sensor box results are relatively accurate compared to the reference data from the traditional laser-based system.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Sean Ye	Grant Number 70NANB15H142
Academic Institution: Northwestern University	Major: Mechanical Engineering & Cognitive Science
Academic Standing Sophomore	(Sept. '15): Future Plans
(School/Career):	Earn B.S. Degree in Chemical Engineering
NIST Laboratory, Division, and Group:	NIST Laboratory, Materials Measurement Lab, Chemical Sciences Division, Chemical Process Measurements Group
NIST Research Advisor:	Greg Vogl
Title of Talk:	Sensor-Based Diagnostics of CNC Linear Axes
Abstract:	<p>Computer Numerical Control (CNC) Linear axes lie at the heart of machine tools which enable them to fabricate parts for a wide range of products. Degradation of linear axes impact the parts produced by manufacturers but degradation patterns are often too time consuming to determine. Diagnosing the motion errors of a single axis can cause large disruptions to production, so it is often inefficient to use traditional approaches. Our project aims to reduce the amount of time for diagnosis of linear axis degradation through use of a relatively cheap sensor box. The box contains two inclinometers, a triaxial rate gyroscope, and three accelerometers. This setup was tested on a linear axis test-bed that contains a servo motor (for position control) and a commercial laser-based system (for purposes of validation and verification).</p> <p>Our linear axis test-bed relies on LabVIEW* software to interface with the sensors and motors. The main challenge was to achieve different sampling rates simultaneously for each sensor along with control of the servomotor. This process involved writing LabVIEW field programmable gate array (FPGA) code so that data could have different sampling rates for each sensor and hardware setup. One challenge was the rate gyroscope, which is a digital device that required special data conversion and supervision of its data packets. All data was formatted so that it could be easily analyzed within MATLAB®. Finally, experiments with controlled degradation patterns were performed using ball bearings with varying diameters to simulate degradation. Data was then analyzed to ensure that the new sensor box results are relatively accurate compared to the reference data from the traditional laser-based system.</p>

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4–6, 2015	
Name: Raef Youssef	Grant Number   70NANB15H172
Academic Institution: University of Maryland, Baltimore County	Major: Computer Engineering
Academic Standing (Sept. '15): Junior	
Future Plans (School/Career): Graduate School	
NIST Laboratory, Division, and Group: Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group	
NIST Research Advisor: Dr. Judith Terrill	
Title of Talk: Automating the Testing of the Computer Assisted Virtual Environment (CAVE) Software System	
<b>Abstract:</b>	
<p>The Computer Assisted Virtual Environment (CAVE) system is an immersive virtual reality environment. It is often used to aid in the visualization of large and complex data sets. Although composed of multiple layers and utilities, at its core the CAVE software system uses Open Graphics Library (OpenGL). The OpenGL standard, however, states that it is not an exact pixel specification. Therefore, it does not guarantee an exact match between images produced by different hardware. This is important when attempting to determine if the software system is functioning properly. Furthermore, having an unknown amount of variation, whether due to OpenGL or to the overall software system, is undesired to many of CAVE's scientific applications which require a precise and repeatable output.</p> <p>My task was to develop and automate rendering tests which would verify that system is working properly even though its environment is constantly changing. The tests cover different aspects of the CAVE software system. Running them on different hardware and software configurations, one is able to measure the variance due to OpenGL alone. The data can also be used as a baseline when determining if the overall system is working properly.</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 5–7, 2014	
	
Name: Carolyn Zhang	Grant Number   70NANB15H169
Academic Institution: Yale University	Major: Physics
Academic Standing (Sept. '15): Junior	
Future Plans (School/Career): Graduate studies in physics, then professorship in physics.	
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Quantum Processes Division, and Metrology Group	
NIST Research Advisor: Dr. Josh Pomeroy	
Title of Talk: Optimizing Plasma Oxidation for Nanoscale Insulating Films in Magnetic Tunnel Junctions	
<b>Abstract:</b>	
<p>Nanoscale insulating films allow quantum mechanical tunneling of spin-polarized current, the basis of magnetic tunnel junctions (MTJs) (ferromagnet-insulator-ferromagnet) and Meservey-Tedrow devices (ferromagnet-insulator-superconductor). These devices form the backbone of the rising field of spintronics, as well as fundamental research in spin polarization, and require highly uniform, stoichiometric, crystalline insulating layers. We analyzed DC oxygen plasma using breakdown voltage, photovoltage, and optical spectrometry to determine the optimal conditions for oxidizing metallic aluminum to insulating aluminum oxide (<math>\text{Al}_2\text{O}_3</math>) in a 3 second process. To produce more stoichiometrically consistent and accurate films of <math>\text{Al}_2\text{O}_3</math> a mere 1.1 nm thick, we maximized the concentration of <math>\text{O}^*</math> radicals, the species most conductive to plasma oxidation. Namely, we surveyed I-V, photovoltage, and light emission trends across set currents of 5 – 160 mA and pressures of 30 – 1100 mtorr. We also constrained our optimization method to avoid sputtering the steel components of the plasma chamber. In addition, we evaluated the effectiveness of using the same plasma conditions for substrate cleaning by taking spectra of the process at closely timed intervals. By comparing the plasma power (i.e. particle momentum) and composition between two different ultra-high vacuum chambers, we also developed a mapping method for maintaining plasma conditions between systems. For device testing, we designed a multipurpose cryogenic dipper for measuring tunnel magneto-resistance (TMR) of MTJs and Zeeman splitting of the density of states (DOS) of Meservey-Tedrow devices, both of which can be used to extrapolate the spin polarization of the ferromagnetic material. Through these efforts we hope to gain a more comprehensive understanding of the connection between MTJ fabrication parameters and device performance for future applications such as magnetic random access memory (MRAM).</p>	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Nicholas Zielinski	Grant Number   70NANB15H168
Academic Institution: University of Maryland College Park	Major: Electrical Engineering
Academic Standing   Sophomore	
(Sept. '15):	I plan to pursue a career in power systems or robotics. I will attend graduate school once I am in a position for a company to pay for it.
Future Plans   (School/Career):	NIST Laboratory, Quantum Measurement Division, Applied Electrical Division, and Group: Metrology Group
NIST Research Advisor:	Allen Goldstein, Richard Steiner
Title of Talk:	Testing of PMU Leap Second Response
<b>Abstract:</b>	
Between June 30, 2015 22:30:00 and July 2, 2015 00:30:00 Coordinated Universal Time (UTC), the National Institute of Standards and Technology (NIST) tested 8 Phasor Measurement Units (PMUs) to investigate their response to the leap second which occurred on June 30, 2015 at 23:59:59 UTC. At the end of the second beginning at UTC 23:59:59, the offset between International Atomic Time (TAI) and UTC time incremented by 1 second from 35 seconds to 36 seconds. NIST tested 8 PMU models.	
The data sent out by the PMUs was processed into files by a program Allen Goldstein created and then analyzed using a program I wrote. The analysis program sorts the data by PMU and allows one to parse through the collected data and see the outputted phasor values at chosen times.	
The leap second testing of 8 PMUs at NIST shows that there should be concern about the interoperability of PMUs during the next leap second and the need for conformance testing of the leap second event. None of the PMUs remained in sync with UTC during the leap second and all of them displayed that there would be missing data and errors in the synchrophasor data due to incorrect Second of Century in the report timestamps.	
<b>Abstract:</b>	
The Computer Assisted Virtual Environment (CAVE) is a part of ITL's High Performance Computing and Visualization Group. It is a three dimensional virtual environment that is used to create high fidelity visualizations of scientific experiments and also for measurement.	
At the lowest level, the CAVE's graphical software is implemented in OpenGL, a cross-language, multi-platform application programming interface (API) for rendering 2D and 3D graphics. The OpenGL standard does not guarantee that two images, although correct, will necessarily be identical.	
Because the hardware and software environment that the CAVE exists on is constantly changing, there is a need to develop a series of tests to ensure that both are functioning properly together. It is also important that we automate these tests as much as possible to relieve time constraints of the Group.	
In this talk, I will describe the process involved in creating and implementing these tests. I will also describe how they are conducted and the ways in which they are automated. In addition, I will show a couple of unrelated ways that I have found to improve the CAVE software suite.	

<b>SURF Student Colloquium</b>	
NIST – Gaithersburg, MD	
August 4-6, 2015	
Name: Jason Zimmerman	Grant Number   70NANB15H113
Academic Institution: Millersville University	Major: Computer Science
Academic Standing   Senior	
(Sept. '15):	Graduate School. Career in Software development.
Future Plans   (School/Career):	NIST Laboratory, Information Technology Laboratory, Applied and Computational Mathematics Division, and Group: High Performance Computing and Visualization Group
NIST Research Advisor:	Judith Terrill
Title of Talk:	OpenGL Software Testing: Ensuring Compatibility Across Platforms
<b>Abstract:</b>	
The Computer Assisted Virtual Environment (CAVE) is a part of ITL's High Performance Computing and Visualization Group. It is a three dimensional virtual environment that is used to create high fidelity visualizations of scientific experiments and also for measurement.	
At the lowest level, the CAVE's graphical software is implemented in OpenGL, a cross-language, multi-platform application programming interface (API) for rendering 2D and 3D graphics. The OpenGL standard does not guarantee that two images, although correct, will necessarily be identical.	
Because the hardware and software environment that the CAVE exists on is constantly changing, there is a need to develop a series of tests to ensure that both are functioning properly together. It is also important that we automate these tests as much as possible to relieve time constraints of the Group.	
In this talk, I will describe the process involved in creating and implementing these tests. I will also describe how they are conducted and the ways in which they are automated. In addition, I will show a couple of unrelated ways that I have found to improve the CAVE software suite.	

## SURF Student Colloquium

NIST – Gaithersburg, MD  
August 4-6, 2015



Name:	Mary Zischkau	Grant Number	70NANB15H161
Academic Institution:	University of Dallas	Major:	Physics
Academic Standing (Sept. '15):	Senior		
Future Plans (School/Career):	Career in optics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory	Sensor Science Division	Thermodynamic Metrology
NIST Research Advisor:	Jacob Ricker		
Title of Talk:	A Determination of the Speed of Sound in DEHS (Di-2-ethylhexyl sebacate)		

### Abstract:

Among the four ultrasonic interferometer manometers (UIM) employed to maintain national pressure standards at the National Institute of Standards and Technology Low Pressure Manometry Laboratory, the oil UIM is in highest demand, calibrating approximately 75% of the devices under test. The oil UIM operates from a range of 1 mPa to 140 Pa in absolute mode and uses Di-2-ethylhexyl sebacate (DEHS), a nontoxic liquid with a low vapor pressure, as the working fluid in comparison to the three other manometers that use mercury, a neurotoxin that is slowly being eliminated from use in the US. Currently, the oil UIM requires comparison with the mercury manometers in order to determine pressure measurement uncertainties since the speed of sound in oil has not been measured. A measurement of the speed of sound in DEHS eliminates the need for traceability to the mercury UIMs which will be phased out in the next 5 years in place of a new optical pressure standard. An apparatus was designed to determine the speed of sound by measuring change in the displacement and time of flight for ultrasound in DEHS using ultrasound and laser interferometry. Due to the variability of the speed of sound with density, the experiment was designed to take place at several different pressures and temperatures to create an equation for speed of sound. The calculations and experiments performed with this apparatus will provide proof of concept for the next generation oil manometer.

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**2015**

**SURF STUDENTS BY  
ORGANIZATIONAL UNIT**

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UNIVERSITY	STUDENT	TITLE OF TALK	OU
Colorado School of Mines	Berntson, Matthew	Functionality for the Dynamic Spectrum Project Website	CTL
George Mason University	Barcklow, Daniel	Software-defined Radio Receiver Design with FPGA-based Hardware Acceleration	CTL
State University of New York Binghamton	Indictor, David	Spectrum Sharing for Wireless Communications with Occupancy Prediction	CTL
State University of New York Binghamton	Calamari, Matthew	Data Analysis and Validation for Sensor-Based Diagnostics of CNC Linear Axes	EL
State University of New York Binghamton	Paulson, William	Data Requirements to Characterize Machine Utilization	EL
College of William and Mary	Cheon, Seong Ik	Hot seat: Fire Protective Performance of Barrier Fabrics	EL
Colorado School of Mines	Craig, Shannon	Calculating Sustainability Performance of Residential Buildings	EL
City College of New York	Sanigepalli, SaiAdiVishnu	Real-Time Data Analytics for Smart Manufacturing Systems Project	EL
Haverford College	Kienzle, Anton	Review of Machine Learning in Manufacturing from 2010 to 2015	EL
Hobart and William Smith Colleges	Orrick, Elizabeth	Community-wide Disaster Recovery: The Choices that Divide Us	EL
Montgomery College	Goh, Justin	Test Method for Evaluating Robotic Hands' Center of Pressure and Normal Force Sensing Modalities	EL
Northwestern University	Ye, Sean	Sensor-Based Diagnostics of CNC Linear Axes	EL
Purdue University	Morgan, Sawyer	Degradation Study of PV Polymeric Materials during Accelerated Laboratory Testing	EL
Rowan University	Dow, Nicholas	Impact of Convective Heat Transfer on Fire Fighter Personal Protective Equipment	EL
Salisbury University	Aboul-Enein, Omar Y.	Inter-System Communication for Multi-Robot Control	EL
St. Olaf College	Stutzman, Mara	Mapping Vulnerability of Regional Economies to Natural Disasters Using Input-Output Data	EL
Texas A&M University	Trujillo Jr, Victor Manuel	Virtual Fusion: Human Presence in Manufacturing Simulation	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
City College of New York	Rahman, Enan	A Case Study of Implementing ISO 15746 Standard for Chemical Process Optimization	EL
Pennsylvania State University	Brockett, Nathan	A Proof-Of-Concept Additive Manufacturing Database	EL
University of California Berkeley	Molla, Nusrat	Turning Up the Heat: Simulating Outdoor Air Temperatures in the Intelligent Agents Laboratory	EL
University of Maryland College Park	Dewey, Moira	Realization Through Visualization: Understanding How Barrier Fabrics Affect Flame Spread on Upholstered Furniture	EL
University of Maryland College Park	Ettehadieh, Leila	Test Methods for Evaluating the Ability of a Robotic Hand to Detect Slip	EL
University of Maryland College Park	Feric, Tony	Modeling Smoke Venting of a Compartment Fire	EL
University of Maryland College Park	Menon, Rahul	Developing MATLAB Functions to Analyze Wind Pressure Coefficients on Building Envelopes	EL
University of Maryland College Park	Xu, Jason	Error Estimates for Gas Velocity Measurements in Ducts and Stacks	EL
University of Maryland Baltimore County	Anderson, Khalil	Meters, Meters and More Meters: The Implementation of the Smart Grid Standard on the NIST Campus	EL
University of Maryland Baltimore County	Hillsley, Brian	One Layer Deep: Investigating Scan Path Strategies for Individual Print Layers	EL
University of Maryland Baltimore County	Hudak, Steven	A Comparison of Standard Representations of Predictive Models	EL
University of Maryland Baltimore County	Kovarek, Matthew	Dynamic Pressure Propagation in a Tubing System	EL
University of Maryland College Park	Amatucci, Luke	Experimental Methods of Pressure Transducer Data Correction	EL
University of Maryland College Park	Green, Elise	Representing Robot Capabilities for Automated Planning of Manufacturing Assembly Robots	EL
University of Maryland College Park	Montgomery, Katelin	Simulation of a Robot Tool Dynamic Impact on Human Skin and Soft Tissue Bio-simulant Artifacts Based on the NIST DITCI Instrument Simulator Test Data	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of New Haven	Meisinger-MacDonald, Jessica	The Effects of High Temperatures on Radio Speaker Microphones	EL
Virginia Polytechnic Institute and State University	Bass, Lindsey	Residual Stress in Metal Additive Manufacturing Parts	EL
Wellesley College	Shaw, Vivienne	Context Awareness for Adaptive Human-Robot Interaction	EL
Worcester Polytechnic Institute	Barolli, Rebecca	Characterization of Exposure Conditions for Wildland/Wildland-Urban Interface Fire Fighters	EL
Worcester Polytechnic Institute	Macsata, Adam	The Effect of Wind-Driven Fires Along Fences on Homes in the Wildland-Urban Interface	EL
University of Maryland Baltimore County	Massey, Joshua	The MML Data Management Plan Tool: Understanding and Reporting Data About Data	ISO
American University	Cerna Sanchez, Juana	3D to 1D: Variances of Tumor Measurements from CT Patient Data Sets with Linear Scale Analysis of Volume Measurements	ITL
American University	Dang, Thinh	Fundamental solution of the Helmholtz Equation in hyperbolic and hyperspherical geometry	ITL
Bowie State University	Jackson, Alauna	Automating the Testing of Immersive Visualizations in a Computer Assisted Virtual Environment (CAVE)	ITL
George Washington University	Berger, Isabelle	Algorithms Behind the Symbolic Search and Verification for Generating Functions of Orthogonal Polynomials	ITL
Georgetown University	Park, Zoe	Generating Random Graphs	ITL
Hampton University	Moore, Zora	Access Control Rule Logic Circuit Simulation: Immediate Fault Detecting System	ITL
Hood College	Kasner, Jillian	Redeveloping the GUM.validate Function in the MetRology Package for R	ITL
Hood College	Traini, Catherine	Verification and Search for Generating Functions for Orthogonal Polynomials in the Askey Scheme	ITL
McLennan Community College	Ratliff, Zachary	The Relationship Between Software Bug Type and Number of Factors Involved in Failures	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Millersville University of Pennsylvania	Helsel, Tyler	Digital Forensics using EXtensible Markup Language (XML)	ITL
Millersville University of Pennsylvania	Rabiega, Daniel	Walk-On-GPU: Implementing Monte-Carlo Algorithms on GPU	ITL
Millersville University of Pennsylvania	Zimmerman, Jason	OpenGL Software Testing: Ensuring Compatibility Across Platforms	ITL
Pennsylvania State University	de la Vega, Jose	Fuzzing bugs out of Wireshark to test static analyzers	ITL
Saint Francis University	Shattuck, Taylor	Personal Data Stores	ITL
Smith College	Stoudt, Sara	“Big Force” Calibrations: An Errors in Variables Approach	ITL
College of New Jersey	Davis, Kyle	Integration of Web-Based 3D Modeling with Leap Motion Tracking and Oculus Rift Virtual Reality	ITL
College of New Jersey	Lessoff, Daniel	Improvements in Routing Security: A BGPSEC Test System	ITL
University Colorado Boulder	Weller, Ryan	Designing 3D GUI Widgets for OOF	ITL
University of the District of Columbia	Mayo, Kamala	Testing Wireshark Protocols for Vulnerabilities using Fuzzed Data	ITL
University of Maryland Baltimore County	Jackson, Malik	Improving the Unigram Classification Model	ITL
University of Maryland Baltimore County	Lagnese, Joseph	Feasibility and Applications of RapidMiner 5 for Estimating the Entropy of an Entropy Source	ITL
University of Maryland Baltimore County	Landen, Matthew	Cloud Rubik’s Cube: NIST’s Cloud Security Reference Tool	ITL
University of Maryland Baltimore County	Rogers, James	Practical Proof Potential: Examining the Algorithm Verification Ability of the Software Assurance Workbench	ITL
University of Maryland Baltimore County	Shahir, Jamshaid	Quantify differences between image feature extraction tools	ITL
University of Maryland Baltimore County	Wong, Celestine	Developing Programs with Hard Coded Passwords to Test Static Analysis Tools	ITL
University of Maryland Baltimore County	Youssef, Raef	Automating the Testing of the Computer Assisted Virtual Environment (CAVE) Software System	ITL
University of Maryland College Park	Wang, Andrew	Characterization of Nanofiber Scaffolds	ITL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Puerto Rico	Collazo-Martis, Ramon	Combinational Circuit Optimization: New Results	ITL
University of Puerto Rico	de la Cruz, Julio	Coloring the Facets of the Cloud Rubik's Cube	ITL
University of Puerto Rico	Dear, Mark	Experiments in Numerical Reproducibility	ITL
University of Puerto Rico	Morales Miranda, Adriana	Counting Large Prime Numbers	ITL
Centre College	Graham, Daniel	Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	MML/NCNR ChemBio
East Carolina University	Niyonzima, Yvonne	Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	MML/NCNR ChemBio
Frostburg State University	Blair, Andrew	MS Analysis of Protein BSA	MML/NCNR ChemBio
Hampton University	Mosley, Matthew	The Application of Gas Chromatography – Mass Spectrometry	MML/NCNR ChemBio
Miami Dade College	Galvin, Connor	Protein Crystallography	MML/NCNR ChemBio
Montgomery College	Blendermann, Anna	Fitness Measurements and Protein Evolution	MML/NCNR ChemBio
Montgomery College	Chaudhry, Maria	Developing Websites using Visual Studio and SQL Server	MML/NCNR ChemBio
Montgomery College	Davis, Kiersta	Using evolution to predict novel N-glycosylation on non-canonical protein motifs	MML/NCNR ChemBio
Montgomery College	Hahm, Grace	Quantification of Anthocyanins in Cranberry Standard Reference Materials by LC-Absorbance-MS	MML/NCNR ChemBio
Montgomery College	Kiryutina, Tatyana	Method Development and Validation of Targeted Metabolomics Approach for Nanotoxicity Assessment	MML/NCNR ChemBio
Montgomery College	Lee, Wai In	Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials	MML/NCNR ChemBio
Morgan State University	Mojibola, Adeolu	Structural Studies of an Inactivating Peptide of Ion Channels in Phospholipid Bilayers	MML/NCNR ChemBio
Purdue University	Browne, Christopher	Optimized detection of Homemade Explosive Precursors and By-products using Ion Mobility Spectrometry	MML/NCNR ChemBio

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Reed College	Underwood, Samuel	Preparation and Characterization of Silver Nanoparticle-loaded Fabrics as Test Materials	MML/NCNR ChemBio
Rose-Hulman Institute of Technology	Pasco, Madeleine	Reproducible, Multispecies, Microbial Biofilms	MML/NCNR ChemBio
State University of New York Polytechnic University	Kamaldinov, Timur	Determination of Mineralizing Phenotype in <i>in vitro</i> Tissue Cultures Using Confocal Laser Scanning Microscopy	MML/NCNR ChemBio
University of Massachusetts Amherst	Deschamps, Melissa	The Effect of Electrolyte Concentration on Irreversible Colloid Adsorption	MML/NCNR ChemBio
University of Massachusetts Amherst	Sim, Brian	Effects of environmental photo-oxidants on the stability of polymeric coatings on nanoparticles	MML/NCNR ChemBio
University of Maryland Baltimore County	Hong, Donald	Analysis of New HDX-ETD Software for Higher Resolution in Epitope Mapping	MML/NCNR ChemBio
University of Maryland Baltimore County	McDonald, Natalie	Statistical Analyses of Data Obtained from the NIST Hydrogen/Deuterium Exchange Mass Spectrometry Inter-laboratory Comparison Project	MML/NCNR ChemBio
University of Maryland College Park	Douti, Lampouguin	Loss of functionalized gold nanoparticles in commonly used containers	MML/NCNR ChemBio
University of Maryland College Park	Lingayat, Akshay	The Gold-Worm Conundrum	MML/NCNR ChemBio
University of Maryland College Park	Rachuri, Swaksha	Molecular Cloning and Characterization of Adenylyl Cyclase Class II Secreted from <i>Pseudomonas Aeruginosa</i>	MML/NCNR ChemBio
University of Maryland College Park	Winston, Shira	STRviz - An informatics pipeline for visualizing Next Generation Sequencing data of Short Tandem Repeats (STRs) of DNA	MML/NCNR ChemBio
Vanderbilt University	Bryant, Carson	Development of a Reproducible Electrochemical Method for Quantifying Oxidative Stress	MML/NCNR ChemBio
Virginia Polytechnic Institute and State University	Rastatter, Brett	Optimizing HPLC- Based Biopharmaceutical Analysis using Design of Experiments	MML/NCNR ChemBio
Virginia Polytechnic Institute and State University	Van Dongen, Kimberly	Resistance of Next Generation Dental Resin to Biological Challenges in an Oral Environment	MML/NCNR ChemBio

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Virginia Polytechnic Institute and State University	Wollman, Sarah	Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook	MML/NCNR ChemBio
The Citadel	Huntington, S. Lee	A Novel Method for Tin Speciation in Complex Biological Matrices	MML/NCNR ChemBio at HML
American Univ	Henrich, Janelle	Inversion of Quasielastic Neutron Scattering Data from Differing Instruments	MML/NCNR MatSci
Boise State University	Correa Hernandez, Andres	Density Functional Theory Studies of Carbon Dioxide Interaction with Oxide Surfaces	MML/NCNR MatSci
Boise State University	Huff, Jonathan	Displacement Metrology for Nanomechanical Testing	MML/NCNR MatSci
California Polytechnic State University	Ross, Alicia	Quantifying the Amount of Diffusion Between 3D Printed Layers	MML/NCNR MatSci
Carnegie Mellon University	Christie, Nathan	Modeling Competition between Polymerization and Phase Separation with a Webtool	MML/NCNR MatSci
Case Western Reserve University	Wade, Matthew	Calculation of Radial Distribution Functions for Polymer Nanocomposites using Parallel Processing on a Graphical Processing Unit	MML/NCNR MatSci
Centre College	Vollbrecht, Cecilia	Synthesis and Characterization of Activatable Dyes for Integration into Polymer Systems	MML/NCNR MatSci
Colorado School Mines	Fischer, John	Understanding Interfacial Structures of Ultrathin Self-Assembled Nafion®	MML/NCNR MatSci
Colorado School Mines	Hillgartner, Kaitlyn	3D Printing Temperature and Speed Effects	MML/NCNR MatSci
Duke University	Gayle, Andrew	Mapping Mechanical Properties of Polymer and Polymer Composites Using Nanoindentation	MML/NCNR MatSci
East Carolina University	Thornton, Lindsay	Can you see my data now?: The Materials Genome Initiative and building data infrastructure	MML/NCNR MatSci
Hamilton College	Baer, Joelle	Here's the (In)Situ-ation: Optimizing and Testing a Prototype for Beamline Helium-3 Polarization	MML/NCNR MatSci
Hood College	Franklin, Ryan	Construction and Molecular Dynamics of a Nanodisc for Membrane Protein Simulation	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Lewis Clark College	Artner, Kodie	Exfoliation and Study of Transition Metal Dichalcogenides	MML/NCNR MatSci
McDaniel College	Wendeu Foyet, Yann	Carbon Nanotube Purification by Specific DNA Sequences	MML/NCNR MatSci
Miami University of Ohio	Brock, Jeffrey	Nanostructure Characterization from X-Ray Scattering Techniques via Inverse Algorithms	MML/NCNR MatSci
Miami University of Ohio	Herrmann, Emily	Dynamic Reliability Assessment of the NIST NBSR Thermal Shield Cooling System	MML/NCNR MatSci
Montgomery College	Lee, Stephen	Effect of film thickness on the network structure of polyamide water desalination membranes	MML/NCNR MatSci
Montgomery College	Uddin, Tareq	Quantitative Prediction of Biodegradable Nanofiber Diameter for use in Tissue Engineering: a Therapy for Age-Related Macular Degeneration	MML/NCNR MatSci
Mount St Mary's University	Lesniewski, Joseph	BLAND: A Stimulating Method for the Analysis of Diffraction Patterns	MML/NCNR MatSci
Northwestern University	Silver, Alexander	Measuring Aggregation in Organic Photovoltaic Solutions	MML/NCNR MatSci
Princeton University	Register, Jeffrey	X-ray and Neutron Reflectivity Studies of Nanoimprinted Polystyrene Bilayers	MML/NCNR MatSci
Purdue University	Scherbarth, Austin	Synthesis and Characterization of Conducting Composite Nanoparticles for Flow Battery Applications	MML/NCNR MatSci
Rochester Institute of Technology	Collini, John	Magnetic Ordering in Ce <sub>1-x</sub> Y <sub>x</sub> RhIn <sub>5</sub> Heavy Fermions as a Function of Doping	MML/NCNR MatSci
Rowan University	Scott, Charles	Data curation software for reproducible results in the FACT Lab	MML/NCNR MatSci
Savannah State University	Lynn, Kurt	Characterizing Radiation Induced Faults in Microprocessors	MML/NCNR MatSci
Smith College	Knobloch, Emmie	Assessing Healing Properties of an Airbrushed Chitosan Wound Dressing	MML/NCNR MatSci
University of Delaware	McAllister, Robert	Shooting Neutrons at Soap: Orientation of Wormlike Micelles Under Extensional Flow	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland Baltimore County	Bleakney, Matthew	Effect of gaps in backing support on ballistic performance of body armor	MML/NCNR MatSci
University of Maryland Baltimore County	Horn, Jarod	Challenges in the reliable measurement of high pressure CO <sub>2</sub> adsorption isotherms	MML/NCNR MatSci
University of Maryland Baltimore County	Poole, Maxwell	Python Scripting and Coffee: Software Development for the Sciences	MML/NCNR MatSci
University of Maryland College Park	Goldman, Joshua	Missing Abstract	MML/NCNR MatSci
University of Maryland College Park	Graybill, Joshua	In-situ hydro-mechanical stress response of aged perfluorinated ionomer (PFSI) membranes for fuel cell applications.	MML/NCNR MatSci
University of Maryland College Park	Isser, Ariel	Predicting Bulk Properties of Photocurable Monomers from Molecular Dynamics Simulations	MML/NCNR MatSci
University of Maryland College Park	Mittal, Rohan	Characterization of High-strength Fibers used in Soft Body Armor	MML/NCNR MatSci
University of Maryland College Park	Nguyen, Khanh	Materials Informatics for Combinatorial Thin Film Libraries	MML/NCNR MatSci
University of Maryland College Park	Pascale, Maria	Control your Spin: Using Chemistry and Pressure to Regulate Magnetic Order	MML/NCNR MatSci
University of Maryland College Park	Sabatelli, Nicole	Developing Standards to Assess Biological Effects of Electronic-Cigarettes	MML/NCNR MatSci
University of Maryland College Park	Young, Jessica	Characterizing Aerosols Absorption Using Photoacoustic Spectroscopy	MML/NCNR MatSci
University of Missouri	Prevost, Dylan	Designing a World-Class Cold Neutron Source: NISTCOR	MML/NCNR MatSci
Virginia Polytechnic Institute and State University	Anderegg, David	Study of dewetting properties of inkjet-printed polymers	MML/NCNR MatSci
West Virginia University	Cain, Megan	Length-Scale Effects on the Mechanical Properties of Soft Materials	MML/NCNR MatSci
West Virginia University	Isaac, Samantha	Monte-Carlo Modeling of Multiplexed Neutron Spectroscopy	MML/NCNR MatSci
Northwestern University	Martinez, Jose	Harmonizing Standards: Reviewing Military and Law Enforcement PPE Performance Standards	ADL/SP





